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INTRODUCTION

Avec le soutien du C.N.R.S et de la D.R.E.D, l'année académique 1990/91 fût une année spéciale consacrée aux méthodes semiclassiques.

A l'origine les méthodes semi-classiques désignaient les techniques utilisées par les physiciens pour essayer de comprendre les relations subtiles existant entre la mécanique classique de Newton et la mécanique quantique de Heisenberg-Schrödinger (lorsque la constante de Planck $\hbar$ devient négligeable par rapport aux autres grandeurs physiques: masse, énergie, distances, ...). L'exemple fondamental est la méthode B.K.W (Brillouin, Kramers, Wentsel) qui consiste à construire des solutions asymptotiques, par rapport à la constante de Planck, de l'équation de Schrödinger. Cette méthode est restée longtemps formelle. La justification mathématique rigoureuse a nécessité l'élaboration de théories sophistiquées qui ont vu le jour dans les années 1970 (indice de Maslov, opérateurs intégraux de Fourier-Hörmander). A partir de ces travaux de base, de nombreux mathématiciens se sont attaqués avec succès à divers problèmes issus de la physique et se traduisant par l'étude spectrale d'opérateurs pseudo-différentiels, dépendant de paramètres. Citons quelques exemples parmi les plus connus:

• le comportement du spectre de l'opérateur de Schrödinger lorsque la constante de Planck tend vers zéro (régle de Bohr-Sommerfeld, effet tunnel)

• le comportement asymptotique des grandes valeurs propres (formules du type Weyl)

• la trace du noyau de la chaleur lorsque la température tend vers zéro et les invariants géométriques associés

• diffusion quantique ou acoustique: problèmes à plusieurs corps, problèmes inverses, résonances

• systèmes périodiques: analyse du spectre de bande, problèmes inverses

• description de certains systèmes quantiques désordonnés: potentiels quasi périodiques, équation de Harper, chaos quantique

• limite thermodynamique.

Durant ces quinze dernières années, les méthodes semi-classiques se sont beaucoup enrichies avec le développement de l'analyse microlocale des équations aux dérivées partielles et de leurs solutions. De nombreux mathématiciens (et physiciens!) ont participé à ce développement. Parmi les travaux que l'on peut considérer comme fondamentaux mentionnons en particulier ceux de S. Agmon, Y. Colin de Verdière, J. Chazarain, L. Hörmander, V. Ivrii, J. Leray,V. Maslov, R. Melrose, J. Sjöstrand, A. Voros (je cite ces noms car il me sem-

ble bien représenter le rapprochement fructueux qui s'est effectué durant cette période entre l'analyse des équations aux dérivées partielles et la physique-mathématique).
Deux volumes de la collection **Astérisque** regroupent les actes de l'Ecole d'Eté et du Colloque International organisés à Nantes, en Juin 1991. L'Ecole d'Eté était centrée sur quatre cours: V. Ivrii (Asymptotiques Spectrales); M.A Shubin (Théorie spectrale sur les variétés non compactes); A. Soffer (Problèmes à N-corps) et G. Ulhmann (Problèmes inverses). Le Colloque International comportait vingt conférences portant sur des thèmes variés, illustrant la puissance des méthodes semi-classiques appliquées aux équations de la mécanique quantique ou à l'équation des ondes acoustiques. Les sujets abordés concernent principalement l'équation de Schrödinger sous différents aspects: N-corps, champs magnétiques, limite thermodynamique, solitons, cristaux. Deux exposés sont consacrés à la diffusion acoustique par un obstacle et à la conjecture de Lax-Philips sur les résonances.

En conclusion, je voudrais remercier les institutions et les personnes qui ont permis le succès de cette année spéciale sur les méthodes semiclassiques, en premier lieu le C.N.R.S en la personne de J.P Ferrier et la D.R.E.D en la personne de J. Giraud. Je remercie également tous ceux qui ont participé à l'organisation des différents colloques qui se sont déroulés entre Novembre 1990 et Juin 1991, en particulier les collègues suivants: J. Bellissard, J.M.Bismut, A. Ben Arous, J.M. Combes, C. Gérard , A. Grigis , J.C Guillot, B. Helffer, A. Martinez, J.F.Nourrigat, F. Pham, J. Sjöstrand, A.Unterberger, A. Voros.
Je remercie l'université de Nantes et le conseil général de Loire-Atlantique pour le soutien qu'ils nous ont apporté.
D. Macé-Ramette a assuré avec dévouement et compétence le secrétariat de cette année spéciale, je l'en remercie.

Nantes, le 21 Décembre 1992

D. Robert

RESUMES

1. AGMON Shmuel . *A representation theorem for solutions of Schrödinger type equations on non compact Riemannian manifolds*
Let X be a real analytic Riemannian manifold with a boundary ∂X. Denote its interior by X and its metric by g. Introduce on X a conformal metric h defined by $h = p^{-2}g$ where $p(x)$ is a real analytic on X such that $p(x) > 0$ in $X, p(x) = 0$ and $dp \neq 0$ on ∂X. Under the metric h, X becomes a complete non-compact Riemannian manifold with a corresponding Laplacian Γ_h. Consider solutions of the differential equation.

$$(*)\ \Gamma_h u + \lambda q(x) u = 0 \quad \text{on} X$$

where $q(x)$ is a real analytic function on ∂X and $\lambda \in \mathbf{C}$.
Our main result is a representation theorem for all solutions of equation (*). The theorem is a generalization of a representation formula established by Helgason and Minemura for solutions of the Helmholtz equation on hyperbolic space.

2. BOUTET de MONVEL Anne-Marie; GEORGESCU Vladimir. *Some developments and applications of the abstract Mourre theory*
Our aim is to present several applications of a version of Mourre theory that we have recently developed. We can easily deduce from it, for example, a very precise form of the limiting absorption principle for perturbations $H = h(P) + V_S + V_L$ of a constant coefficient pseudo-differential operator $h(P)$ by short-range and long-range *non local* potentials V_S and V_L. The perturbations V_S, V_L are quite singular locally (the sum above is required to exist only in form-sense) and the assumptions concerning their behaviour at infinity are essentially optimal (e.g V_S is of Enss type). Furthermore, if such an H is perturbed by another short-range potential, the relative wave operators exist and are complete. The theory works aslo for systems (like Dirac operators). Other applications are to division theorems, i.e.properties of the operators of multiplication by $(h(x) \pm io)^{-1}$, under minimal regularity assumptions on h. In particular these examples show that the regularity assumptions we make in our abstract version of Mourre theory are essentially optimal.

3. BUSLAEV Vladimir; PERELMAN Gregor. *On nonlinear scattering of states which are close to a soliton*
Under some conditions on the function F the nonlinear Schroedinger equation

$$i\psi_t = -\psi_{xx} + F(|\psi|^2)\psi, \psi = \psi(x,t) \in \mathbf{C},$$

admits a class of bounded solutions $w(x|\sigma(t))$, which parameters $\sigma = \sigma(t) \in \mathbf{R}^4$ depend explicitely on time t. The Cauchy problem for the Schroedinger equation with the initial data

$$\psi(x,0) = w(x|\sigma_0(0)) + \chi_0(x)$$

is considered where χ_0 is assumed to have the sufficiently small norm

$$N = \|(1+x^2)\chi_0\|_2 + \|\chi_0'\|_2.$$

If the spectrum of the linearization of the Schroedinger equation on the soliton $w(\cdot|\sigma_0(0))$ has the simplest structure in some natural sense, the asymptotic behavior of ψ as $t \to +\infty$ is given by the formula (in $\mathbf{L}_2$-norm):

$$\psi = w(\cdot|\sigma_+(t)) + \exp(-il_0 t)f_+ + o(1),$$

here $\sigma_+(0)$ is close to $\sigma_0(0), l_0 = -\partial_x^2, f_+ \in \mathbf{L}_2(\mathbf{R})$ and is sufficiently small.

4. BRUNING Jochen; SUNADA Toshikazu. *On the spectrum of gauge-periodic elliptic operators*
We consider a symmetric elliptic operator, D, on a complete Riemannian manifold which admits a properly discontinuous action of a group Γ, with compact quotient. We assume that D is "gauge periodic" i.e. commutes with the group action twisted by a gauge; a typical example is the Schrödinger operator with constant magnetic field. We associate a C^*-algebra with this situation and prove that the spectrum of (the closure) D has band sructure if this C^*-algebra has the "Kadison property". For the magnetic Schrödinger operator, we can derive an optimal upperbound on the number of gaps for rational flux.

5. GEORGESCU Vladimir; BOUTET de MONVEL Anne-Marie. *Graded C^*-algebras and many-body perturbation theory:* II. *The Mourre estimate*
Let $\mathcal{L}$ be a finite lattice with largest element X and $\mathcal{A}$ a C^*-algebra. We say that $\mathcal{A}$ is $\mathcal{L}$-graded if a family $\{\mathcal{A}(Y)\}_{Y\in\mathcal{L}}$ of C^*-subalgebras has been given such that $\mathcal{A} = \sum_{Y\in\mathcal{L}} \mathcal{A}(Y)$ (direct sum) and $\mathcal{A}(Y)\mathcal{A}(Z) \subset \mathcal{A}(Y \vee Z)$ for $Y, Z \in \mathcal{Z}$. The Hamiltonians usually considered in the many-body problems are affiliated to such an algebra. If $\mathcal{A}$ is realized on a Hilbert space $\mathcal{H}$, the many-channel structure of a self-adjoint operator H(in general non densely defined) affiliated to $\mathcal{A}$ may be described as follows : for each $Y \in \mathcal{L}, \mathcal{A}_Y = \sum_{Z\leq Y} \mathcal{A}(Z)$ is a C^*-algebra, the natural projection $\mathcal{P}_Y : \mathcal{A} \to \mathcal{A}_Y$ is a $*$-homomorphism and there is a unique self-adjoint operator H_Y such that $\mathcal{P}_Y(f(H)) = f(H_Y)$ for all

$f \in C_\infty(\mathbf{R})$. Let A be a self-adjoint operator such that $e^{-iA\alpha}\mathcal{A}(Y)e^{iA\alpha} \subset \mathcal{A}(Y)$ for all Y and α. Assume that $D(H_Y)$ is invariant under $e^{iA\alpha}$ for all Y and $\frac{d}{d\alpha}e^{-iA\alpha}He^{iA\alpha}$ exists in norm in $B(D(H), D(H)^*)$ and H has a spectral gap. Our main result is that,under a further assumption on $\mathcal{A}$ which is independent of H and trivially verified in the N-body case. A is conjugate to H at a point $\lambda \in \mathbf{R}$ if it is conjugate to each H_Y with $Y \neq X$ at λ.

6. GUILLEMIN Victor. *The homogeneous Monge-Ampere equation on a pseudoconvex domain*
In the first three sections of this article I give a new proof of a theorem of Jack Lee which says that if M is a compact strictly pseudoconvex domain with a real-analytic boundary, one can find a defining function on the boundary which satisfies the homogeneous complex Monge-Ampere equation. The proof involves complexifying a solution of a related real Monge-Ampere equation.
The rest of this article is devoted to a generalization of a theorem of L. Boutet de Monvel. Boutet's theorem says that if X is a compact manifolf equipped with a real-analytic Riemannian metric and f is a real-analytic function of M then the following are equivalent

(1) f can be extended holomorphically to a Grauert of radius r, about X.

(2) The diffusion equation, $\frac{\partial u}{\partial t} = \Delta^{\frac{1}{2}}u$, can be solved *backwards* in time over the interval,$-r \leq t \leq 0$ with initial data :

$$u(0, x) = f(x).$$

In the second half of this article I show that this theorem has a generalization in which Grauert tubes are replaced by a family ,$\phi = r$, of strictly pseudoconvex domains, ϕ satisfying homogeneous Monge-Ampere.

7. HAGEDORN George. *Classification and normal forms for quantum mechanical eigenvalue crossings*
In the analysis of molecular systems, one is led to the study of a quantum mechanical Hamiltonian for the electrons that is a function of n parameters that describe the positions of the nuclei. As the parameters are varied, the spectrum of the electron Hamiltonian can change.The way in which the graphs of the discrete eigenvalues cross one another depends on the symmetry group of the Hamiltonian function. We classify generic crossings of minimal multiplicity eigenvalues under all possible symmetry circumstances. For each of the eleven types of crossings, we derive a normal form for the Hamiltonian function near the crossing.

8. HELFFER Bernard; SJÖSTRAND Johannes. *Semiclassical expansions of the thermodynamic limit for a Schrödinger equation*
We give a proof of the semi-classical expansion of the thermodynamic limit for a model introduced in statistical mechanics by M.Kac. For this family

(parametrized by m) of Schrödinger operators $P^{(m)}(h) = -\sum_{k=1}^{m} h^2\partial^2/\partial x_k^2 + V^{(m)}(x)$ defined on $\mathbf{R}^m$, this corresponds to the study of the expansion in power of h of $lim_{m\to\infty}\lambda(m,h)/m$ where $\lambda(m,h)$ is the first eigenvalue of $P^{(m)}(h)$.

9. HEMPEL Reiner. *Eigenvalue asymptotics related to impurities in crystals*

As a mathematical model for energy levels produced by impurities in a crystal, we study perturbations of a (periodic) Schrödinger operator $H = -\Delta + V$ by a potential λW, where λ is a real coupling constant and W decays at infinity. Assuming that H has a spectral gap, we ask for the number of eigenvalues which are moved into the gap and cross a fixed level E in the gap, as λ increases. Such "impurity levels" are a basic ingredient in the quantum mechanical theory of the color of crystals (insulators) and of the conductivity of (doped) semi-conductors in solid state physics.

In the general case where W is allowed to change its sign, we discuss upper and lower asymptotic bounds for the eigenvalue counting function.

We also provide bounds for the total number of eigenvalues crossing E as the height of a repulsive "barrier", living on a compact set K, tends to ∞. While quasi-classical arguments give some useful hints, it turns out that, in particular, lower bounds are very sensitive and depend highly on the structure of the set K. Here decoupling via natural Dirichlet boundary conditions tends to play a dominating rôle, e.g. if the set K has many small holes ("swiss cheese").

10. HISLOP Peter. *Singular perturbations of Dirichlet and Neumann domains and resonances for obstacle scattering*

We consider the problem of proving the existence of and estimating the location of scattering poles for a class of trapping obstacles known as Helmholtz resonators with both Dirichlet and Neumann boundary conditions. We treat the case when the diameter of the tube linking the cavity to the exterior is made small and the high energy behavior of resonances when the tube diameter is fixed. The latter case gives an example of the Lax-Phillips conjecture.

11. IKAWA Mitsuru. *Singular perturbation of symbolic flows and the modified Lax-Phillips conjecture*

In order to consider the modified Lax-Phillips conjecture for scattering by obstacles consisting of several convex bodies, the zeta functions of a dynamical system in the exterior of the obstacle play an important role.

In this paper we develope a theory for singular perturbations of symbolic dynamics and consider the zeta functions associated with dynamical systems. We give a sufficient condition for the existence of poles of the zeta functions of the singularity perturbed dynamics.

As the application of this theory, the validity of the modified Lax-Philipps conjecture for obstacles consisting of small balls is proved.

12. LIEB Elliott. *Large atoms in large magnetic fields*
The ground state energy of an atom of nuclear charge Ze and in a magnetic field B is evaluated exactly in the asymptotic regime $Z \to \infty$. We present the results of a rigorous analysis that reveals the existence of 5 regions as $Z \to \infty$: $B \ll Z^{4/3}$, $B \approx Z^{4/3}$, $Z^{4/3} \ll B \ll Z^3$, $B \approx Z^3$, $B \gg Z^3$. Different regions have different physics and different asymptotic theories. Regions 1,2,3,5 are described exactly by a simple density functional theory, but only in regions 1,2,3 is it of the semiclassical Thomas-Fermi form. Region 4 cannot be described exactly by any simple density functional theory; surprisingly, it can be described by a simple *density matrix* functional theory, as found after this talk was presented. [There are two more recent references: Phys. Rev. Lett. **69**, 749-752 (1992) and Commun. Pure Appl. Math. (in press for the McKean issue).] A surprising conclusion is that although the magnetic field has a profound effect on the atomic energy in regions 2,3,4 and 5, the atom remains spherical (to leading order) in regions 2 and 3.

13. NAKAMURA Shu. *Resolvent estimates and time-decay in the semiclassical limit*
We consider resolvent estimates for Schrödinger operators in the semiclassical limit. We construct a semiclassical analogue of the theory of multiple commutator estimates by Jensen, Mourre and Perry [JMP]. Then we apply it to the barrier-top energy and nontrapping energies to obtain semiclassical estimates for powers of the resolvent. As a consequence, we also obtain estimates for the time-decay in the semiclassical limit.

14. RALSTON James. *Magnetic breakdown*
This article constructs time-dependent asymptotic solutions to the magnetic Schrödinger equation in the weak magnetic field limit in the case of "interband magnetic breakdown". This means that there is an eigenvalue crossing in the (Bloch) spectrum of the zero magnetic field operator and interband tunnelling effects occur.

15. SHUBIN Michael; GROMOV Michael. *Near-cohomology of Hilbert complexes and topology of non-simply connected manifolds*
Near cohomologies of Hilbert complexes are obtained heuristically by taking cochains with small coboundaries modulo cochains which are close to cocycles. Rigorously this leads to a family of closed cones depending on a small real parameter up to an equivalence relation. It is proved that the near cohomologies are homotopy invariants of a Hilbert complex with respect to the chain homotopy equivalence defined by morphism and homotopy operators which are bounded linear operators. Applying this to the Hilbert de Rham complex on the universal covering of a non-simply connected manifold gives homotopy invariants of this manifold. A von Neumann algebra stucture on a Hilbert complex allows to convert near-cohomologies to number homotopy invariants of the

complex. For the Hilbert de Rham complex they coincide with the invariants introduced and investigated by the authors in an earlier paper and include heat kernel decay exponents by S.P. Novikov and M.A. Shubin.

16. SIMON Barry. *The Scott correction and the quasi-classical limit*
The Scott correction is the second term in a large Z asymptotic expansion of the total binding energy of an atom with nuclear charge Z. The atom is complicated system with multiparticle correlations among the electrons. Nevertheless, the proof of the Scoot correction can be reduced to the study of the semi-classical limit of a one-body system where the electron-electron interaction is replaced by an averaged self-consistent potential.

17. SJÖSTRAND Johannes. *Exponential convergence of the first eigenvalue divided by the dimension, for certain sequences of Schrödinger operators*
We consider certain sequences of Schrödinger operators

$$-h^2\Delta + V^{(m)}(x), x \in \mathbf{R}^m, m = 1, 2, ...$$

Our assumptions imply that $V^{(m)}$ is strictly convex. If $\mu(m,h)$ denotes the lowest eigenvalue, we study the exponential convergence of $\mu(m,h)/m$ when m tends to ∞.

18. VAINBERG Boris. *Scattering of waves in a medium depending periodically on time*
The asymptotic behaviour as $t \to \infty, |x| \leq a < \infty$ of solutions of exterior mixed problems for hyperbolic equations and systems is obtained when the boundary of a domain and coefficients of the equations depend periodically on time. It is supposed that the coefficients are constant in a neigborhood of infinity and that the non-trapping condition is fulfilled. The method of the research is based on using a special parametrix, Fourier-Bloch transform and analytical properties of an integral eguation which arises. This method can be regarded as an alternative one to the Lax-Phillips scattering theory. Then the asymptotic behavior of the solutions is used to prove existence of the wave operators and of the scattering operator, if the general energy of any solution is uniformly bounded for $t \geq 0$ provided that it is bounded at $t = 0$.

19. WHITE Denis. *Long range scattering and the Stark effect*
We prove the completeness of Dollard's modified wave operators for the Stark effect Hamiltonians $H_0 = -(1/2\Delta - x_1$ and $H = H_0 + V$ where V is a general long range potential. As a consequence, the "unmodified" wave operators do not exist if V is not short range. In one space dimension this quantum mechanical result differs from the classical result : Jensen and Ozawa have shown that the usual wave operators in classical mechanics do exist. We show however that

this mathematical difference cannot be detected by any quantum mechanical observable. We derive the existence and completeness of the modified wave operators (in arbitrary space dimensions) from the comparable result for two Hilbert space wave operators by a stationary phase argument.

20. YAFAEV Dimitri. *Radiation conditions and scattering theory for three-particle Hamiltonians*
The correct form of radiation conditions is found in scattering problem for three-particle Hamiltonians H. For example, in a cone Γ of the configuration space where all pair potentials are vanishing the radiation conditions-estimate has the following forme. Let $\nabla^{(s)}$,

$$\nabla^{(s)}u(x) = \nabla u(x) - |x|^{-2} < \nabla u(x), x > x,$$

be the projection of the gradient ∇ on the plane, orthogonal to x, and let ξ be the characteristic function of Γ. Then the operator

$$\xi(|x|) + 1)^{-1/2}\nabla^{(s)}$$

is locally (away from thresholds and eigenvalues of H) H-smooth (in the sense of T.Kato). In cones where some of pair potentials are not vanishing radiation conditions-estimates have similar (though weaker) form with the gradient replaced by its projection on a certain subspace. Such estimates allows us to give an elementary proof of the asymptotic completeness for three-particle systems in the framework of the theory of smooth perturbations.

Astérisque

SHMUEL AGMON

A representation theorem for solutions of Schrödinger type equations on non-compact Riemannian manifolds

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A Representation Theorem for Solutions of Schrödinger Type Equations on Non-compact Riemannian Manifolds

SHMUEL AGMON

1. Introduction

In this paper we describe a representation theorem for solutions of the differential equation

$$\Delta u + \lambda q(x) u = 0 \tag{1.1}$$

on certain non-compact real analytic Riemannian manifolds. Here Δ is the Laplace-Beltrami operator, λ a complex number and $q(x)$ is a positive real-analytic function. The theorem is a generalization of a representation theorem for solutions of the Helmholtz equation on hyperbolic space proved by Helgason [3; 4] and Minemura [5]. By way of introduction we recall this special representation theorem.

We take for the hyperbolic n-space the Poincaré model of the unit ball $\mathbb{B}^n = \{x \in \mathbb{R}^n : |x| < 1\}$ with the Riemannian metric

$$ds^2 = \left(\frac{1-|x|^2}{2}\right)^{-2} |dx|^2. \tag{1.2}$$

$\mathbb{B}^n$ is a complete non-compact Riemannian manifold with an ideal boundary $\partial\mathbb{B}^n$ identified with the sphere $S^{n-1} \subset \mathbb{R}^n$. The Laplace-Beltrami operator on $\mathbb{B}^n$, denoted by Δ_h, is given in Euclidean global coordinates by

$$\Delta_h = \left(\frac{1-|x|^2}{2}\right)^2 \Delta + (n-2)\frac{1-|x|^2}{2} \sum_{i=1}^{n} x_i \partial_i \tag{1.3}$$

where Δ is the Laplacian on $\mathbb{R}^n$, $\partial_i = \partial/\partial x_i$.

Consider the equation

$$\Delta_h u + \lambda u = 0 \text{ in } \mathbb{B}^n. \tag{1.4}$$

The Helmholtz equation (1.4) has a distinguished class of solutions known as the generalized eigenfunctions of $-\Delta_h$. Given any $s \in \mathbb{C}$ and $\omega \in \partial\mathbb{B}^n$ there is a unique (normalized) generalized eigenfunction denoted by $E(x,\omega;s)$, $x \in \mathbb{B}^n$. In Euclidean coordinates it has the explicit form

$$E(x,\omega;s) = (\frac{1-|x|^2}{|x-\omega|})^s \tag{1.5}$$

for $|x| < 1$, $\omega \in S^{n-1}$. The function $u(x) = E(x,\omega;s)$ is a solution of equation (1.4) with $\lambda = s(n-1-s)$. The problem arises whether any solution u of equation (1.4) can be represented by an integral formula of the form

$$u(x) = \int_{S^{n-1}} \Phi(\omega) E(x,\omega;s)d\omega,$$

for s satisfying $s(n-1-s) = \lambda$, where Φ is some generalized function on S^{n-1}. This problem was solved in the affirmative by Helgason [3;4] and by Minemura [5]. Their main result can be stated as follows,

THEOREM 1.1. *Let $u(x)$ be a solution of the Helmholtz equation*

$$\Delta_h u + s(n-1-s)u = 0 \textit{ in } \mathbb{B}^n \tag{1.6}$$

where s is some complex number such that $s \neq (n-1-j)/2$ for $j = 1,2,\ldots$ Then there exists a unique hyperfunction Φ_u on S^{n-1} such that

$$u(x) = \langle \Phi_u, E(x,\cdot;s)\rangle \tag{1.7}$$

for $x \in \mathbb{B}^n$. Moreover, the map: $u \to \Phi_u$ is a bijection of the space of solutions of (1.6) on the space of hyperfunctions on S^{n-1}.

In this paper we generalize Theorem 1.1 and show that a similar representation theorem holds for solutions of equations (1.1) on a general class of non-compact Riemannian manifolds of which hyperbolic space is a special case. We use a P.D.E. oriented approach. When restricted to the special situation of Theorem 1.1 our approach yields a new proof of the theorem which is not using the special structure of $\mathbb{B}^n$ as a symmetric space (see also [1]). The general set up of our study is as follows. Let X be a real-analytic compact Riemannian manifold with a boundary ∂X. Let g denote the Riemannian metric on X and let Δ_g denote the corresponding Laplace-Beltrami operator. Set

$$\overset{\circ}{X} = X \setminus \partial X.$$

Introduce on $\overset{\circ}{X}$ a new Riemannian metric h, conformal with g, defined by

$$h = \rho^{-2} g \tag{1.8}$$

where $\rho(x)$ is a real-analytic function on X such that

$$\begin{aligned} &\rho(x) > 0 \text{ on } \overset{\circ}{X}, \\ &\rho(x) = 0 \text{ and } d\rho \neq 0 \text{ on } \partial X. \end{aligned} \tag{1.9}$$

Denote by Δ_h the Laplace-Beltrami operator on $\overset{\circ}{X}$ in the metric h. It is given by

$$\Delta_h = \rho^2 \Delta_g - (n-2)\rho(\nabla_g \rho) \tag{1.10}$$

where throughout the paper n denotes the dimension of X and where $\nabla_g \rho$ denotes the gradient vector field in the metric g. As usual $\nabla_g \rho$ is identified with a first order differential operator given in local coordinates by

$$\nabla_g \rho = \sum_{i,j} g^{ij} \frac{\partial \rho}{\partial x_i} \frac{\partial}{\partial x_j}. \tag{1.11}$$

We denote by $|\nabla_g \rho(x)|$, the norm of the vector $\nabla_g \rho(x)$ induced by g. In local coordinates

$$|\nabla_g \rho(x)|^2 = \sum_{i,j} g^{ij}(x) \frac{\partial \rho}{\partial x_i} \frac{\partial \rho}{\partial x_j}. \tag{1.12}$$

We consider solutions of the differential equation

$$\Delta_h u + \lambda q(x) u = 0 \text{ in } \overset{\circ}{X} \tag{1.13}$$

where $q(x)$ is a positive real-analytic function on X and λ is a complex number. We shall derive a representation theorem similar to Theorem 1.1 for solutions of (1.13). It will involve the generalized eigenfunctions of the operator $q^{-1}\Delta_h$ which will be defined in section 2.

REMARK: We note that the main result of this paper (the representation theorem) holds under weaker smoothness assumptions than those imposed above. The result holds if one assumes for instance that X, ρ and q are of class C^2 and that in addition X, ρ and q are real analytic in some neighborhood of ∂X.

In this paper we are going to impose on the function q a boundary condition. We shall assume that

$$q(x) = |\nabla_g \rho(x)|^2 \text{ on } \partial X. \tag{1.14}$$

We note that this condition is not necessary for the validity of the main representation theorem. However assumption (1.14) simplifies considerably many details in the proof of the theorem. Observe that equation (1.6) on hyperbolic n-space belongs to the class of equations introduced above. We conclude this introduction by noting that the representation theorem described in this paper for solutions of (1.13) can be shown to hold for solutions of a much wider class of equations of the form

$$\rho^2 \Delta_g u + \rho B u + C u = 0 \text{ in } \overset{\circ}{X}$$

where B is a real-analytic vector field on X satisfying some conditions on ∂X and C is a real-analytic function on X.

The main part of this paper is divided into two sections. In section 2 we discuss the Green's function associated with equation (1.13). The asymptotic and related real-analyticity properties of the Green's function play a crucial role in our study. These are described in Theorem 2.1. Using the theorem we define the generalized eigenfunctions which form a distinguished class of solutions of equation (1.13) and which are the building blocks in the representation theorem for any solution of that equation. The representation theorem is stated and proved in section 3. We note that the proof of the theorem is composed of the following two main ingredients. (i) Asymptotic and real-analyticity properties of the Green's function described in Theorem 2.1. (ii) A theorem of Baouendi and Goulaouic [2] on the solvability of the Cauchy problem on a characteristic initial hypersurface for certain P.D.E. of Fuchsian type.

2. Asymptotic properties of Green's functions and related results

When studying solutions of (1.13) it will be convenient to introduce the differential operator P on $\overset{\circ}{X}$ defined by

$$P = -q^{-1}\Delta_h. \tag{2.1}$$

We associate with P the measure dm on $\overset{\circ}{X}$ defined by

$$dm := q d\mu_h = q\rho^{-n} d\mu_g \tag{2.2}$$

where $d\mu_h$ (resp. $d\mu_g$) is the measure induced by the metric h (resp. g) on $\overset{\circ}{X}$. Considering P as a symmetric operator in $L^2(\overset{\circ}{X}; dm)$ with domain $C_0^\infty(\overset{\circ}{X})$ it is not difficult to show that $\bar{P}$ (the closure of P) is a self-adjoint operator in $L^2(\overset{\circ}{X}; dm)$. Furthermore, it can be shown that the spectrum of $\bar{P}$ has the following properties.

(i) $$\sigma_{ess}(\bar{P}) = [(\frac{n-1}{2})^2, \infty), \quad n = dim X.$$

(ii) $\sigma_p(\bar{P})$ consists of a finite number of eigenvalues contained in the interval $[0, (\frac{n-1}{2})^2)$.

Next, it will be convenient to replace the parameter λ in (1.13) by a parameter s related by

$$s(n-1-s) = \lambda. \tag{2.3}$$

Thus we rewrite equation (1.13) in the form

$$Pu - s(n-1-s)u = 0. \tag{2.4}$$

Note that the map: $s \to \lambda$ defined by (2.3) takes the half-plane $Res > (n-1)/2$ onto the domain $\mathbb{C} \setminus \sigma_{ess}(\bar{P})$. We shall denote by $\mathcal{E}$ the set of points $\{s_i\}$ in the half-plane $Res > (n-1)/2$ such that $s_i(n-1-s_i)$ is an eigenvalue of $\bar{P}$. From (ii) above it follows that $\mathcal{E}$ is a finite set of points contained in the interval $(\frac{n-1}{2}, n-1]$.

From now on we shall assume that s is some fixed number in the half-plane $Res > (n-1)/2$ such that $s \notin \mathcal{E}$. We shall denote by $G(x,y;s)$ the Green's function associated with equation (2.4) in $\overset{\circ}{X}$. It is the kernel (with respect to the measure dm) of the resolvent operator

$$(2.6) \qquad G(s) = (\bar{P} - s(n-1-s))^{-1}.$$

From the ellipticity of P in $\overset{\circ}{X}$ and the real-analyticity of the manifold (X, g) and the functions ρ and g, it follows that $G(x,y;s)$ is real-analytic in $x, y \in \overset{\circ}{X}$ for $x \neq y$. This property can be extended in some generalized sense to the (ideal) boundary of $\overset{\circ}{X}$. In this connection we introduce the following notation. For any two sets $X_i \subset X, \quad i = 1, 2$, we define

$$(X_1 \times X_2)' = \{(x_1, x_2) : x_1 \in X_1, x_2 \in X_2, x_1 \neq x_2\}.$$

The following "extension theorem" has a basic role in this paper.

THEOREM 2.1. *Let $F(x,y;s)$ be the real-analytic function on $(\overset{\circ}{X} \times \overset{\circ}{X})'$ defined by*

$$(2.7) \qquad F(x,y;s) = \rho(x)^{-s}\rho(y)^{-s}G(x,y;s).$$

Then $F(x,y;s)$ admits a real-analytic extension from $(\overset{\circ}{X} \times \overset{\circ}{X})'$ to $(X \times X)'$.

The proof of Theorem 2.1 is quite long and technical. For reasons of brevity we shall not give the proof in this paper. We plan to give the proof in another publication. Note that in the special case of equation (1.6) on the hyperbolic space $\mathbb{B}^n$ the Green's function is known explicitly and Theorem 2.1 can be verified by inspection.

Now define a family of solutions of equation (2.4) as follows. For any $\omega \in \partial X$ and $x \in \overset{\circ}{X}$ set

$$(2.8) \qquad E(x,\omega;s) = \lim_{\substack{y \to \omega \\ y \in \overset{\circ}{X}}} \rho(y)^{-s}G(x,y;s).$$

In view of Theorem 2.1 it is clear that $E(x,\omega;s)$ is a well defined real-analytic function of (x,ω) on $\overset{\circ}{X}\times\partial X$. Furthermore, for a fixed ω the function $E(x,\omega;s)$ is a solution of equation (2.4) in $\overset{\circ}{X}$. We shall refer to the family $E(x,\omega;s)$ (parameterized by $\omega\in\partial X$) as the generalized eigenfunctions of P with eigenvalue $s(n-1-s)$. These functions are the building blocks of the general representation theorem (Theorem 3.1). Note that in the special case of equation (1.6) on hyperbolic n-space the generalized eigenfunctions defined by (2.8) are (up to a multiplicative constant) those defined previously by (1.5).

We conclude this section by introducing some classes of real-analytic functions on ∂X. Let Λ be the Laplace-Beltrami operator on ∂X in the Riemannian metric induced by g. For any number $d>0$ we denote by $\mathcal{A}_d(\partial X)$ the class of C^∞ functions $\varphi(\omega)$ on ∂X satisfying the inequalities

$$(2.9)\qquad |\Lambda^j\varphi(\omega)|\le C(2j)!d^{2j}\text{ for } j=0,1,\ldots,$$

and all $\omega\in\partial X$ where C is some constant depending on φ. $\mathcal{A}_d(\partial X)$ is a Banach space under the norm

$$\|\varphi\|_d=\text{smallest constant } C \text{ for which (2.9) holds.}$$

We denote by $\mathcal{A}(\partial X)$ the class of real-analytic functions on ∂X. It is well known that

$$\mathcal{A}_d(\partial X)\subset\mathcal{A}(\partial X)\text{ for all } d>0$$

and that

$$(2.10)\qquad \mathcal{A}(\partial X)=\lim_{d\uparrow\infty}\mathcal{A}_d(\partial X).$$

We consider $\mathcal{A}(\partial X)$ as a topological linear space with the inductive limit topology induced by (2.10) and the given topologies on the Banach spaces $\mathcal{A}_d(\partial X)$.

Let $\mathcal{A}'(\partial X)$ be the dual of $\mathcal{A}(\partial X)$. Any member of $\mathcal{A}'(\partial X)$ is called a hyperfunction on ∂X. Thus a hyperfunction on ∂X is a linear functional Φ on $\mathcal{A}(\partial X)$ such that for any $d>0$ and any $\varphi\in\mathcal{A}_d(\partial X)$ the following inequality holds

$$(2.11)\qquad |\langle\Phi,\varphi\rangle|\le C_d\|\varphi\|_d$$

where C_d is a constant depending only on Φ and d.

3. The representation theorem.

We come now to the main result of this paper.

THEOREM 3.1. *Let $u(x)$ be any solution of equation (2.4) on $\overset{\circ}{X}$. Then there exists a unique hyperfunction Φ_u on ∂X such that the following representation holds*

$$u(x) = \langle \Phi_u, E(x, \cdot; s) \rangle \tag{3.1}$$

for $x \in \overset{\circ}{X}$. Moreover the map: $u \to \Phi_u$ is a bijection of the space of solutions of (2.4) on $\mathcal{A}'(\partial X)$.

REMARK 1: It can be shown that (3.1) holds with Φ_u a Schwartz distribution on ∂X if and only if

$$|u(x)| \leq \text{Const.} \rho(x)^{-N} \text{ on } \overset{\circ}{X} \tag{3.2}$$

for some $N \geq 0$. Moreover, this variant of the representation theorem can be shown to hold under weaker smoothness assumptions. Namely, it is enough to assume that X is a C^∞ Riemannian manifold and that ρ and q are C^∞ functions on X.

REMARK 2: Using Theorem 2.1 and some related estimates one can show that $E(x, \omega; s)$ is a meromorphic function of s in the half-plane $Res > (n-1)/2$ with simple poles contained in $\mathcal{E}$. Furthermore, it can be shown that $E(x, \omega; s)$ admits a meromorphic continuation in s into the whole complex plane. The last (deep) result can be used to extend Theorem 3.1 to all complex values of the parameter s which are not poles of $E(x, \omega; s)$. Thus in general solutions of equation (2.4) admit two representations of the form (3.1). One representation involves the family of solutions $E(x, \omega; s)$ and the other representation involves the family $E(x, \omega; n-1-s)$.

The proof of Theorem 3.1 will be based on Theorem 2.1 and on Theorem 3.2 below which deals with the analytic Cauchy problem for a differential equation related to (2.4) with initial data given on the characteristic manifold

∂X. Before stating the result we introduce the following notation. For any $\varepsilon > 0$ we denote by Ω_ε a neighborhood of ∂X in X defined by

$$\Omega_\varepsilon = \{x \in X : 0 \leq \rho(x) \leq \varepsilon\}.$$

We also set

$$X_\varepsilon = X \setminus \Omega_\varepsilon = \{x \in X : \rho(x) > \varepsilon\}.$$

We now state

THEOREM 3.2. *Given $\varphi \in \mathcal{A}_d(\partial X)$, $d > 0$, there exists a unique function $v_\varphi(x)$, defined and real-analytic in Ω_δ for some $\delta = \delta(d) > 0$, (δ depending on d but not on φ) such that the following holds:*

(i) v_φ is a solution in Ω_δ of the differential equation

$$\rho^{-s}P(\rho^s v) - s(n-1-s)v = 0. \tag{3.3}$$

(ii) v_φ satisfies the initial condition

$$v_\varphi = \varphi \text{ on } \partial X. \tag{3.4}$$

Moreover, the map: $\varphi \to v_\varphi$ is a continuous map from $\mathcal{A}_d(\partial X)$ to $C^k(\Omega_\delta)$ for $k = 0, 1, \ldots$

Theorem 3.2 follows as an easy corollary from a general theorem dealing with the initial value problem for Fuchsian type partial differential equations proved by Baouendi and Goulaouic ([2]; see Theorem 3 with $m = 2, k = 1$ and $h = 0$). In this connection note that the two indicial exponents associated with equation (2.4) at the boundary are s and $n - 1 - s$. This implies that equation (3.3) can be written in the form

$$\rho\Delta_g v + Bv + Cv = 0 \text{ in } \Omega_\delta \tag{3.5}$$

where B is a real-analytic field on X and C is a real-analytic function on X. It is this form of equation (3.3) which allows one to deduce Theorem 3.2 from the results of [2].

We turn to the

PROOF OF THEOREM 3.1: Observe that since $E(x,\omega;s)$ is a real-analytic function in (x,ω) on $\overset{\circ}{X} \times \partial X$ it is clear that the function $u(x) = \langle \Phi, E(x,\cdot;s)\rangle$ is a well defined solution of (2.4) in $\overset{\circ}{X}$ for any $\Phi \in \mathcal{A}'(\partial X)$. To establish the converse we introduce some notation.

For any $\varphi \in \mathcal{A}(\partial X)$ we set

$$w_\varphi(x) = \rho^s v_\varphi(x) \tag{3.6}$$

where $v_\varphi(x)$ is the solution of the initial value problem described in Theorem 3.2. With no loss of generality we shall assume in the following that $\varphi \in \mathcal{A}_d(\partial X)$ for some $d > 0$ and that $v_\varphi(x)$ is defined in $\Omega_{\delta(d)}$ for some $\delta(d) > 0$. We shall also assume that $\delta(d) \le \delta_0$ where $\delta_0 > 0$ is chosen sufficiently small so that $(d\rho)(x) \ne 0$ for $x \in \Omega_{\delta_0}$. It follows form (3.6) and (3.3) that $w_\varphi(x)$ is a well defined solution of (2.4) in $\mathrm{int}(\Omega_{\delta(d)})$.

Let now $u(x)$ be a given solution of equation (2.4) in $\overset{\circ}{X}$. For any $\varphi \in \mathcal{A}_d(\partial X)$ and $0 < \varepsilon < \delta(d)$, we set

$$I_u^\varepsilon(\varphi) := \int_{\partial X_\varepsilon} (w_\varphi D_\nu u - u D_\nu w_\varphi) d\mu_h^\varepsilon(x) \tag{3.7}$$

where D_ν denotes a derivation in the direction of the outward unit normal vector (in the metric h) at the boundary ∂X_ε. Here $d\mu_h^\varepsilon$ denotes the measure on ∂X_ε induced by $d\mu_h$. We claim that $I_u^\varepsilon(\varphi)$ is independent of ε; i.e.

$$I_u^{\varepsilon_1}(\varphi) = I_u^{\varepsilon_2}(\varphi) \text{ for } 0 < \varepsilon_1 < \varepsilon_2 < \delta(d). \tag{3.8}$$

Indeed, we have

$$w_\varphi \Delta_h u - u \Delta_h w_\varphi = 0 \text{ in } \mathrm{int}(\Omega_{\delta(d)}). \tag{3.9}$$

Integrating (3.9) on the domain $X_{\varepsilon_1} \setminus X_{\varepsilon_2}$, applying Green's formula, one obtains (3.8).

Next we define a hyperfunction Φ_u on ∂X as follows: For any $\varphi \in \mathcal{A}(\partial X)$ we set

$$\langle \Phi_u, \varphi \rangle := \lim_{\varepsilon \to 0} I_u^\varepsilon(\varphi). \tag{3.10}$$

That Φ_u is a well defined linear functional on $\mathcal{A}(\partial X)$ is clear in view of (3.8) and the linearity of w_φ in φ. That Φ_u is also continuous on $\mathcal{A}(\partial X)$ one sees by noting that for a given $d > 0$ there exists a $\delta = \delta(d) > 0$ such that for any $\varepsilon \in (0, \delta)$ I_u^ε is a well defined continuous linear functional on $\mathcal{A}_d(\partial X)$. This observation follows easily from the definition of I_u^ε and Theorem 3.2.

Finally we shall show that the hyperfunction Φ_u defined by (3.10) yields the representation (3.1). To this end fix a point $y \in \overset{\circ}{X}$ and set

$$\psi(\omega) = E(y, \omega; s). \tag{3.11}$$

From (2.8), Theorem 2.1 and Theorem 3.2 it follows that the unique solution v_ψ of equation (3.3) with the initial data $\psi(\omega)$ on ∂X is given by

$$v_\psi(x) = \rho(x)^{-s} G(x, y; s),$$

so that

$$w_\psi(x) = G(x, y; s) \text{ for } x \in int(\Omega_\delta) \tag{3.12}$$

(we can take $\delta = \rho(y)$). Combining (3.7) to (3.12), taking ε sufficiently small, we get

$$\begin{aligned} \langle \Phi_u, \psi \rangle &= I_u^\varepsilon(\psi) \\ &= \int\limits_{\partial X_\varepsilon} (G(x, y; s) D_\nu u(x) - u(x) D_\nu G(x, y; s)) d\mu_h^\varepsilon(x) \\ &= u(y), \end{aligned} \tag{3.13}$$

where the last equality follows by application of Green's formula to u and the Green's function. This yields formula (3.1) and proves the existence part of Theorem 3.1.

It remains to show that the representation (3.1) is unique. This is an easy consequence of the following

LEMMA 3.3. *Given $\varphi \in \mathcal{A}(\partial X)$ there exists a function $f \in C_0^\infty(\overset{\circ}{X})$ such that*

$$\varphi(\omega) = \int\limits_{\overset{\circ}{X}} f(x) E(x, \omega; s) dm(x). \tag{3.14}$$

Deferring the proof of the lemma we establish the uniqueness of the representation (3.1) by showing that if $\Phi \in \mathcal{A}'(\partial X)$ satisfies

$$\langle \Phi, E(x; \cdot; s)\rangle = 0 \text{ for all } x \in \overset{\circ}{X} \tag{3.15}$$

then

$$\langle \Phi, \varphi\rangle = 0 \text{ for all } \varphi \in \mathcal{A}(\partial X), \tag{3.15 $'$}$$

Indeed, it follows from (3.15) that for any function $f \in C_0^\infty(\overset{\circ}{X})$ we have

$$\begin{aligned} 0 &= \int_{\overset{\circ}{X}} f(x)\langle \Phi, E(x, \cdot; s)\rangle dm(x) \\ &= \langle \Phi, \int_{\overset{\circ}{X}} f(x) E(x, \cdot; s) dm(x)\rangle, \end{aligned} \tag{3.16}$$

where the change of order of "integrations" in (3.16) is easily justified. Combining (3.16) with Lemma 3.3 we obtain (3.15$'$). This establishes uniqueness and completes the proof of Theorem 3.1.

We conclude with the

PROOF OF LEMMA 3.3: As before we shall associate with the given function $\varphi \in \mathcal{A}(\partial X)$ the solution $v_\varphi(x)$ of the initial value problem described in Theorem 3.2. Thus in particular v_φ is a real-analytic function defined in some $\Omega_\delta, \quad \delta > 0$. Next we pick a function $\zeta(x) \in C^\infty(X)$ such that

$$\zeta(x) = 1 \text{ for } x \in \Omega_{\delta/3}, \quad \zeta(x) = 0 \text{ for } x \in X \setminus \Omega_{\delta/2} \tag{3.17}$$

and define a function $w \in C^\infty(\overset{\circ}{X})$ by

$$\begin{aligned} w(x) &= \zeta(x)\rho(x)^s v_\varphi(x) \text{ for } x \in \Omega_{\delta/2} \setminus \partial X, \\ w(x) &= 0 \text{ for } x \in X \setminus \Omega_{\delta/2}. \end{aligned} \tag{3.18}$$

Set

$$f(x) := (P - s(n-1-s))w(x). \tag{3.19}$$

Since v_φ is a solution of (3.3) in Ω_δ it follows from (3.19), (3.18) and (3.17) that $f(x) = 0$ in $\Omega_{\delta/3}$ and thus $f \in C_0^\infty(\overset{\circ}{X})$. We also observe that $w \in L^2(\overset{\circ}{X}; dm)$ (since $Res > (n-1)/2$). These remarks and (3.19) imply that

$$w = G(s)f \tag{3.20}$$

where $G(s)$ denotes the resolvent operator (2.6). Rewriting (3.20) in terms of the Green's function (the kernel of $G(s)$), using (3.17), (3.18) and the symmetry of the Green's function, we find that for any $y \in \Omega_{\delta/3}/\partial X$ the following formula holds

$$v_\varphi(y) = \int_{\overset{\circ}{X}} f(x)G(x,y;s)\rho(y)^{-s}\,dm(x). \tag{3.21}$$

Now fix a point $\omega \in \partial X$ and let $y \to \omega$ in (3.21). Using (3.4), (2.8) and Theorem 2.1 we find that

$$\begin{aligned}\varphi(\omega) = \lim_{y\to\omega} v_\varphi(y) &= \lim_{y\to\infty} \int_{\overset{\circ}{X}} f(x)G(x,y;s)\rho(y)^{-s}\,dm(x) \\ &= \int_{\overset{\circ}{X}} f(x)E(x,\omega;s)dm(x).\end{aligned}$$

This proves the lemma.

REFERENCES

[1] S. Agmon, *On the representation theorem for solutions of the Helmholtz equation on the hyperbolic space*, Preprint 1990.

[2] M. S. Baouendi and C. Goulaouic, *Cauchy problems with characteristic initial hypersurface*, Comm. Pure Appl. Math., 26, 1973, pp. 455-475.

[3] S. Helgason, *A duality for symmetric spaces with applications to group representations*, Advan. Math., 5, 1970, pp. 1-154.

[4] S. Helgason, *Eigenspaces of the Laplacian; Integral representations and irreducibility*, J. Func. Analysis, 17, 1974, pp. 328-353.

[5] K. Minemura, *Eigenfunctions of the Laplacian on a real hyperbolic space*, J. Math. Soc. Japan, 27, 1975, pp. 82-105.

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Some developments and applications of the abstract Mourre theory

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Some Developments and Applications of the Abstract Mourre Theory

Anne Boutet de Monvel-Berthier and Vladimir Georgescu [1]

1. Introduction

In 1979 Eric Mourre introduced the concept of locally conjugate operator and invented a very efficient method of proving the limiting absorption principle (L.A.P.). His ideas opened the way to a complete solution of the N-body problem: detailed spectral properties have been obtained by Perry, Sigal and Simon and asymptotic completeness has been proved by Sigal and Soffer. The abstract side of Mourre theory has been further developped by Perry, Sigal and Simon [PSS] (they eliminated an assumption on the first commutator which was annoying in applications) and by Mourre [M] and Jensen and Perry [JP] (the L.A.P was established in better spaces).

In [ABG] efforts were made in order to avoid the use of the second commutator of the hamiltonian with the conjugate operator. Optimal, in some sense, results in this direction were obtained in [BGM2] and [BG1]. In [BGM2] the space $\mathcal{G}$ which appears below is the domain of the hamiltonian and the main theorem is easy to apply in the N-body case with short-range and long-range interactions of a very general nature. In [BG1,2] the space $\mathcal{G}$ is the form-domain of the hamiltonian (the domain is not assumed invariant under the group generated by the conjugate operator, this being compensated by a stronger condition on the first commutator) and the theory is applied to pseudo-differential operators. In both cases, the L.A.P. is established in "optimal" (in some sense) spaces, which allows one to get without any further effort very good criteria for the existence and completeness of relative, local wave operators.

The main part of this article is devoted to an exposition of several applications of a version of the locally conjugate operator method which we developed in [BG1,2]. In fact, theorems 3.1 and 3.2 below are the main results got in [BG1] and in sections 4 and 5 we show their force and also fineness. In the preliminary section 2 we introduce and discuss the most important notion we have isolated, that of operator of class $\mathcal{C}^1$ with respect to a unitary group. This is a quite general property and in section 5 we show in some simple cases that it is almost impossible to be replaced by a weaker one without loosing the strong form of the L.A.P. given

[1] Lecture delivered by A. Boutet de Monvel-Berthier

in theorem 3.1. Moreover, in section 5 we show how to deal with hamiltonians with very singular interactions (this part will be treated more thoroughly in a later publication). But section 4 contains the most important results. Although their formulation is abstract, it is trivial to apply them to many-body hamiltonians. After the Nantes conference, as A. Soffer raised the problem of the spectral analysis of hard-core N-body hamiltonians, we decided to formulate, in this paper, several consequences of theorem 3.1 such as to cover non-densely defined hamiltonians (in fact we use pseudo-resolvents in place of resolvents). The particular case of hard-core N-body hamiltonians is the subject of a in-preparation-joint-paper with A. Soffer. Finally, an appendix contains a technical estimate related to Littlewood-Paley theory which seemes to us quite powerful in various situations.

2. Unitary Groups in Friedrichs Couples

In our approach, the natural framework for the "locally conjugate operator method" is a triplet $(\mathscr{G},\mathscr{H};W)$ consisting of two Hilbert spaces $\mathscr{G},\mathscr{H}$ such that $\mathscr{G}\subset\mathscr{H}$ continuously and densely, and a strongly continuous unitary one-parameter group $W=\{W_\alpha\}_{\alpha\in\mathbb{R}}$ in $\mathscr{H}$ which leaves $\mathscr{G}$ invariant: $W_\alpha\mathscr{G}\subset\mathscr{G}$ for all $\alpha\in\mathbb{R}$ .The Hilbert spaces are always complex but not necessarily separable. In our applications, $\mathscr{G}$ will be either the domain of the hamiltonian, or its form domain, or it will be just $\mathscr{H}$ (although, in this last case, the hamiltonian could be unbounded and even non-densely defined).

A triplet $(\mathscr{G},\mathscr{H};W)$ with the preceding properties will be called a *unitary group in a Friedrichs couple* , the pair of spaces $(\mathscr{G},\mathscr{H})$ being called a *Friedrichs couple.* In this section we shall fix such a system $(\mathscr{G},\mathscr{H};W)$ and we shall study some notions related to it.

Let $\mathscr{G}^*$ be the adjoint (or antidual) space of $\mathscr{G}$; identify $\mathscr{H}^*=\mathscr{H}$ by using Riesz lemma and embed as usual $\mathscr{G}\subset\mathscr{H}\subset\mathscr{G}^*$. Then define $\mathscr{G}^s=[\mathscr{G},\mathscr{G}^*]_{(1-s)/2}$ by complex interpolation for $-1\leq s\leq 1$, so that $\mathscr{G}^1=\mathscr{G}$, $\mathscr{G}^0=\mathscr{H}$ and $\mathscr{G}^{-1}=\mathscr{G}^*$. Observe that we have canonical identifications $(\mathscr{G}^s)^*=\mathscr{G}^{-s}$. We shall denote $\mathscr{X}=B(\mathscr{G},\mathscr{G}^*)$ the Banach space of continuous linear operators from $\mathscr{G}$ to $\mathscr{G}^*$ and $\|\cdot\|_{\mathscr{X}}$ its norm; observe that $\mathscr{X}$ is equipped with an isometric involution $T\mapsto T^*$. For each $s,t\in[-1,+1]$ we have canonical embeddings $B(\mathscr{G}^s,\mathscr{G}^t)\subset\mathscr{X}$. Then the norm in $\mathscr{G}^s$, resp. in $B(\mathscr{G}^s,\mathscr{G}^t)$, will be denoted $\|\cdot\|_s$, resp. $\|\cdot\|_{s,t}$, and we abbreviate $\|\cdot\|_0=\|\cdot\|$, $\|\cdot\|_{0,0}=\|\cdot\|$.

The following fact will be often used below:

LEMMA 2.1: *Let* $\mathbf{E},\mathbf{F}$ *be Hilbert spaces such that* $\mathbf{E}\subset\mathbf{F}$ *continuously and let* $W_\alpha(\alpha)=e^{iA\alpha}$, $\alpha\in\mathbb{R}$, *be a* C_0-*group in* $\mathbf{F}$ *which leaves* $\mathbf{E}$ *invariant*: $W_\alpha\mathbf{E}\subset\mathbf{E}$

$(\forall\alpha\in\mathbb{R})$.*Denote* $W_\alpha^{\mathbf{E}}=W_\alpha|_{\mathbf{E}}$ *considered as operator in* $\mathbf{E}$. *Then* $\{W_\alpha^{\mathbf{E}}\}_{\alpha\in\mathbb{R}}$ *is a* C_0-*group in* $\mathbf{E}$ *and its infinitesimal generator is the closed, densely defined operator* $A^{\mathbf{E}}$ *in* $\mathbf{E}$ *defined as the restriction of* A *to* $D(A^{\mathbf{E}})=\{u\in D(A)\cap\mathbf{E}|\ Au\in\mathbf{E}\}$.

Proof: The lemma has been proved in [ABG] under the assumption that $\mathbf{E},\mathbf{F}$ are separable. We shall reduce ourselves to this case. The only problem is to prove the continuity of $\alpha\mapsto W_\alpha u\in\mathbf{E}$ when $u\in\mathbf{E}$. Let $\mathbf{E}_0$ (resp. $\mathbf{F}_0$) be the closed subspace of $\mathbf{E}$ (resp.$\mathbf{F}$) generated by $\{W_\alpha u|\ \alpha\in\mathbb{R}\}$. Then $\mathbf{E}_0\subset\mathbf{F}_0$ continuously and densely, W leaves $\mathbf{E}_0$ and $\mathbf{F}_0$ invariant and it is strongly continuous in $\mathbf{F}_0$. Moreover, $\mathbf{F}_0$ is separable because $\alpha\mapsto W_\alpha u\in\mathbf{F}_0$ is continuous and its image is a total subset of $\mathbf{F}_0$. Since $\mathbf{F}_0^*\subset\mathbf{E}_0^*$ continuously and densely, we see that $\mathbf{E}_0^*$ is separable, hence $\mathbf{E}_0$ is separable too. Now we may apply lemmas 1.1.3 and 1.1.4 from [ABG1] to $(\mathbf{E}_0,\mathbf{F}_0;W|_{\mathbf{F}_0})$. ■

Let us apply this lemma in the case of the unitary group W in the Friedrichs couple $(\mathscr{G},\mathscr{H})$. Denote A the self-adjoint operator in $\mathscr{H}$ such that $W_\alpha=e^{iA\alpha}$. The notations $W_\alpha^{\mathscr{G}}$, $A^{\mathscr{G}}$ have the same signification as in the preceding lemma. Now let $W_\alpha^{\mathscr{G}^*}=(W_{-\alpha}^{\mathscr{G}})^*\in B(\mathscr{G}^*)$. Since for a group weak and strong continuity are equivalent, $\{W_\alpha^{\mathscr{G}^*}\}_{\alpha\in\mathbb{R}}$ will be a C_0-group in $\mathscr{G}^*$; we denote $A^{\mathscr{G}^*}$ its generator (closed, densely defined operator in $\mathscr{G}^*$ such that $W_\alpha^{\mathscr{G}^*}=\exp(i\alpha A^{\mathscr{G}^*})$).

It is easily shown that $W_\alpha^{\mathscr{G}^*}|_{\mathscr{H}}=W_\alpha$ and an application of lemma 2.1 shows that A is just the restriction of $A^{\mathscr{G}^*}$ to $\{u\in D(A^{\mathscr{G}^*})\cap\mathscr{H}\ |\ A^{\mathscr{G}^*}u\in\mathscr{H}\}$. Interpolating between $\mathscr{G}$ and $\mathscr{G}^*$, we see that $W^{\mathscr{G}^*}$induces a C_0-group $W^{\mathscr{G}^s}$ in each $\mathscr{G}^s$, the infinitesimal generators of these groups being the natural restrictions of $A^{\mathscr{G}^*}$. It will be obvious in later arguments that no confusion arises if we drop the index which indicates the space in which the operators are considered. We summarize these facts in:

PROPOSITION 2.2: *Let* $(\mathscr{G},\mathscr{H};W)$ *be a unitary group in a Friedrichs couple. Then , for each* $\alpha\in\mathbb{R}$, *the operator* W_α *in* $\mathscr{H}$ *is continuous when* $\mathscr{H}$ *is equipped with the topology induced by* $\mathscr{G}^*$ *and, if we denote again by* W_α *its unique extension to a continuous operator on* $\mathscr{G}^*$, *the application* $\alpha\mapsto W_\alpha\in B(\mathscr{G}^*)$ *is a* C_0-*group in* $\mathscr{G}^*$ *which leaves invariant and induces a* C_0-*group in each space* $\mathscr{G}^s$. *Let* A *be the infinitesimal generator of the group* W *in* $\mathscr{G}^*$, i.e. A *is the unique closed, densely defined operator in* $\mathscr{G}^*$ *such that* $W_\alpha=e^{iA\alpha}$; *denote* $D(A;\mathscr{G}^*)$ *its domain. Then for each* $s\in[-1,+1]$, *the restriction of* A *to*

(2.1) $\quad D(A;\mathscr{G}^s) = \{u \in \mathscr{G}^s \mid u \in D(A;\mathscr{G}^*)$ *and* $Au \in \mathscr{G}^s\}$

is a closed, densely defined operator in $\mathscr{G}^s$ *which is just the infinitesimal generator of the* C_0*-group* $W_\alpha|_{\mathscr{G}^s}$.

We shall always consider $D(A;\mathscr{G}^s)$ as a Hilbert space, the norm being the graph norm associated to A in $\mathscr{G}^s$: $\|u\|_s^A = [\ \|u\|_s^2 + \|Au\|_s^2\ ]^{1/2}$. It follows from a well-known lemma of Nelson (see theorem 1.9 in [D]) that $D(A;\mathscr{G}) \subset D(A;\mathscr{G}^s) \subset \mathscr{G}^s$ continuously and *densely* for all $s \in [-1,+1]$. Moreover, the operator A with domain $D(A;\mathscr{H})$ is self-adjoint in $\mathscr{H}$.

Finally, let us remark that the equality $W_\alpha^* = W_{-\alpha}$ has to be interpreted in the following sense: if $-1 \le s \le 1$, then the adjoint of the operator $W_\alpha|_{\mathscr{G}^s} \in B(\mathscr{G}^s)$ is equal to $W_{-\alpha}|_{\mathscr{G}^{-s}} \in B(\mathscr{G}^{-s})$, the identification $(\mathscr{G}^s)^* = \mathscr{G}^{-s}$ being assumed.

Let us consider now the group of automorphisms of the Banach space $\mathscr{X} = B(\mathscr{G},\mathscr{G}^*)$ induced by W, namely $\mathscr{W}_\alpha(T) = W_\alpha T W_\alpha^*$ for $T \in \mathscr{X}$. Observe that $\alpha \mapsto \mathscr{W}_\alpha(T) \in \mathscr{X}$ is continuous only when $\mathscr{X}$ is equipped with the strong operator topology, hence $\{\mathscr{W}_\alpha\}_{\alpha \in \mathbb{R}}$ is not a C_0-group on $\mathscr{X}$. However, one has $\mathscr{W}_\alpha = e^{i\mathscr{A}\alpha}$, with $\mathscr{A}(T) = [A,T]$, in a sense which we shall explain below.

DEFINITION 2.3: *Let* $0 < \theta \le 1$. *We shall say that an operator* $T \in B(\mathscr{G},\mathscr{G}^*)$ *is of class* $C^\theta(A;\mathscr{G},\mathscr{G}^*)$, *and we shall write* $T \in C^\theta(A;\mathscr{G},\mathscr{G}^*)$, *if the function* $\alpha \mapsto \mathscr{W}_\alpha(T) \in \mathscr{X}$ *is Hölder continuous of order* θ, *i.e. there is* $c < \infty$ *such that* $\|W_\varepsilon T W_\varepsilon^* - T\|_{\mathscr{X}} \le c|\varepsilon|^\theta$ *for* $|\varepsilon| \le 1$. *For* $\theta = +0$ *we replace Hölder-continuity by Dini-continuity, more precisely we write* $T \in C^{+0}(A;\mathscr{G},\mathscr{G}^*)$ *if* $\int_0^1 \|W_\varepsilon T W_\varepsilon^* - T\|_{\mathscr{X}}\, \varepsilon^{-1} d\varepsilon < \infty$.

Remark that we could replace here $W_\varepsilon T W_\varepsilon^* - T$ by the commutator $[T,W_\varepsilon] = TW_\varepsilon - W_\varepsilon T = (W_\varepsilon T W_\varepsilon^* - T)W_\varepsilon$. One can refine the notion and define $T \in C^\theta(A;\mathscr{G}^s,\mathscr{G}^t)$ for some $-1 \le s,t \le 1$ by replacing the norm $\|\cdot\|_{\mathscr{X}}$ with the norm $\|\cdot\|_{s,t}$.

If $T: \mathscr{G} \to \mathscr{G}^*$ is a linear continuous operator, we shall denote $[A,T] \equiv -[T,A]$ the continuous sesquilinear form on $D(A;\mathscr{G})$ defined by the formula $\langle u|[A,T]v\rangle = \langle Au|Tv\rangle - \langle u|TAv\rangle$. Taking into account that W is a C_0-group in $\mathscr{G}$

and that $\alpha \mapsto W_\alpha u \in \mathcal{G}$ is strongly differentiable for each $u \in D(A;\mathcal{G})$ it is trivial to see that

$$(2.2) \qquad W_\alpha T W_\alpha^* - T = i \int_0^\alpha W_\tau [A,T] W_\tau^* \, d\tau$$

as sesquilinear forms on $D(A;\mathcal{G})$. In particular, denoting $A_\alpha = (i\alpha)^{-1}(W_\alpha - 1)$ for $\alpha \neq 0$, we get

$$(2.3) \qquad [A_\alpha, T] = \alpha^{-1} \int_0^\alpha W_\tau [A,T] W_{\alpha-\tau} \, d\tau.$$

as forms on $D(A;\mathcal{G})$. In the next lemma we shall summarize some easy consequences of these formulas.

LEMMA 2.4: *An operator* $T \in B(\mathcal{G}, \mathcal{G}^*)$ *is of class* $C^1(A;\mathcal{G},\mathcal{G}^*)$ *if and only if one of the following equivalent properties is fulfilled* :

(a) $\liminf_{\varepsilon \to +0} \|[A_\varepsilon, T]\|_{\mathcal{X}} < \infty$;

(b) *the function* $\alpha \mapsto W_\alpha T W_\alpha^* \in B(\mathcal{G},\mathcal{G}^*)$ *is weakly derivable at* $\alpha = 0$;

(c) *the preceding function is strongly continuously derivable* ;

(d) *the sesquilinear form* $[A,T]$ *is continuous for the topology induced by* $\mathcal{G}$ *on* $D(A;\mathcal{G})$;

(e) $\lim_{\varepsilon \to 0} [A_\varepsilon, T]$ *exists weakly in* $B(\mathcal{G},\mathcal{G}^*)$;

(f) $\lim_{\mu \to +0} \int_\mu^1 (W_{2\varepsilon} T W_{2\varepsilon}^* - 2W_\varepsilon T W_\varepsilon^* + T)\, \varepsilon^{-2} d\varepsilon$ *exists weakly (hence also strongly) in* $B(\mathcal{G},\mathcal{G}^*)$.

Under these conditions, if we denote by the same symbol $[A,T]$ *the continuous sesquilinear form on* $\mathcal{G}$ *which extends the form* $[A,T]$ *given on* $D(A;\mathcal{G})$ *and the continuous operator* $\mathcal{G} \to \mathcal{G}^*$ *associated to it, then:*

$$(2.4) \qquad [A,T] = -i \frac{d}{d\alpha} W_\alpha T W_\alpha^* |_{\alpha=0} = \lim_{\varepsilon \to 0} [A_\varepsilon, T] ,$$

the derivative and the limit being taken in the strong operator topology of $B(\mathcal{G},\mathcal{G}^*)$. *Moreover, we shall have* $[A,T] \in B(\mathcal{G}^s, \mathcal{G}^t)$ *for some* $-1 \leq s,t \leq 1$, *if and only if* $T \in C^1(A;\mathcal{G}^s,\mathcal{G}^t)$ *and in this case* (2.2) *will hold strongly in* $B(\mathcal{G}^s,\mathcal{G}^t)$.

Proof: (2.2) and (2.3) show that $\varepsilon^{-1}(W_\varepsilon T W_\varepsilon^* - T) \to [iA,T]$ and $[A_\varepsilon,T] \to [A,T]$ weakly as forms on $D(A;\mathcal{G})$ (W is strongly continuous on $D(A;\mathcal{G})$ also). So (b) $\Leftrightarrow$ (e) $\Leftrightarrow$ (d) $\Leftrightarrow$ (c) (use (2.2) again). From (a) and the compacity of closed balls of $\mathcal{X}$ in the weak operator topology, we see that $\varepsilon_j^{-1}(W_{\varepsilon_j} T W_{\varepsilon_j}^* - T)$ is weakly convergent in $B(\mathcal{G},\mathcal{G}^*)$ for some sequence $\varepsilon_j \to 0$, so we get (d) again. It remains to show that (f) is equivalent with the other assertions (see [BB] for the technique which we shall use). Let $J_\tau:\mathscr{X}\to\mathscr{X}$ be defined by $J_\tau=\tau^{-1}\int_0^\tau \mathscr{W}_\alpha d\alpha$ and let $S_\mu=(\ell n2)^{-1}\int_\mu^{2\mu}(\mathscr{W}_\varepsilon(T)-T)\varepsilon^{-2}d\varepsilon$. A simple calculation gives:

$$(2.5)\qquad J_\tau(S_\mu)=(\ell n2)^{-1}\int_\mu^{2\mu}J_\alpha[\tau^{-1}(\mathscr{W}_\tau(T)-T)]\,\alpha^{-1}d\alpha.$$

If (b) is fulfilled, taking into account that $\lim_{\tau\to 0} J_\tau=1$ in the strong operator topology of $\mathscr{X}=B(\mathscr{G},\mathscr{G}^*)$, we get $S_\mu=(\ell n2)^{-1}\int_\mu^{2\mu}J_\alpha(i[A,T])\alpha^{-1}d\alpha$ which easily implies that $\lim_{\mu\to 0}S_\mu=[iA,T]$ strongly. Now observe that:

$$(2.6)\qquad 2\ell n2\ S_\mu = 2\int_\mu^1(\mathscr{W}_\varepsilon(T)-T)\,\varepsilon^{-2}d\varepsilon - 2\int_{2\mu}^1(\mathscr{W}_\varepsilon(T)-T)\,\varepsilon^{-2}d\varepsilon =$$
$$= 2\int_{1/2}^1(\mathscr{W}_\varepsilon(T)-T)\varepsilon^{-2}d\varepsilon - \int_\mu^{1/2}(\mathscr{W}_{2\varepsilon}(T)-2\mathscr{W}_\varepsilon(T)+T)\,\varepsilon^{-2}d\varepsilon\ ,$$

hence the limit in (f) exists strongly. Reciprocally, assume (f). Then (2.6) shows that $\lim_{\mu\to 0} S_\mu\equiv S$ exists weakly. But (2.5) implies (with no assumption on T) that $\lim_{\mu\to 0} J_\tau(S_\mu)=\tau^{-1}(\mathscr{W}_\tau(T)-T)$ strongly. So we get $\tau^{-1}(\mathscr{W}_\tau(T)-T)=J_\tau(S)\to S$ strongly as $\tau\to 0$, in particular (b) is fulfilled. ■

COROLLARY 2.5 (Virial theorem): *If* $T:\mathscr{G}\to\mathscr{G}^*$ *is symmetric and of class* $C^1(A;\mathscr{G},\mathscr{G}^*)$, *and if* $u,v\in\mathscr{G}$ *are such that* $Tu=\lambda u$, $Tv=\lambda v$ *for some* $\lambda\in\mathbb{R}$, *then* $\langle u|[A,T]v\rangle=0$.

Proof: Using the second equality in (2.5) we have:

$$\langle u|[A,T]v\rangle=\lim_{\varepsilon\to 0}\langle u|[A_\varepsilon,T]v\rangle=\lim_{\varepsilon\to 0}(\langle u|A_\varepsilon Tv\rangle-\langle Tu|A_\varepsilon v\rangle)=0.\ ■$$

In order to arrive at deeper aspects of Mourre theory (namely a precise form of the limiting absorption principle) the C^1 regularity property is not enough. One can introduce a stronger notion, namely to ask that $\alpha\mapsto W_\alpha TW_\alpha^*\in B(\mathscr{G},\mathscr{G}^*)$ be *norm* derivable at $\alpha=0$; *we then say that* T *is of class* $C_u^1(A;\mathscr{G},\mathscr{G}^*)$ (i.e. it is of class C^1 in the uniform topology). This is equivalent with asking, besides $T\in C^1(A;\mathscr{G},\mathscr{G}^*)$, that $\alpha\mapsto W_\alpha[A,T]W_\alpha^*$ be norm-continuous. Unfortunately, even this assumption is not strong enough, as our example from section 5 shows. However, the sufficient assumption we have been able to isolate, is only slightly stronger than this one. In fact, the proof of lemma 2.4 shows that $T\in C_u^1(A;\mathscr{G},\mathscr{G}^*)$ *if and only if the limit in* (f) *exists in norm.* Our condition is the following:

DEFINITION 2.6: *An operator* $T\in B(\mathscr{G},\mathscr{G}^*)$ *is said to be of class* $\mathscr{C}^1(A;\mathscr{G},\mathscr{G}^*)$ *if:*

$$(2.7)\qquad \int_0^1 \|W_{2\varepsilon}TW_{2\varepsilon}^*-2W_\varepsilon TW_\varepsilon^*+T\|_{\mathscr{X}}\ \varepsilon^{-2}d\varepsilon<\infty.$$

It is clear that the expression under the norm above may be replaced by the more symmetrical $W_\varepsilon T W_\varepsilon^* + W_{-\varepsilon} T W_{-\varepsilon}^* - 2T$ or by $[W_\varepsilon,[W_\varepsilon,T]]$. In fact $W_{2\varepsilon} T W_{2\varepsilon}^* - 2W_\varepsilon T W_\varepsilon^* + T = [W_\varepsilon,[W_\varepsilon,T]]W_{2\varepsilon}^*$. Using the notation $A_\varepsilon = (i\varepsilon)^{-1}(W_\varepsilon - 1)$ introduced above, (2.7) can be expressed in the equivalent from

(2.8) $\quad \int_0^1 \|[A_\varepsilon,[A_\varepsilon,T]]\|_{\mathcal{X}}\, d\varepsilon < \infty.$

The remark we made just before the definition implies $\mathscr{C}^1(A;\mathcal{G},\mathcal{G}^*) \subset C_u^1(A;\mathcal{G},\mathcal{G}^*)$. In order to compare the assumption $T \in \mathscr{C}^1$ with other assumptions made in the development of Mourre theory, it is useful to introduce the classes $C^s(A;\mathcal{G},\mathcal{G}^*)$ for $1<s\leq 2$ or $s=1+0$.

DEFINITION 2.7: *Let* $s \in]1,2]$ *or* $s=1+0$; *denote* $\theta=s-1$ *in the first case and* $\theta=+0$ *in the second one. We shall say that* $T \in B(\mathcal{G},\mathcal{G}^*)$ *is of class* $C^s(A;\mathcal{G},\mathcal{G}^*)$ *if* $T \in C^1(A;\mathcal{G},\mathcal{G}^*)$ *and* $[A,T] \in C^\theta(A;\mathcal{G},\mathcal{G}^*)$.

So $T \in C^{1+0}(A;\mathcal{G},\mathcal{G}^*)$ means that $\alpha \longmapsto W_\alpha T W_\alpha^* \in B(\mathcal{G},\mathcal{G}^*)$ is derivable and its derivative is a Dini-continuous function. We have for $0<\theta\leq 1$:

(2.9) $\quad \mathscr{C}^1(A;\mathcal{G},\mathcal{G}^*) \supset C^{1+0}(A;\mathcal{G},\mathcal{G}^*) \supset C^{1+\theta}(A;\mathcal{G},\mathcal{G}^*).$

Only the first inclusion is not completely trivial, but it follows easily from:

$$W_\varepsilon T W_\varepsilon^* + W_{-\varepsilon} T W_{-\varepsilon}^* - 2T = i \int_0^\varepsilon \{W_\tau[A,T]W_\tau^* - W_{-\tau}[A,T]W_{-\tau}^*\}\, d\tau.$$

By lemma 2.4, $T \in C^2(A;\mathcal{G},\mathcal{G}^*)$ means that $[A,T]$ and $[A,[A,T]]$ belong to $B(\mathcal{G},\mathcal{G}^*)$; this is, essentially, the situation considered by Mourre and Perry, Sigal and Simon. The case $0<\theta<1$ was studied in [ABG] while the class $\mathscr{C}^1$ is implicit in the definition of "admissibility" given in section 4 of [BGM].

We shall not explain here how the assumption $T \in \mathscr{C}^1(A;\mathcal{G},\mathcal{G}^*)$ is verified in applications. In fact this is quite easy if one uses the technique presented in [BG2] together with the estimate proved in the appendix at the end of this paper (see [BG2] for examples).

3. The Limiting Absorption Principle

In this section we shall summarize the results of our Note [BG1]. Let $(\mathcal{G},\mathcal{H};W)$ be a unitary group in a Friedrichs couple and H a self-adjoint operator in $\mathcal{H}$ with $\mathcal{G}$ as form-domain (i.e. $\mathcal{G}=D(|H|^{1/2})$ algebraically; by closed graph theorem the equality will hold on a topological level too). Then H extends to a continuous symmetric operator (denoted by the same symbol) $H:\mathcal{G}\to\mathcal{G}^*$ and, if E is the spectral measure of H, then $E(J)\in B(\mathcal{G})\cap B(\mathcal{G}^*)$ for any Borel set $J\subset\mathbb{R}$.

DEFINITION 3.1 : *We shall say that* A *is conjugate to* H *on an open subset* $J\subset\mathbb{R}$ *(in form sense) if* $H\in C^1(A;\mathcal{G},\mathcal{G}^*)$ *and there is a strictly positive number* a *and a compact operator* $K:\mathcal{G}\to\mathcal{G}^*$ *such that* $E(J)[iH,A]E(J)\geq aE(J)+K$ *(as operators* $\mathcal{G}\to\mathcal{G}^*$*). If* $K=0$, *we say that* A *is strictly conjugate to* H *on* J. *If* $\lambda\in\mathbb{R}$ *and* A *is (strictly) conjugate to* H *on a neighbourhood of* λ, *we say that* A *is (strictly) conjugate to* H *at* λ. *If* A *is (strictly) conjugate to* H *at all points of an open set* J, *then we say that* A *is locally (strictly) conjugate to* H *on* J.

Using the virial theorem (corollary 2.5) it is a trivial matter to show that, under the conditions of the first part of the preceding definition, H *has in* J *a finite number of eigenvalues (counting multiplicities)*. We shall denote J_0 the set of $\lambda\in J$ such that λ is not an eigenvalue of H. Then we put $\mathbb{C}^{\pm}=\{z\in\mathbb{C}\mid \pm\mathrm{Im}\ z>0\}$. Clearly $\mathbb{C}^{\pm}\ni z\mapsto (z-H)^{-1}\in B(\mathcal{G}^*,\mathcal{G})$ as a holomorphic function. In order to control its boundary values on J_0, we shall need the following space:

$$\mathcal{E} = (\mathcal{G}^*,D(A;\mathcal{G}^*))_{1/2,1}\ . \tag{3.1}$$

Here $(\cdot,\cdot)_{\theta,p}$ is the real interpolation functor which makes sense if $0<\theta<1$ and $1\leq p\leq\infty$. Hence $\mathcal{E}$ is a Banach space such that $D(A;\mathcal{G}^*)\subset\mathcal{E}\subset\mathcal{G}^*$ continuously and densely. Taking adjoints we get $\mathcal{G}\subset\mathcal{E}^*$ continuously but not densely in general, because $\mathcal{E}$ could be non-reflexive. We shall denote $\mathring{\mathcal{E}}^*$ the closure of $\mathcal{G}$ in $\mathcal{E}^*$; it is known that $(\mathring{\mathcal{E}}^*)^*=\mathcal{E}$. Observe that we have a natural continuous embedding $B(\mathcal{G}^*,\mathcal{G})\subset B(\mathcal{E},\mathcal{E}^*)$, in particular we may consider the holomorphic function $\mathbb{C}^{\pm}\ni z\mapsto (z-H)^{-1}\in B(\mathcal{E},\mathcal{E}^*)$.

THEOREM 3.1: *Assume that* $H\in\mathcal{C}^1(A;\mathcal{G},\mathcal{G}^*)$ *and that* A *is conjugate to* H *on the open subset* $J\subset\mathbb{R}$. *Then the function* $\mathbb{C}^{\pm}\ni z\mapsto (z-H)^{-1}\in B(\mathcal{E},\mathcal{E}^*)$ *extends as a weak*-continuous function on* $\mathbb{C}^{\pm}\cup J_0$. *In particular,* H *has no singularly continuous spectrum in* J *and the function* $J_0\ni\lambda\mapsto(\lambda\pm i0-H)^{-1}\in B(\mathcal{E},\mathcal{E}^*)$ *is well defined and weak*-continuous.*

THEOREM 3.2: *Let* $(\mathcal{G}_j,\mathcal{H};W_j)$, $j=1,2$, *be two unitary groups in Friedrichs couples with the same Hilbert space* $\mathcal{H}$. *Let* H_j *be a self-adjoint operator in* $\mathcal{H}$ *with* $\mathcal{G}_j$ *as form-domain and such that* $H_j\in\mathcal{C}^1(A_j;\mathcal{G}_j,\mathcal{G}_j^*)$. *Assume that* A_j *is conjugate to* H_j *on an open subset* $J\subset\mathbb{R}$ *(independent of* j*). Let* $\mathcal{E}_j=(\mathcal{G}_j^*,D(A_j;\mathcal{G}_j^*))_{1/2,1}$ *and assume that* *there is a continuous operator* $V:\overset{\circ}{\mathcal{E}}_1^*\to\mathcal{E}_2$ *such that* $H_2=H_1+V$ *as forms on* $D(H_1)\times D(H_2)$. *Finally, denote* E_j^c *the continuous component of the spectral measure of* E_j. *Then the following relative wave operators exist (hence are complete):*

$$W_1^{\pm}=\text{s-lim}_{t\to\pm\infty}e^{iH_2t}e^{-iH_1t}E_1^c(J);\qquad W_2^{\pm}=\text{s-lim}_{t\to\pm\infty}e^{iH_1t}e^{-iH_2t}E_2^c(J). \tag{3.2}$$

4. Pseudo-resolvents with a Spectral Gap

The theorems 3.1 and 3.2, as we stated them, do not seem to give optimal results for N-body Schrödinger hamiltonians. In fact, in this case $\mathcal{H}=L^2(\mathbb{R}^n)$ and one tries to take as conjugate operator the generator of dilations $A=\frac{1}{2}(PQ+QP)$, where $P=-i\nabla$ is the momentum and Q is the position observable (multiplication by $x\in\mathbb{R}^n$). The hamiltonian has the form $H=\frac{1}{2}P^2+V(Q)$ where V is a real distribution on $\mathbb{R}^n$ such that $V(Q)$ (the operator of multiplication by V) is a continuous operator $\mathcal{H}^1(\mathbb{R}^n)\to\mathcal{H}^{-1}(\mathbb{R}^n)$ (usual Sobolev spaces). A natural choice for the form-domain of H is $\mathcal{G}=\mathcal{H}^1(\mathbb{R}^n)$. Then $[iH,A]=P^2-QV'(Q)=2H-(2V(Q)+QV'(Q))$ (where $V'=\nabla V$) as sesquilinear forms on $\mathcal{S}(\mathbb{R}^n)$. Clearly $H\in C^1(A;\mathcal{H}^1,\mathcal{H}^{-1})$ if and only if $QV'(Q)\in B(\mathcal{H}^1,\mathcal{H}^{-1})$. But this condition is, locally, stronger than needed (although it covers many examples in which the sum defining H exists only in form sense, so the usual Mourre theory does not apply). Our purpose now is to overcome this problem, in particular to recover the results of [BGM] from theorem 3.1. Observe that, if H is a N-body hamiltonian with short and long range interactions, then H is lower semibounded, so it has a spectral gap. We shall now study operators with spectral gaps but which are very singular: they need not be densely defined and we shall not require that their domains or form-domains be invariant under the group W_α. In particular, N-body Schrödinger hamiltonians with hard-core interactions are covered by this formalism (cf.joint work with A.Soffer).

Let $\mathcal{H}$ be a Hilbert space and $W_\alpha=e^{iA\alpha}$ a strongly continuous unitary group in $\mathcal{H}$, so A is a densely defined, self-adjoint operator in $\mathcal{H}$. We denote $D(A;\mathcal{H})$ the domain of A equipped with the graph-norm. Then $D(A;\mathcal{H})$ is a Hilbert space continuously and densely embedded in $\mathcal{H}$, hence we may define by real interpolation the Banach space:

$$\mathcal{F}=(\mathcal{H},D(A;\mathcal{H}))_{1/2,1}\ . \tag{4.1}$$

Then $D(A;\mathcal{H})\subset\mathcal{F}\subset\mathcal{H}$ continuously and densely. After the identification $\mathcal{H}\cong\mathcal{H}^*$, we get $\mathcal{F}\subset\mathcal{H}\subset\mathcal{F}^*$ continuously, in particular $B(\mathcal{H})\subset B(\mathcal{F},\mathcal{F}^*)$ continuously.

Let $\{R(z) | z \in \mathbb{C}\setminus\mathbb{R}\}$ be a *self-adjoint pseudo-resolvent* in $\mathcal{H}$, i.e. a family of bounded operators such that $R(z_1)-R(z_2)=(z_2-z_1)R(z_1)R(z_2)$ and $R(z^*)=R(z)^*$. It is known (see [HP]) that the closure of the image of $R(z)$ is a subspace $\mathcal{H}_0$ of $\mathcal{H}$ independent of z, and there is a self-adjoint, densely defined in $\mathcal{H}_0$ operator H such that $R(z)|_{\mathcal{H}_0}=(z-H)^{-1}$ and $R(z)|_{\mathcal{H}\ominus\mathcal{H}_0}=0$ (formally, think that $H=\infty$ on $\mathcal{H}\ominus\mathcal{H}_0$). It is clear that $R(z)$ is a holomorphic function of $z\in\mathbb{C}\setminus\mathbb{R}$. We shall say that *the pseudo-resolvent* $\{R(z)\}$ *has a spectral gap at the point* $\lambda_0\in\mathbb{R}$ if this function extends to an holomorphic function on a neighbourhood of λ_0. Of course, this is equivalent with saying that λ_0 is in the resolvent set of the operator H in $\mathcal{H}_0$.

LEMMA 4.1: *If the operator* $R(z_0)$ *is of class* $\mathscr{C}^1(A;\mathcal{H})$ *for some* z_0 *in the domain of holomorphy of* $\{R(z)\}$, *then* $R(z)$ *will be of class* $\mathscr{C}^1(A;\mathcal{H})$ *for all* z *in this domain.*

Proof: The hypothesis means, according to (2.8):

(4.2) $$\int_0^1 \|[A_\varepsilon,[A_\varepsilon,R(z_0)]]\|_{B(\mathcal{H})}\, d\varepsilon < \infty\ .$$

Then this will be true if A_ε is replaced by $A_{-\varepsilon}$ too. Since $(A_\varepsilon)^*=A_{-\varepsilon}$ and $R(z_0)^*=R(z_0^*)$, it will follow that $R(z_0^*)\in\mathscr{C}^1(A;\mathcal{H})$. Hence, by an analytic continuation argument, it is enough to show that $R(z)\in\mathscr{C}^1(A;\mathcal{H})$ for z near z_0. If $|z-z_0|\,\|R(z_0)\|<1$, then $R(z)=R(z_0)[1+(z-z_0)R(z_0)]^{-1}$. So it is enough to prove two things: (i) if $S\in B(\mathcal{H})$ is bijective and $S\in\mathscr{C}^1(A;\mathcal{H})$, then $S^{-1}\in\mathscr{C}^1(A;\mathcal{H})$; (ii) if $S,T\in B(\mathcal{H})$ are of class $\mathscr{C}^1(A;\mathcal{H})$, then $ST\in\mathscr{C}^1(A;\mathcal{H})$. But:

(4.3) $$[A_\varepsilon,[A_\varepsilon,S^{-1}]] = 2S^{-1}[A_\varepsilon,S]S^{-1}[A_\varepsilon,S]S^{-1}-S^{-1}[A_\varepsilon,[A_\varepsilon,S]]S^{-1}$$

(4.4) $$[A_\varepsilon,[A_\varepsilon,ST]] = 2[A_\varepsilon,S][A_\varepsilon,T] + [A_\varepsilon,[A_\varepsilon,S]]T + S[A_\varepsilon,[A_\varepsilon,T]].$$

It remains to observe that $\|[A_\varepsilon,S]\|\le$const. if $S\in\mathscr{C}^1(A;\mathcal{H})$, because this implies $S\in C^1(A;\mathcal{H})$ and we may use (e) of lemma 2.4. ■

If the assertions of lemma 4.1 are true, we shall say that *the pseudo-resolvent* $\{R(z)\}$ *is of class* $\mathscr{C}^1(A)$. In the applications it is sometimes useful to be able to express this property directly in terms of the self-adjoint operator H. The next criterion is efficient in the N-body case.

PROPOSITION 4.2: *Assume that* $\{R(z)\}$ *is the resolvent of a self-adjoint, densely defined operator* H *in* $\mathcal{H}$ *with domain invariant under* W. *Denote* $\mathcal{G}$ *the domain of* H *equipped with graph-norm and identify* $\mathcal{G}\subset\mathcal{H}\subset\mathcal{G}^*$. *Then the pseudo-resolvent* $\{R(z)\}$ *is of class* $\mathscr{C}^1(A)$ *if and only if* $H\in\mathscr{C}^1(A;\mathcal{G},\mathcal{G}^*)$.

Proof: Assume $H\in\mathscr{C}^1(A;\mathscr{G},\mathscr{G}^*)$. Let $z_0\in\mathbb{C}$ not in the spectrum of H Then $H-z_0\equiv S$ is an isomorphism of $\mathscr{G}$ onto $\mathscr{H}$ and $\mathscr{H}$ onto $\mathscr{G}^*$. Since A_ε is a bounded operator in each $\mathscr{G}^s$, it is easy to show that (4.3) is valid. We have to prove (4.2). The last term in (4.3) is integrable because it is bounded by $c\|[A_\varepsilon,[A_\varepsilon,H]]\|_{1,-1}$. The first term in the r.h.s. of (4.3) has norm in $B(\mathscr{H})$ bounded by

$$c\|[A_\varepsilon,H]\|_{1/2,-1}\ \|[A_\varepsilon,H]\|_{1,-1/2}=c\|[A_\varepsilon,H]\|^2_{1,-1/2}\leq c'\,\varepsilon^{-2}\|W_\varepsilon HW^*_\varepsilon-H\|^2_{1,-1/2}\,.$$

Hence it is enough to prove that the last expression is integrable. We use the identity $2(\mathscr{W}_\varepsilon-1)=(\mathscr{W}_{2\varepsilon}-1)-(\mathscr{W}_\varepsilon-1)^2$ in order to obtain for $0<\varepsilon<1$:

$$2\|W_\varepsilon HW^*_\varepsilon-H\|_{1,-1/2}\leq\|W_{2\varepsilon}HW^*_{2\varepsilon}-H\|_{1,-1/2}+c\varepsilon^2\|[A_\varepsilon[A_\varepsilon,H]]\|_{1,-1/2}. \tag{4.5}$$

Hence

$$2[\,\textstyle\int_0^1\varepsilon^{-2}\,\|W_\varepsilon HW^*_\varepsilon-H\|^2_{1,-1/2}\,d\varepsilon]^{1/2}\leq[\,\int_0^1\varepsilon^{-2}\,\|W_{2\varepsilon}HW^*_{2\varepsilon}-H\|^2_{1,-1/2}\,d\varepsilon]^{1/2} + c[\int_0^1\varepsilon^2\,\|[A_\varepsilon[A_\varepsilon,H]]\,\|^2_{1,-1/2}\,d\varepsilon]^{1/2}. \tag{4.6}$$

In the first integral of the r.h.s. make the change of variable $2\varepsilon=\tau$; the contribution of the integral over $\tau\in(1,2)$ is finite, whereas the integral over $\tau\in(0,1)$ is $2^{-1/2}$ times the l.h.s. of (4.6). So, it is enough to prove that the last term above is finite. But we have, by complex interpolation:

$$\begin{aligned}\varepsilon^2\|[A_\varepsilon,[A_\varepsilon,H]]\|^2_{1,-1/2}&\leq\varepsilon^2\|[A_\varepsilon,[A_\varepsilon,H]]\|_{1,0}\,\|[A_\varepsilon,[A_\varepsilon,H]]\|_{1,-1}\\&\leq c\|[A_\varepsilon,[A_\varepsilon,H]]\|_{1,-1}\,,\end{aligned} \tag{4.7}$$

which finishes the proof of (4.2). In order to prove the converse ($S^{-1}\in\mathscr{C}^1(A;\mathscr{H})\Rightarrow S\in\mathscr{C}^1(A;\mathscr{G},\mathscr{G}^*)$), a similar argument is applied to (4.3) with S replaced by S^{-1}. ■

Remark: There is a variant of this proposition for the case when W leaves invariant only the form-domain of H, i.e. the space $\mathscr{G}^{1/2}$. In order to be able to use this in applications, one needs some informations about D(H), which can be obtained by more refined methods if H is, say, an elliptic operator (see [GT]; observe that $\mathscr{G}$, the domain of H, could be a rather pathological space even if $\mathscr{G}^{1/2}$, its form-domain, is quite simple).

The next result is an easy corollary of theorem 3.1.

PROPOSITION 4.3: *Let* $\{R(z)\}$ *be a self-adjoint pseudo-resolvent of class* $\mathscr{C}^1(A)$. *Assume that* $\{R(z)\}$ *has a spectral gap at some point* $\lambda_0\in\mathbb{R}$ *and let* J *be an open subset of* $\mathbb{R}$ *such that* λ_0 *does not belong to its closure. Finally, suppose that* A *is conjugated to* $R(\lambda_0)$ *on* $\tilde{J}=\{(\lambda_0-\lambda)^{-1}\mid\lambda\in J\}$. *Then there is* $J_0\subset J$, *with* $J\setminus J_0$ *a finite set* *such that the holomorphic function* $\mathbb{C}^{\pm}\ni z\mapsto R(z)\in B(\mathcal{F},\mathcal{F}^*)$ *extends to a weak*-continuous function on* $\mathbb{C}^{\pm}\cup J_0$. *If* A *is strictly conjugated to* $R(\lambda_0)$ *on* J, *then* $J_0=J$.

Remark: $J\setminus J_0$ coincides with the set of eigenvalues in J of the self-adjoint (non-densely defined in general) operator H; these eigenvalues are of finite multiplicity and the associated eigenvectors belong to the range of R(z) (which is independent of z). If the domain of H is invariant under W, proposition 3.3 of [BG3] shows how to verify the fact that A is conjugated to $R(\lambda_0)$.

Proof: Observe first that $R(\lambda_0)$ is a bounded, self-adjoint operator.A number $\mu\in\tilde{J}$ is an eigenvalue of $R(\lambda_0)$ if and only if $\lambda_0-\mu^{-1}$ is an eigenvalue of H (in $\mathcal{H}_0$; observe that $0\notin\tilde{J}$) the multiplicities being the same. We apply theorem 3.1 with $\mathcal{G}=\mathcal{H}$ and H replaced by $R(\lambda_0)$; hence $\mathcal{E}=\mathcal{F}$. Then remark that for non-real z we have

$$R(z) = (z-\lambda_0)^{-1}R(\lambda_0)[R(\lambda_0)+(z-\lambda_0)^{-1}]^{-1}.$$

In fact, for $|z-\lambda_0|\,\|R(\lambda_0)\|<1$ this follows from the equation defining the notion of pseudo-resolvent and for arbitrary z it remains true by holomorphy. Finally, use the fact that $z\mapsto(\lambda_0-z)^{-1}$ is a homeomorphism of $\mathbb{C}^{\pm}\cup J_0$ onto $\mathbb{C}^{\pm}\cup(\tilde{J}\setminus\{$eigenvalues of $R(\lambda_0)\})$. ■

The space $\mathcal{F}$ in which the limiting absorption principle has been proved is too small for several important applications. In order to improve it, we follow [PSS] and use the formula

$$(4.8)\qquad R(z) = R(\lambda_0) + (\lambda_0-z)R(\lambda_0)^2 + (\lambda_0-z)^2R(\lambda_0)R(z)R(\lambda_0)$$

obtained after an iteration from $R(z)=R(\lambda_0)+(\lambda_0-z)R(\lambda_0)R(z)$ (sometimes the form $R(z)=R(\lambda_0)+(\lambda_0-z)R(\lambda_0)^{1/2}R(z)R(\lambda_0)^{1/2}$, with $R(\lambda_0)^{1/2}$ conveniently defined, is of simpler use). As an example, we state the following general form of the limiting absorption principle:

PROPOSITION 4.4: *Assume that the conditions of Proposition* 4.3 *are fulfilled. Let* $\mathcal{K},\mathcal{K}_1$ *be Hilbert spaces such that* $\mathcal{K}_1\subset\mathcal{K}$ *and* $\mathcal{H}\subset\mathcal{K}$ *continuously and densely. Identify* $\mathcal{K}^*\subset\mathcal{H}\cong\mathcal{H}^*\subset\mathcal{K}$ *and assume that* $R(\lambda_0)$ *extends to a continuous operator* $\mathcal{K}\to\mathcal{K}^*$ *with the property* $R(\lambda_0)\mathcal{K}_1\subset D(A;\mathcal{H})$. *Denote* $\mathcal{K}_{1/2,1}=(\mathcal{K},\mathcal{K}_1)_{1/2,1}$ *(real interpolation) and observe that* $\mathcal{K}_{1/2,1}\subset\mathcal{K}$ *continuously and densely, so that* $\mathcal{K}^*\subset\mathcal{K}^*_{1/2,1}$ *and* $B(\mathcal{K},\mathcal{K}^*)\subset B(\mathcal{K}_{1/2,1},\mathcal{K}^*_{1/2,1})$ *continuously. Then* :

(i) $R(z)\in B(\mathcal{K},\mathcal{K}^*)$ *for each* $z\in\mathbb{C}^{\pm}$ *and the function* $\mathbb{C}^{\pm}\ni z\mapsto R(z)\in B(\mathcal{K},\mathcal{K}^*)$ *is holomorphic* ;

(ii) *When considered with values in* $B(\mathcal{K}_{1/2,1},\mathcal{K}^*_{1/2,1})$, *the preceding application extends to a weak***-continuous function on* $\mathbb{C}^{\pm}\cup J_0$.

Proof: The assertion (i) follows trivially from (4.8). Closed graph theorem implies $R(\lambda_0)\in B(\mathcal{K}_1,D(A;\mathcal{H}))$. Since $R(\lambda_0)\in B(\mathcal{K},\mathcal{H})$ also, we get $R(\lambda_0):\mathcal{K}_{1/2,1}\to\mathcal{F}$ continuously by interpolation. Then taking adjoints and using the symmetry of $R(\lambda_0)$ we obtain $R(\lambda_0):\mathcal{F}^*\to\mathcal{K}^*_{1/2,1}$. Hence (4.8) and proposition 4.3 imply (ii).■

Let us consider, as an example, a situation which covers the N-body Schrödinger hamiltonians with very singular (even hard-core) interactions. Let $\mathcal{H}=L^2(\mathbb{R}^n)$, $\mathcal{K}=\mathcal{H}^{-1}(\mathbb{R}^n)$, $\mathcal{K}^*=\mathcal{H}^1(\mathbb{R}^n)$. We take $A=\frac{1}{2}(PQ+QP)$ the generator of dilations. If $\mathcal{H}^s_t=\{u\in\mathcal{S}^*(\mathbb{R}^n)\mid \langle P\rangle^s\langle Q\rangle^t u\in\mathcal{H}\}$ are the usual weighted Sobolev spaces, we take $\mathcal{K}_1=\mathcal{H}^{-1}_1$. The spaces $\mathcal{K}_{1/2,1}$ can be explicitely described as follows (see [BG2]). Let $\theta,\eta\in C_0^\infty(\mathbb{R}^n)$ be such that $\theta(x)>0$ if $2^{-1}<|x|<2$ and $\theta(x)=0$ otherwise; $\eta(x)>0$ if $|x|<2$ and $\eta(x)=0$ otherwise. For any $s,t\in\mathbb{R}$ and $1\le p\le\infty$ let $\mathcal{H}^s_{t,p}$ be the Banach space of all temperate distributions u such that:

$$\|\langle P\rangle^s\eta(Q)u\|_{\mathcal{H}} + \left[\int_1^\infty \|\langle P\rangle^s r^t\,\theta(r^{-1}Q)\,u\|^p_{\mathcal{H}}\, r^{-1}dr\right]^{1/p} < \infty.$$

Then $\mathcal{K}_{1/2,1}=\mathcal{H}^{-1}_{1/2,1}$ and $\mathcal{K}^*_{1/2,1}=\mathcal{H}^1_{-1/2,\infty}$.

If $\{R(z)\}$ is a pseudo-resolvent in $\mathcal{H}$ such that $R(\lambda_0)\in B(\mathcal{H}^{-1},\mathcal{H}^{+1})$, in order to get the results of proposition 4.4 we have to ask $R(\lambda_0)\mathcal{H}^{-1}_1\subset D(A;\mathcal{H})$. For this $PQR(\lambda_0)\mathcal{H}^{-1}_1\subset\mathcal{H}$ would be enough and this condition is a consequence of $[Q_j,R(\lambda_0)]\mathcal{H}^{-1}\subset\mathcal{H}^1$.

COROLLARY 4.5: *Let* $\{R(z)\}$ *be a self-adjoint pseudo-resolvent on the Hilbert space* $\mathcal{H}=L^2(\mathbb{R}^n)$. *Assume that* $\{R(z)\}$ *has a spectral gap at* $\lambda_0\in\mathbb{R}$ *and that* $R(\lambda_0)$ *and* $[Q_j,R(\lambda_0)]$ *belong to* $B(\mathcal{H}^{-1},\mathcal{H}^1)$ $(j=1,\dots,n)$. *Moreover, assume that a closed countable set* $\tau(H)\subset\mathbb{R}$ *is given such that* $A=\frac{1}{2}(PQ+QP)$ *is locally conjugated to* $R(\lambda_0)$ *on* $\{(\lambda_0-\lambda)^{-1}\mid\lambda\notin\tau(H)\}$ *and that* $\{R(z)\}$ *is of class* $\mathcal{C}^1(A)$. *Then there is a closed countable set* $c(H)\subset\mathbb{R}$ *such that the holomorphic function* $\mathbb{C}^{\pm}\ni z\mapsto R(z)\in B(\mathcal{H}^{-1}_{1/2,1},\mathcal{H}^1_{-1/2,\infty})$ *extends to a weak***-continuous function on* $\mathbb{C}^{\pm}\cup(\mathbb{R}\setminus c(H))$.

If one uses the main idea of the proof of theorem 3.2 in the preceding context (the fact that the Banach space $\mathcal{H}^{-1}_{1/2,1}$ is of cotype 2; see [BG2]) one immediately obtains a very precise criterion for the existence and the completeness of the wave operators. We state it only for densely defined operators, although the general case is very similar.

COROLLARY 4.6: *Let* H_1, H_2 *be two self-adjoint, bounded from below densely defined operators in* $\mathcal{H}=L^2(\mathbb{R}^n)$ *with* $\mathcal{H}^1$ *as form-domain and such that* $[Q_j,H_k]\in B(\mathcal{H}^1,\mathcal{H}^{-1})$ *if* $j=1,\dots,n$; $k=1,2$. *Assume that* $H_1-H_2:\mathcal{H}^1\to\mathcal{H}^{-1}$ *extends to a bounded operator from the closure of* $\mathcal{H}^1$ *in* $\mathcal{H}^1_{-1/2,\infty}$ *into* $\mathcal{H}^{-1}_{1/2,1}$. *Finally, assume that for some* $\lambda_0\in\mathbb{R}$ *the operators* $(\lambda_0-H_1)^{-1}$ *and* $(\lambda_0-H_2)^{-1}$ *are of class* $\mathscr{C}^1(A)$, $A=\frac{1}{2}(PQ+QP)$, *and that* A *is locally conjugated to them outside a closed countable set. Then* H_1, H_2 *have no singularly continuous spectrum and the wave operators* $\text{s-lim}_{t\to\pm\infty}e^{iH_2t}e^{-iH_1t}E_1^c$ *exist and have* $E_2^c\mathcal{H}$ *as range* (E_k^c *is the projection on the subspace of continuity of* H_k).

5. Examples . Optimality of the Results .

The results of the preceding section are corollaries of the theorems 3.1 and 3.2 and are formulated in a form suited to N-body type hamiltonians. In this section we shall consider other situations and obtain results which demonstrate not only the power of the theorem 3.1 but also its fineness (especially in connection with the $\mathscr{C}^1(A)$ assumption). We first prove a very precise division theorem (only the one-dimensional case is treated because of lack of space).

PROPOSITION 5.1: *Let* $h:\mathbb{R}\to\mathbb{R}$ *be such that* $\int_0^1 \varepsilon^{-2}\omega_2(\varepsilon)d\varepsilon<\infty$, *where* $\omega_2(\varepsilon)=\sup_{x\in\mathbb{R}}|h(x+\varepsilon)-2h(x)+h(x-\varepsilon)|$ *is the second modulus of continuity of* h. *Then* h *is of class* C^1. *Assume that* h *is a homeomorphism and that* h' *is bounded. Then for each* $\lambda\in\mathbb{R}$ *the limits* $\lim_{\varepsilon\to0}(h(x)-\lambda\mp i\varepsilon)^{-1}\equiv(h(x)-\lambda\mp io)^{-1}$ *exist in the sense of distributions. Moreover, the operator of multiplication by the distribution* $(h(x)-\lambda\mp io)^{-1}$ *belongs to* $B(\mathcal{H}^{1/2,1}(\mathbb{R}),\mathcal{H}^{-1/2,\infty}(\mathbb{R}))$ *and depend* $*$*-weakly continuously on* λ. *In particular, the Besov space* $\mathcal{H}^{1/2,1}(\mathbb{R})$ *consists of continuous functions and the distribution* $\mathrm{VP}h(x)^{-1}$ *belongs to the Besov space* $\mathcal{H}^{-1/2,\infty}(\mathbb{R})$.

Proof: Let us mention first that $\mathcal{H}^{s,p}(\mathbb{R})$ are the Besov spaces denoted $B^{s,p}_2(\mathbb{R})$ in [T]. In the Hilbert space $\mathcal{H}=L^2(\mathbb{R})$ we consider the tranlation group $(W_\alpha u)(x)=u(x-\alpha)$. Then $W_\alpha=e^{-i\alpha P}$ and we take $A=-P=i\frac{d}{dx}$, $H=h(Q)$ the operator of multiplication by h in $\mathcal{H}$ (we assume, without loss of generality, that $h'(x)>0$ for all $x\in\mathbb{R}$). We have to take $\mathscr{G}=D(|H|^{1/2})=\{u\in\mathcal{H}\mid(1+|h(Q)|)^{1/2}u\in\mathcal{H}\}$. Since h is Lipschitz, $\mathscr{G}$ is invariant under W. Observe that

$$\|W_\varepsilon H W_\varepsilon^* - 2H + W_{-\varepsilon} H W_{-\varepsilon}^*\|_{B(\mathcal{H})} = \omega_2(\varepsilon),$$

so that $H \in \mathscr{C}^1(A;\mathscr{G},\mathscr{G}^*)$. A remark made after definition 2.6 implies that the function $\alpha \mapsto W_\alpha h(Q) W_\alpha^* = h(Q-\alpha) \in B(\mathscr{G},\mathscr{G}^*)$ is norm-C^1. In particular h is of class C^1 (for another proof of this fact, see theorem 3.3, p.87 of [Sh]). Then $[iH,A]=h'(Q)$ which easily implies the Mourre estimate (if $I \subset \mathbb{R}$ is compact, $h^{-1}(I)$ is also compact and the inf of h' on compact sets is strictly positive). Finally, observe that

$$\mathscr{E} = (\mathscr{G}^*, D(A;\mathscr{G}^*))_{-1/2,1} \supset (\mathscr{H}, D(A;\mathscr{H}))_{1/2,1} = (\mathscr{H},\mathscr{H}^1)_{1/2,1} = \mathscr{H}^{1/2,1}(\mathbb{R})$$

and $(\mathscr{H}^{1/2,1})^* = \mathscr{H}^{-1/2,\infty}$. Taking $h(x)=x$ we see that $\mathscr{H}^{1/2,1}(\mathbb{R}) \subset C^0(\mathbb{R})$. ■

This proposition allows us to make some comments concerning the degree of optimality of theorem 3.1. Two different questions have to be considered: 1) is the space $\mathscr{E}$ optimal, i.e. is it, in some sense, the largest space, in which the L.A.P. holds? 2) Is the regularity assumption $H \in \mathscr{C}^1(A;\mathscr{G},\mathscr{G}^*)$ optimal, or could it be replaced by $H \in C^1_n(A;\mathscr{G},\mathscr{G}^*)$? Let us discuss these questions in the setting of proposition 5.1. Example 2, page 50, of [P] shows that the best (i.e. smallest) local Besov space $\mathscr{H}^{s,p}_{loc}(\mathbb{R})$ which could contain the distributions $(x\pm io)^{-1}$ is obtained for $s=-1/2$, $p=\infty$ (because the imaginary part of $\mp\pi^{-1}(x\pm io)^{-1}$ is the Dirac measure at zero) and we have proved that in fact they do belong to this space. So in the scale of Besov spaces our space $\mathscr{E}$ gives the optimal result in this example. However, as explained at the end of section 4 of [BGM2], there is a Banach space $\mathscr{K}$ such that $\mathscr{H}^{1/2,1} \subset \mathscr{K} \subset \mathscr{H}$ strictly and the L.A.P. is valid in $B(\mathscr{K},\mathscr{K}^*)$ (but this space is not comparable with $\mathscr{H}^{1/2}$). Let us pass now to the second question. Consider a C^1-diffeomorphism $h:\mathbb{R}\to\mathbb{R}$ and $\lambda \in \mathbb{R}$. Even if the distribution $(h(x)-\lambda+io)^{-1}$ exists, then it does not belong to $\mathscr{H}^{-1/2,\infty}_{loc}$ in general, because the derivative of h could be any (positive) continuous function and the space $\mathscr{H}^{-1/2,1}_{loc}$ is not stable under multiplication by continuous functions (otherwise it would be just $C^0(\mathbb{R})$) (the derivative of h appears when the action on test functions of the distribution $(h(x)-\lambda+io)^{-1}$ is calculated). But something much worse can happen. Using an example due to Lusin (see §13, ch.VIII in [Be]) it is easy to construct a C^1-diffeomorphism h with absolutely continuous derivative such that for every rational number $\lambda \in [0,2\pi]$ the limit of $(h(x)-\lambda+i\varepsilon)^{-1}$ as $\varepsilon \to +0$ does not exist in $\mathscr{D}'(\mathbb{R})$, i.e. in distribution sense (or one can use theorem 5.2 from [Ga] in order to construct a strictly positive, bounded, uniformly continuous function g with Hilbert transform equal to infinity on a dense set and then define h by $h'(x) = (g(h(x))^{-1})$. Finally, let us mention that a condition essentially weaker than $\int_0^1 \varepsilon^{-2}\omega_2(\varepsilon)d\varepsilon < \infty$

cannot force the uniform continuity of h′, i.e. the modulus of continuity of h′ can be made of order $\int_0^\varepsilon t^{-2}\omega_2(t)dt$ (see page 88 of [Sh]).

The next proposition is a remark which concerns the generality of the locally conjugate operator method. We mention it because of the obvious connection with proposition 5.1 and because the construction we make explains the terminology "locally conjugate operator".

PROPOSITION 5.2: *Assume that a self-adjoint operator* H *has a purely absolutely continuous spectrum of constant multiplicity on an open interval* $I\subset\mathbb{R}$. *Then there is an operator* A *which is strictly conjugate to* H *on any compact subset of* I (*and the derivative of the function* $\alpha\mapsto W_\alpha H W_\alpha^*$ *is a* $B(\mathscr{H})$*-valued* C^∞ *function*).

Proof: The assumption we made on H means that there is a Hilbert space $\mathscr{K}$ such that HE(I) is unitarily equivalent to the operator Q of multiplication by the variable x in the Hilbert space $\mathscr{H}_0=L^2(I,dx;\mathscr{K})$ of square-integrable $\mathscr{K}$-valued functions on I. Let $F:I\to\mathbb{R}$ be a bounded function of class C^∞ with all derivatives bounded, with $F(x)>0$ for $x\in I$ and such that $\int_a^c F(x)^{-1}dx=\int_c^b F(x)^{-1}dx=\infty$ (where $a<c<b$ and $I=(a,b)$). Then $A_0=-1/2(F(Q)P+PF(Q))$ is a self-adjoint operator in $\mathscr{H}_0$ such that $[iQ,A_0]=F(Q)$ is strictly positive on each compact subset of I. We take A equal to $U^{-1}A_0U$ on $E(I)\mathscr{H}$ (U is the unitary operator $E(I)\mathscr{H}\to\mathscr{H}_0$ which transforms HE(I) in Q) and equal to zero on $E(\mathbb{R}\setminus I)\mathscr{H}$. Observe that if we take $F(x)=0$ for $x\notin I$, we shall have $[iH,A]=F(H)$. ■

We shall now give a simple example of a hard-core type situation, in which neither the domain nor the form-domain of the hamiltonian are invariant under W, but the conjugate operator method can be used if one works directly with the resolvent. In $\mathscr{H}=L^2(\mathbb{R})$ let $H_0=P^2=-\frac{d^2}{dx^2}$ and $R_0=(H_0+1)^{-1}$. We would like to study the operator $H_\infty=H_0+V_\infty$ where, formally, $V_\infty(x)=+\infty$ if $x<0$ and $V_\infty(x)=0$ if $x>0$. Rigorously, this operator is the limit in the norm-resolvent sense as $\kappa\to+\infty$ of $H_\kappa=H_0+\kappa(1-E)$ where E is the operator of multiplication by the characteristic function of $(0,\infty)$. Let $\phi(x)=2^{-1/2}E(x)e^{-x}$. Then $R_\infty=\lim_{\kappa\to\infty}(H_\kappa+1)^{-1}=ER_0E-\phi\otimes\phi$ where $\phi\otimes\phi$ is the rank one operator which sends u into $\phi\langle\phi|u\rangle$. We shall calculate the order of regularity of R_∞ with respect to the translation group (we do this because the result is simpler; in fact the dilation group must be used in order to have an example relevant for the N-body case; however, if the point zero, where the potential becomes infinite, is replaced by an arbitrary non-zero point, the order of regularity of R_∞ with respect to the translation or the dilation group are obviously the same). If $T_\alpha=e^{iP\alpha}$, then $T_\alpha R_\infty T_{-\alpha}=E_\alpha R_0 E_\alpha-\phi_\alpha\otimes\phi_\alpha$ where E_α is the operator of multiplication by the characteristic function of $(-\alpha,\infty)$ and

$\phi_\alpha=T_\alpha\phi$. Calculating the derivative at $\alpha=0$ one gets $[iP,R_\infty]=2\phi\otimes\phi$, hence R_∞ is of class $C^1(P;\mathscr{H})$.Then $T_\alpha[iP,R_\infty]T_{-\alpha}=2\phi_\alpha\otimes\phi_\alpha$ and $\|\phi_\alpha-\phi\|_{\mathscr{H}}=2^{-1/2}|1-e^{-\alpha}|^{1/2}\sim\alpha^{1/2}$. To conclude, R_∞ is of class $C^{3/2}(P;\mathscr{H})$ and not more.

We mention now another explicitly soluble example in which the conjugate operator method works but the domain of the hamiltonian is not invariant under the group. Let δ be Dirac measure at zero on $\mathbb{R}$. Let $\mathscr{H}$ and H_0 as above and $H=H_0+g\delta$ with $g\in\mathbb{R}\setminus\{0\}$ (form-sum). The form-domain of H is $\mathscr{H}^1(\mathbb{R})$, but the functions in the domain of H have to verify $u'(+0)-u'(-0)=gu(0)$, so that the domain is not invariant under the dilation group W. If $g<0$, then H has a bound state of energy $-g^2/4$, if $g>0$ then H has no bound states and it always has a purely absolutely continuous spectrum equal to $[0,\infty)$.The form-domain of H is obviously invariant under W and $W_\alpha H W_\alpha^*=e^{-2\alpha}P^2+e^\alpha g\delta$ as forms on $\mathscr{H}^1$ (because δ is homogeneous of degree $-n$ in $\mathbb{R}^n$; or use $\langle u|Hu\rangle=\int |u'(x)|^2dx+g|u(0)|^2$). Hence H is of class $C^\infty(A;\mathscr{H}^1,\mathscr{H}^{-1})$ and $[iH,A]=2H-3g\delta$. Since $\delta:\mathscr{H}^1\to\mathscr{H}^{-1}$ is a continuous operator of rank one, A will be conjugate (strictly if $g<0$) to H on (ε,∞) and $-A$ will be conjugate (strictly if $g>0$) to H on $(-\infty,-\varepsilon)$ for each $\varepsilon>0$. Hence we get all spectral properties of H from theorem 3.1.

Our final topic is an improvement of the perturbative method of verifying Mourre estimate presented in proposition 7.6 of [BG2]. This allows one to treat locally very singular potentials. We begin with the following simple remark:

LEMMA 5.3: *Let* H,H_0 *be self-adjoint ,not necessarily densely defined, operators, in some Hilbert space* $\mathscr{H}$. *If* $(H-z)^{-m}-(H_0-z)^{-m}$ *is compact for some fixed* $m\geq1$ *and for all* $z\in\mathbb{C}\setminus\mathbb{R}$, *then* $f(H)-f(H_0)$ *is compact for each* $f:\mathbb{R}\to\mathbb{C}$ *continuous and convergent to zero at infinity. In this case* H *and* H_0 *have the same essential spectrum.*

Proof: Let $R(z)=(H-z)^{-1}$, $R_0(z)=(H_0-z)^{-1}$ the associated pseudo-resolvents. If $f=g^{(m-1)}$ for some $g\in C_0^\infty(\mathbb{R})$, formula (6) from [BG1] gives:

$$f(H)=\Sigma_{k=0}^{n-1}\frac{(-1)^{m-1}(m-1)!}{\pi k!}\int_{\mathbb{R}} g^{(k)}(\lambda)\mathrm{Im}[i^k R^m(\lambda+i)]d\lambda +$$

$$+\frac{(-1)^{m-1}(m-1)!}{\pi(n-1)!}\int_0^1\varepsilon^{n-1}d\varepsilon\int_{\mathbb{R}} g^{(n)}(\lambda)\ \mathrm{Im}[i^n R^m(\lambda+i\varepsilon)]d\lambda.$$

Here $n\geq m+1$ in order to have norm-convergent integrals. A similar formula for $f(H_0)$ shows that $f(H)-f(H_0)$ is compact for such f. Let

$$C_\infty(\mathbb{R})=\{\varphi:\mathbb{R}\to\mathbb{C}\mid\varphi\text{ continuous and }\varphi(x)\to0\text{ if }|x|\to\infty\}$$

with the sup norm. Since $C_\infty(\mathbb{R}) \ni \varphi \mapsto \varphi(H)-\varphi(H_0) \in B(\mathscr{H})$ is norm-continuous, it is enough to show that $\mathscr{N}=\{g^{(m-1)} \mid g \in C_0^\infty(\mathbb{R})\}$ is a dense subspace of $C_\infty(\mathbb{R})$, or of $C_0^\infty(\mathbb{R})$ equipped with the sup norm. But $f \in \mathscr{N}$ if and only if

$$\int f(x)dx = \int xf(x)dx = \ldots = \int x^{m-2}f(x)dx = 0$$

and $f \mapsto \int x^j f(x)dx$ are linear functionals on C_0^∞ which are not continuous for the sup norm, so the intersection ($j=0,\ldots,m-2$) of their kernels is dense for this norm. Since λ does not belong to the essential spectrum of H if and only if there is $f \in C_0^\infty(\mathbb{R})$ with $f(\lambda) \neq 0$ and $f(H)$=compact, the last assertion is trivial. ■

The assumption of Lemma 5.3 is easy to verify and allows quite singular perturbations H of H_0 (see the discussion in section 8 of [Pe]). In the next proposition we shall say that a pseudo-resolvent $\{R(z)\}$ is of class $C_n^1(A)$ if R(z) is of class $C_n^1(A;\mathscr{H})$ for some z in the domain of holomorphy; the proof of lemma 4.1 shows that this will remain true for all such z.

PROPOSITION 5.4: *Let $\{R_0(z)\}$, $\{R(z)\}$ be two self-adjoint pseudo-resolvents which are of class $C_n^1(A)$ for some self-adjoint, densely defined operator A. Assume that $R(z)-R_0(z)$ is compact for some z and that one of them has a spectral gap, so that they have a common spectral gap at some point $\lambda_0 \in \mathbb{R}$. Then A is conjugated to $R(\lambda_0)$ at some point $\lambda \in \mathbb{R}$ if and only if it is conjugated to $R_0(\lambda_0)$ at λ.*

Proof: Write $R=R(\lambda_0)$, $R_0=R_0(\lambda_0)$. Since

$$[iA,R]-[iA,R_0]=\lim_{\varepsilon\to 0}\varepsilon^{-1}\left[W_\varepsilon(R-R_0)W_\varepsilon^*-(R-R_0)\right]$$

is norm limit of compact operators, it will also be compact. Let us write $S \sim T$ if $S-T$ is compact. Then $\varphi(R) \sim \varphi(R_0)$ for each continuous function φ. Hence $\varphi(R)[iA,R]\varphi(R) \sim \varphi(R_0)[iA,R_0]\varphi(R_0)$. From this the assertion of the proposition follows easily. ■

If $\{R_0(z)\}$ is of class $\mathscr{C}^1(A)$, then one may deduce that $\{R(z)\}$ has the same property by applying theorem 6.2 or 6.3 from [BG2] to the difference $R(z)-R_0(z)$ for some fixed z. Then theorems 3.1 and 3.2 will give a detailed spectral and scattering theory for H. For example, results like theorem 8.1 of [Pe] are easily obtained. Observe that one has to put conditions only on the difference of the resolvents of H and H_0 (as in Kato's criterion for the existence of wave operators), so H could be very singular with respect to H_0 (for example a differential operator of higher order). Remark that not only short-range, but also long-range singular perturbations are allowed. Moreover, the unperturbed operator H_0 can be quite complicated (e.g. a N-body hamiltonian), a situation in which usual Enss method (as presented in [Pe] for example) does not work.

Appendix: A Tauberian Estimate

We shall prove here an estimate which plays an important role in the applications we have in mind and which improves the tauberian theorem described in [BG2]. Below we denote $BC(\mathbb{R}^n)$ the C^*-algebra of bounded, continuous functions on $\mathbb{R}^n$ equipped with the norm $\|f\|_\infty=\sup\{|f(x)| \mid x\in\mathbb{R}^n\}$. $C_0^\infty(\mathbb{R}^n)$ is equipped with the usual Schwartz topology.

We shall consider a subalgebra $\mathscr{M}\subset BC(\mathbb{R}^n)$, which contains the constants, and which is equipped with a norm $|\cdot|_{\mathscr{M}}$ for which $\mathscr{M}$ is a Banach space with continuous multiplication (i.e. $\exists M<\infty$ such that $|fg|_{\mathscr{M}}\le M|g|_{\mathscr{M}}$ for all f,g in $\mathscr{M}$). We assume that $C_0^\infty(\mathbb{R}^n)\subset\mathscr{M}\subset BC(\mathbb{R}^n)$ the embeddings being continuous. Let us denote $f^\sigma(x)=f(\sigma x)$ for each function f on $\mathbb{R}^n$ and each $\sigma\ge 0$. Our final assumption is that $\mathscr{M}$ is invariant under dilations, i.e. $f^\sigma\in\mathscr{M}$ if $f\in\mathscr{M}$ and $\sigma>0$, and that there are constants $0<M,N<\infty$ such that

$$\text{(A.1)}\qquad |f^\sigma|_{\mathscr{M}} \le M<\sigma>^N|f|_{\mathscr{M}} \quad \text{for all } f\in\mathscr{M} \quad (<\sigma>=(1+\sigma^2)^{1/2}).$$

THEOREM: *Assume that* **E** *is a Banach space and that a continuous, unital homomorphism* $\mathscr{M}\ni f\longmapsto f(\Lambda)\in B(E)$ *is given. Denote* $f(\sigma\Lambda)\equiv f^\sigma(\Lambda)$. *Let* $\rho\in\mathscr{M}$ *and assume that there is a number* $\ell>N$ *such that for any function* $\theta\in C_0^\infty(\mathbb{R}^n\backslash\{0\})$ *we have* $|\rho^\tau\theta|_{\mathscr{M}} \le c(\theta)\tau^\ell$ if $0<\tau<1$. *Let* $\xi:\mathbb{R}^n\to\mathbb{R}$ *be a function of class* C^∞ *and such that* $\xi(x)=0$ (*resp.* $\xi(x)=1$) *in a neighbourhood of zero* (*resp. of infinity*). *Denote* $\eta(x)=x\nabla\xi(x)$. *Then there is a constant* c *such that for all* $u\in E$ *and all* $0<\varepsilon<1$:

$$\text{(A.2)}\qquad \|\rho(\varepsilon\Lambda)u\| \le c\|\xi(\varepsilon\Lambda)u\| + c\varepsilon^\ell \int_\varepsilon^1 \|\eta(\tau\Lambda)u\|\,\tau^{-1-\ell}\,d\tau + c\varepsilon^\ell\|u\|.$$

Remarks: Here Λ has to be interpreted as a symbol which helps to distinguish the function $f\in\mathscr{M}$ and the operator acting in **E** associated to it by the homomorphism. However, in applications Λ is in fact an operator or a finite set of operators in **E**. Observe that $\eta\in C_0^\infty(\mathbb{R}^n\backslash\{0\})$ so it belongs to $\mathscr{M}$, and $\xi-1\in C_0^\infty(\mathbb{R}^n)$, so that ξ belongs to $\mathscr{M}$ too. Hence all terms in (A.2) are well defined and (A.2) is an estimate of the rate of decay of $\|\rho(\varepsilon\Lambda)u\|$ as $\varepsilon\to 0$ in terms of the rate of decay of $\|\xi(\varepsilon\Lambda)u\|$ and $\|\eta(\varepsilon\Lambda)u\|$. The condition we put on ρ is satisfied if there are $\omega\in C^\infty(\mathbb{R}^n\backslash\{0\})$ and $\rho_0\in\mathscr{M}$ such that $\rho(x)=\omega(x)\rho_0(x)$ for $x\ne 0$ and $\omega(\tau x)=\tau^\ell\omega(x)$ for $\tau>0$ and $x\ne 0$. In fact, we shall then have:

$$|\rho^\tau\theta|_{\mathscr{M}} = |\omega^\tau\rho_0^\tau\theta|_{\mathscr{M}} = \tau^\ell|\omega\theta\rho_0^\tau|_{\mathscr{M}} \le M\tau^\ell|\omega\theta|_{\mathscr{M}}|\rho_0^\tau|_{\mathscr{M}} \le c\tau^\ell$$

for $0<\tau\leq 1$, because $\omega\theta\in C_0^\infty\subset\mathcal{M}$. Observe that ρ has a zero of finite order ℓ at zero in this example, while ξ and η have zeroes of infinite order: this explains why we call (A.2) a "tauberian estimate". Let us mention that in all the applications $\|\rho(\varepsilon\Lambda)\|$ is a constant independent of ε. For example, if Λ is an unbounded self-adjoint operator in a Hilbert space E, then $\|\rho(\varepsilon\Lambda)\|=\text{const.}$ while, if supp θ is included in $0<a\leq|x|\leq b<\infty$, then $\|\rho(\tau\Lambda)\theta(\Lambda)\|\leq \sup_x|\rho(\tau x)\theta(x)|\leq c\sup\{|\rho(\lambda)| \mid a\tau\leq|\lambda|\leq b\tau\}$. Finally, let us observe that if $\zeta\in C_0^\infty(\mathbb{R}^n\setminus\{0\})$ and $\zeta(x)=1$ on supp η, then $\|\eta(\tau\Lambda)u\|=\|\eta(\tau\Lambda)\zeta(\tau\Lambda)u\|\leq \|\eta(\tau\Lambda)\|\,\|\zeta(\tau\Lambda)u\|\leq C\|\zeta(\tau\Lambda)u\|$ for $\tau\leq 1$, hence the precise form of η is irrelevant. Moreover, if ξ_1 is a function with properties similar to ξ, then there is $\mu>0$ such that $\xi_1(\mu x)=1$ for $x\in$ supp ξ, hence $\|\xi(\varepsilon\Lambda)u\|=\|\xi(\varepsilon\Lambda)\xi_1(\varepsilon\mu\Lambda)u\|\leq c\|\xi_1(\varepsilon\mu\Lambda)u\|$ for $\varepsilon\leq 1$, so the precise form of ξ is also irrelevant.

Proof of the theorem : Observe first that for $0<a<b<\infty$ and $x\neq 0$ we have $\xi(bx)-\xi(ax)=\int_a^b \eta(tx)t^{-1}dt$. In particular $1=\xi(x)+\int_1^\infty \eta(tx)\, t^{-1}dt$ if $x\neq 0$, which implies

(A.3) $\quad \rho^\varepsilon(x) = \rho^\varepsilon(x)\xi^\varepsilon(x)+\int_1^\infty \rho^\varepsilon(x)\eta^{\varepsilon t}(x)\, t^{-1}dt \qquad (x\neq 0).$

The application $\sigma\mapsto\eta^\sigma\in C_0^\infty(\mathbb{R}^n)$ is continuous on $(0,\infty)$, hence $t\mapsto\eta^{\varepsilon t}\in\mathcal{M}$ has the same property. Moreover, for $t\geq 1$:

(A.4) $\quad |\rho^\varepsilon\eta^{\varepsilon t}|_{\mathcal{M}} = |(\rho t^{-1}\eta)^{\varepsilon t}|_{\mathcal{M}} \leq M\langle\varepsilon t\rangle^N|\rho t^{-1}\eta|_{\mathcal{M}} \leq c(\varepsilon)t^{N-\ell},$

because $\eta\in C_0^\infty(\mathbb{R}^n\setminus\{0\})$.

Hence $\int_1^\infty |\rho^\varepsilon\eta^{\varepsilon t}|_{\mathcal{M}}\, t^{-1}dt<\infty$, so that the integral $\int_1^\infty \rho^\varepsilon\eta^{\varepsilon t}\, t^{-1}dt$ exists in $\mathcal{M}$ (in norm). Using (A.3) we obtain:

(A.5) $\quad \rho^\varepsilon = \rho^\varepsilon\xi^\varepsilon + \int_1^\infty \rho^\varepsilon\eta^{\varepsilon t}\, t^{-1}dt$

equality in $\mathcal{M}$ (in fact, since all the terms are in $\mathcal{M}$ and $\mathcal{M}$ consists of continuous functions, it is enough to show that the values at each $x\neq 0$ of the right and left side are equal, which is assured by (A.3)). The continuity of the homomorphism $f\mapsto f(\Lambda)$ implies now:

(A.6) $\quad \rho(\varepsilon\Lambda) = \rho(\varepsilon\Lambda)\xi(\varepsilon\Lambda) + \int_1^\infty \rho(\varepsilon\Lambda)\eta(\varepsilon t\Lambda)\, t^{-1}dt$

(the integral exists in norm in B(E) due to (A.4)).

Consider now some $u\in E$ and let us apply (A.6) to it. Since $\|\rho(\varepsilon\Lambda)\|\leq c|\rho^\varepsilon|_{\mathcal{M}}\leq$ const. for $0<\varepsilon\leq 1$, we get:

(A.7) $\quad \|\rho(\varepsilon\Lambda)u\| \leq c\|\xi(\varepsilon\Lambda)u\| + \int_1^\infty \|\rho(\varepsilon\Lambda)\eta(\varepsilon t\Lambda)u\|\, t^{-1}dt =$

$$= c\|\xi(\varepsilon\Lambda)u\| + \int_\varepsilon^1 \|\rho(\varepsilon\Lambda)\eta(\sigma\Lambda)u\|\,\sigma^{-1}d\sigma + \int_1^\infty \|\rho(\varepsilon\Lambda)\eta(\sigma\Lambda)u\|\,\sigma^{-1}d\sigma.$$

In order to estimate the first integral above, let $\theta\in C_0^\infty(\mathbb{R}^n\setminus\{0\})$ be such that $\theta\eta=\eta$. Then

$$\|\rho(\varepsilon\Lambda)\eta(\sigma\Lambda)u\| = \|\rho(\varepsilon\Lambda)\theta(\sigma\Lambda)\eta(\sigma\Lambda)u\| \le \|(\rho^\varepsilon\theta^\sigma)(\Lambda)\|\,\|\eta(\sigma\Lambda)u\| \le$$

$$\le c|\rho^\varepsilon\theta^\sigma|_{\mathcal{M}}\|\eta(\sigma\Lambda)u\| = c|(\rho^{\varepsilon\sigma^{-1}}\theta)^\sigma|_{\mathcal{M}}\,\|\eta(\sigma\Lambda)u\|$$

$$\le cM\langle\sigma\rangle^N|\rho^{\varepsilon\sigma^{-1}}\theta|_{\mathcal{M}}\,\|\eta(\sigma\Lambda)u\| \le c_1\langle\sigma\rangle^N(\varepsilon/\sigma)^\ell\|\eta(\sigma\Lambda)u\|.$$

If we use this estimate in the first integral from the last member of (A.7), we obtain the second term from the right-hand side of (A.2). Finally, we estimate the last integral from (A.7) using (observe that $\eta\in C_0^\infty(\mathbb{R}^n\setminus\{0\})$ and $\sigma\ge1$):

$$\|\rho(\varepsilon\Lambda)\eta(\sigma\Lambda)u\| \le c|\rho^\varepsilon\eta^\sigma|_{\mathcal{M}}\|u\| = c|(\rho^{\varepsilon\sigma^{-1}}\eta)^\sigma|_{\mathcal{M}}\,\|u\| \le$$

$$\le c_1\sigma^N|\rho^{\varepsilon\sigma^{-1}}\eta|_{\mathcal{M}}\,\|u\| \le c_2\sigma^{N-\ell}\varepsilon^\ell\|u\|.$$

Since $\ell>N$, we shall obtain the last term of (A.2). ■

REFERENCES

[ABG1] W.O.Amrein, A.Boutet de Monvel-Berthier and V.Georgescu: *Notes on the N-body problem, I*, preprint de l'Université de Genève, UGVA-DPT 1988/11-598 a (1988), p.1-156.

[ABG2] W.O.Amrein, A.Boutet de Monvel-Berthier and V.Georgescu: *On Mourre's approach to spectral theory*, Helv. Phys. Acta, **62** (1) (1989), p.1-21.

[Ba] N.K.Bary: *A treatise on trigonometric series*, Pergamon Press, 1964.

[BB] P.L.Butzer and H.Berens: *Semigroups of operators and approximation*, Springer-Verlag, Berlin, 1967.

[BG1] A.Boutet de Monvel-Berthier and V.Georgescu: *Locally conjugate operators, boundary values of the resolvent and wave operators*, C.R.Acad.Sci.Paris **313**, Série I (1991), p.13-18.

[BG2] A.Boutet de Monvel-Berthier and V.Georgescu: *Spectral and scattering theory by the conjugate operator method,* Algebra and Analysis, **3** (1992), p.73-116 (= St Petersburg Math.J.) — Preprint Universität Bielefeld, B.I.B.O.S n°487/1991.

[BG3] A.Boutet de Monvel-Berthier and V.Georgescu: *Graded C^*-Algebras and Many-Body Perturbation Theory: II. The Mourre Estimate*, these proceedings.

[BGM1] A.Boutet de Monvel-Berthier, V.Georgescu and M.Mantoiu: *Mourre's theory in a Besov space setting*, C.R.Acad.Sci.Paris, **310**, Série I (1990), p.233-237.

[BGM2] A.Boutet de Monvel-Berthier, V.Georgescu and M.Mantoiu: *Locally smooth operators and the limiting absorption principle for N body hamiltonians,* Reviews in Math. Phys. (1992), to appear — Preprint Universität Bielefeld, B.I.B.O.S. n°433/1990.

[D] E.B.Davies: *One parameter semigroups*, Academic Press, 1980.

[Ga] J.B.Garnett: *Bounded Analytic Functions*, Academic Press, 1981.

[GT] D.Gilberg and N.S.Trudinger: *Elliptic Partial Differential Equations of Second Order*, Springer-Verlag, 1977.

[JP] A.Jensen and P.Perry: *Commutator methods and Besov space estimates for Schrödinger operators*, J.Operator.Th., **14** (1) (1985), p.181-189.

[M1] E.Mourre: *Absence of singular continuous spectrum for certain self-adjoint operators*, Comm. Math. Phys., **78** (1981), p.391-408.

[M2] E.Mourre: *Opérateurs conjugués et propriétés de propagation*, Comm. Math. Phys., **91** (1983), p.279-300.

[P] J.Peetre: *New thoughts on Besov spaces,* Duke University Math. Series I, Durham, 1976.

[PPS] P.Perry, I.M.Sigal and B.Simon: *Spectral analysis of N body Schrödinger operators*, Ann. Math., **114** (1981), p.519-567.

[Pe] P.Perry: *Scattering theory by the Enss method*, Math. Reports, vol. 1, Harwood Academic Publishers, 1983.

[Sh] H.S.Shapiro: *Smoothing and Approximation of Functions*, Van Nostrand, 1969.

[T] H.Triebel: *Interpolation theory, function spaces, differential operators*, VEB, Deutscher-Verlag, Berlin, 1978.

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On nonlinear scattering of states which are close to a soliton

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ON NONLINEAR SCATTERING OF STATES WHICH ARE CLOSE TO A SOLITON

V.S.Buslaev and G.S.Perelman

1 Solitons

Consider the nonlinear Schroedinger equation

$$i\psi_t = -\psi_{xx} + F(|\psi|^2)\psi, \psi = \psi(x,t) \in \mathbf{C}, \tag{1.1}$$

$x, t \in \mathbf{R}$. Assume that
i)F is a given smooth ($\in C^\infty$) real function bounded from below,
ii)the point $\xi = 0$ is a (sufficiently strong) root of the function F:

$$F(\xi) = F_1\xi^p(1 + O(\xi)), p > 0. \tag{1.2}$$

Further consider the function

$$U(\phi, \alpha) = -\frac{1}{8}\alpha^2\phi^2 - \frac{1}{2}\int_0^{\phi^2} F(\xi)d\xi. \tag{1.3}$$

If $\alpha \neq 0$ this function is negative for sufficiently small ϕ. The next assumption on F will be given in a sligtly implicit, but absolutely elementary form:
iii)for α from some interval, $\alpha \in A \subset \mathbf{R}_+$, the function $\phi \to U(\phi, \alpha)$ has a positive root; if $\phi_0(= \phi_0(\alpha))$ is the smallest positive root then $U_\phi(\phi_0, \alpha) > 0$.

Under all these assumptions there exists the unique even positive solution $y \to \phi(y)$ of the equation

$$\phi_{yy} = -U_\phi = \frac{1}{4}\alpha^2\phi + F(\phi^2)\phi \tag{1.4}$$

vanishing at infinity. More precisely

$$\phi = \phi(y|\alpha) \sim \phi_\infty exp(-\frac{1}{2}\alpha|y|), y \to \infty. \tag{1.5}$$

The following functions of x can be called the *soliton states*:

$$w(x|\sigma) = exp(-i\beta + i\frac{1}{2}vx)\phi(x - b|\alpha), \tag{1.6}$$

here

$$\sigma = (\beta, \omega, b, v), \omega = \frac{1}{4}(v^2 - \alpha^2), \tag{1.7}$$

$\beta, \omega, b, v \in \mathbf{R}, \alpha \in A$. The set of the allowable σ will be denoted by Σ. If σ is a solution of the Hamiltonian system:

$$\beta' = \omega, \omega' = 0, b' = v, v' = 0. \tag{1.8}$$

the function $w(x|\sigma(t))$ is a solution of the equation (1.1) called the *soliton*.

2 The linearization of equation (1.1)

Consider the linearization of the equation (1.1) on the soliton $w(x|\sigma(t))$:

$$i\chi_t = -\chi_{xx} + F(|w|^2)\chi + F'(|w|^2)w(\bar{w}\chi + w\bar{\chi}). \tag{2.1}$$

Instead of χ introduce the function f:

$$\chi(x,t) = exp(i\Phi)f(y,t), \Phi = -\beta(t) + \frac{1}{2}vx, y = x - b(t). \tag{2.2}$$

The function f obeys the following equation:

$$if_t = L(\alpha)f, \tag{2.3}$$

where

$$L(\alpha)f = -f_{yy} + \frac{1}{4}\alpha^2 f + F(\phi^2)f + F'(\phi^2)\phi^2(f + \bar{f}), \tag{2.4}$$

$\phi = \phi(y|\alpha)$. Equation (2.3) is only a real-linear equation. Introduce its complexification:

$$i\vec{f}_t = H(\alpha)\vec{f}, \vec{f} = \begin{pmatrix} f \\ \bar{f} \end{pmatrix}, \tag{2.5}$$

$$H(\alpha) = H_0(\alpha) + V(\alpha), H_0(\alpha) = (-\partial_y^2 + \frac{1}{4}\alpha^2)\sigma_3, \tag{2.6}$$

$$V(\alpha) = \left[F(\phi^2) + F'(\phi^2)\phi^2\right]\sigma_3 + iF'(\phi^2)\phi^2\sigma_2, \tag{2.7}$$

σ_2, σ_3 are the standard Pauli matrices:

$$\sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{2.8}$$

3 Properties of the operator $H(\alpha)$

The operator $H(\alpha)$ can be treated as a linear operator in $\mathbf{L}_2(\mathbf{R} \to \mathbf{C}^2)$. Define it on the domain where $H_0(\alpha)$ is self-adjoint. It possesses the properties:

$$\sigma_3 H = H^* \sigma_3, \sigma_2 H = -H^* \sigma_2, \sigma_1 H = -H\sigma_1. \tag{3.1}$$

As a result the spectrum of H is invariant with respect to the following transformations: $E \to \bar{E}, E \to -E$.

The continuous spectrum consists of two half-axis $[E_0, \infty)$ and $(-\infty, -E_0]$, $E_0 = \frac{1}{4}\alpha^2$. Its multiplicity is equal to 2.

Owing to the exponential decay of the potential term $V(\alpha)$ at infinity the discrete spectrum of $H(\alpha)$ contains only a finite number of eigenvalues and the corresponding *root subspaces* have only finite dimension.

The point $E = 0$ is always a point of the discrete spectrum. One can indicate two *eigenfunctions*

$$\vec{\xi}_1 = \begin{pmatrix} u_1 \\ \bar{u}_1 \end{pmatrix}, \vec{\xi}_3 = \begin{pmatrix} u_3 \\ \bar{u}_3 \end{pmatrix}, \tag{3.2}$$

where

$$u_1 = -i\phi(y|\alpha), u_3 = -\phi_y, \tag{3.3}$$

and two *adjoint functions*:

$$\vec{\xi}_2 = \begin{pmatrix} u_2 \\ \bar{u}_2 \end{pmatrix}, \vec{\xi}_4 = \begin{pmatrix} u_4 \\ \bar{u}_4 \end{pmatrix}, \tag{3.4}$$

where

$$u_2 = -\frac{2}{\alpha}\phi_\alpha, u_4 = \frac{i}{2}y\phi. \tag{3.5}$$

They obey the relations:

$$H\vec{\xi}_1 = H\vec{\xi}_3 = 0, H\vec{\xi}_2 = i\vec{\xi}_1, H\vec{\xi}_4 = i\vec{\xi}_3. \tag{3.6}$$

Actually, the spectrum of $H(\alpha)$ can lie only in the real axis and in the imaginary axis of the E-plane, see [Wc2], for example. It is known also that the spectrum of $H(\alpha)$ is real and the root subspace corresponding to the point $E = 0$ is generated by the vectors $\vec{\xi}_1, \vec{\xi}_2, \vec{\xi}_3, \vec{\xi}_4$ if and only if

$$\partial_\alpha \|\phi\|^2 > 0. \tag{3.7}$$

Consider the resolvent $R(E) = (H - E)^{-1}$. Its kernel $R(y, y'|E)$ is an analytic function in the *extended* E-plane: it admits an analytic continuation through the continuous spectrum as a meromorphic function. The resolvent kernel goes to infinity when E tends to the branch points $\mp E_0$ if the equation $H(\alpha)\psi = \mp E_0\psi$, treated as a differential equation, has nontrivial solutions bounded at infinity. In this case the points $\mp E_0$ will be called *resonances*.

4 Nonlinear equation

Consider the Cauchy problem for equation (1.1) with the initial data

$$\psi(x,0) = \psi_0(x), \tag{4.1}$$

where $\psi_0 \in H^1, H^1$ is the standard Sobolev space with the norm:

$$\|f\|_{H^1}^2 = \|f\|_2^2 + \|f'\|_2^2. \tag{4.2}$$

The problem has a solution $\psi = \psi(x,t)$ which belongs to H^1 with respect to x for each t, moreover $\psi \in C(\mathbf{R} \to H^1)$. Any such solution ψ obeys two *conservation laws*:

$$\int |\psi(x,t)|^2 dx = const, \int \left[|\psi_x(x,t)|^2 + U(|\psi(x,t)|)\right] dx = const, \tag{4.3}$$

where U is the function (1.3). The second formula (4.3) leads to the following estimate:

$$\|\psi(\cdot,t)\|_{H^1} \le c\left(\|\psi_0\|_{H^1}\right) \|\psi_0\|_{H^1}, \tag{4.4}$$

here $c = \mathbf{R}_+ \to \mathbf{R}_+$ is a smooth function. If in addition ψ_0 has the finite norm: $\|(1+|x|)\psi_0\|_2 < \infty$, the solution ψ also has the finite , but growing in time, similar norm:

$$\|(1+|x|)\psi(x,t)\|_2 \le c(\|\psi_0\|_{H^1}) \left[\|(1+|x|)\psi\|_2 + t\|\psi_0\|_{H^1}\right]. \tag{4.5}$$

5 Theorem

Let $\sigma_0 = (\beta_0, \omega_0, b_0, v_0) \in \Sigma, \omega_0 = \frac{1}{4}(v_0^2 - \alpha_0^2)$. Consider the Cauchy problem for equation (1.1) with the initial data:

$$\psi_0(x) = w(x|\sigma_0) + \chi_0(x). \tag{5.1}$$

Our aim is to describe the asymptotic behavior of the solution ψ as $t \to \infty$. Assume that:

T_1) the norm

$$N = \|(1+x^2)\chi_0\|_2 + \|\chi_0'\|_2 \tag{5.2}$$

is sufficiently small;

T_2) $E = 0$ is the only point of the discrete spectrum of $H(\alpha_0)$ and the dimension of the corresponding root subspace is equal to 4;

T_3)the points $\mp E_0$ are not resonances;
T_4)the function F is a polynomial[1] and $p \geq 4$.

Then there exist $\sigma_+ \in \Sigma$ and $f_+ \in \mathbf{L}_2 \cap \mathbf{L}_\infty$ such that

$$\psi = w(\cdot, \sigma_+(t)) + exp(-il_0 t) + o(1) \tag{5.3}$$

as $t \to \infty$. In this formula: $\sigma_+(t)$ is the trajectory of the system (1.8) with the initial data $\sigma_+(0) = \sigma_+$; $l_0 = -\partial_x^2$; $o(1)$ is meant $\mathbf{L}_2$ -norm. Moreover σ_+ in (5-3) is sufficiently close to σ_0 and f_+ is sufficiently small.

It is worth to note that the operator $H(\alpha)$ possesses theses two properties T_2) and T_3) if α is sufficiently close to α_0 and the operator $H(\alpha_+)$ possesses both these properties naturally.

6 Literature

Of course, simple formulas (1.6-8) for the soliton are well known. But in many dimensional x-space the situation is quite different,see,for example, [Str2, Be-Li]. Properties of the spectrum of the operator $H(\alpha)$ were considered in [We2]. The Cauchy problem for equation (1.1) was considered in the space H^1 in [G-V, K] and in some other works. The Cauchy problem with the initial data of the form (5.1) was treated in [Sh-Str, Ca-Li, We1, We2]. The main result states that for the Cauchy data (5.1) the solution always remains in a small H^1-vicinity of the orbit generated by the trajectory $\sigma_0(t), \sigma_0(0) = \sigma_0$. As for the scattering behavior of the solution when $t \to \infty$, some series of works devoted to the scattering in the absence of bound states should be mentioned [Str1, G-V]. The only result which is close to formula (5.3) is contained in [Sof-We]. The authors of the work have considered the equation

$$i\psi_t = - \triangle \psi + [V(x) + \lambda|\psi|^{m-1}]\psi,$$
$$\psi = \psi(x,t), x \in \mathbf{R}^n, 1 < m < \frac{n+2}{n-2}, n = 2, 3.$$

In this situation the soliton appears as the perturbation of an eigenfunction of the operator $\psi \to - \triangle \psi + V(x)\psi$, which is supposed to be unique and simple. The main difference between the theorem of [Sof-We] and our theorem is generated by the fact that in the first case the center of the soliton is *stable*. As a result our work containes some number of technical detailes which differ it from [Sof-We] although the main line is the same. However, it is worth to emphasize that this common mane line is also similar to the corresponding one in the investigation of asymptotic regimes for nonlinear parabolic equations,see[He].

[1]This assumption is not crucial, it is accepted only for the simplicity

7 Separation of motions

Consider a trajectory $\sigma(t) = (\beta(t), \omega(t), b(t), v(t)) \in \Sigma$ which generally is not a solution of system (1.8).Consider the corresponding trajectory in the set of soliton states

(7.1) $$w(x|\sigma(t)) = \exp(i\Phi)\phi(y|\alpha),$$

$$\Phi = -\beta(t) + \frac{1}{2}v(t)x, y = x - b(t), \alpha = \alpha(t).$$

Write the solution ψ of the Cauchy problem (1.1),(5.1) as the sum

(7.2) $$\psi(x,t) = w(x|\sigma(t)) + \chi(x,t).$$

Instead of the equation (1.1) one can get a system for σ and χ introducing some conditions on the splitting (7.2). Let w_σ be the derivative of $w(x|\sigma)$ with respect to the parameter σ and $w_\sigma(t) = w_\sigma(\cdot|\sigma(t))$. One will use the following condition to fix the splitting:

(7.3) $$\langle \vec{\chi}(t), \sigma_3 \vec{w}_\sigma(t) \rangle = 0,$$

here $\langle \cdot, \cdot \rangle$ is the scalar product in the space $\mathbf{L}_2(\mathbf{R} \to \mathbf{C}^2)$. Note that

(7.4) $$\vec{w}_\beta = \exp(i\sigma_3\Phi)\vec{\xi}_1, \ \vec{w}_\omega = \exp(i\sigma_3\Phi)\vec{\xi}_2,$$

(7.5) $$\vec{w}_b = \exp(i\sigma_3\Phi)\vec{\xi}_3, \ \vec{w}_v = \exp(i\sigma_3\Phi)(\vec{\xi}_4 - \frac{1}{2}b\vec{\xi}_1 - \frac{1}{2}v\vec{\xi}_2).$$

So conditions (7.3) can be represented in the form:

(7.6) $$\langle \vec{f}(t), \sigma_3 \vec{\xi}_i(t) \rangle = 0,$$

where

(7.7) $$\chi(x,t) = \exp(i\Phi)f(y,t), \vec{\xi}_i(t) = \vec{\xi}_i(y|\alpha(t)).$$

A different but an equivalent form of the splitting condition is

(7.8) $$im(f(t), u_i(t)) = 0.$$

The geometrical sense of (7.3)=(7.6)=(7.8) is very simple: condition (7.6) implies that $\vec{f}(t)$ belongs to the subspace of the continuous spectrum of the operator $H(\alpha(t))$. Actually the condition leads to decomposition which is in accordance with the asymptotic behavior (5.3).

Write down the system for σ and χ (or f) in more explicit form. Replace the set $\sigma = (\beta, \omega, b, v)$ by some other set of variables (γ, ω, c, v), where

(7.9) $$b = \int_0^t v(\tau)d\tau + c, \ \beta = \int_0^t \omega(\tau)dt + \gamma.$$

In terms of new variables system (1.8) acquires the form:

$$\gamma' = 0, \omega' = 0, c' = 0, v' = 0. \tag{7.10}$$

Rewrite equation (1.1) in terms of f:

$$if_t = L(\alpha)f + N(\phi, f) + l(\sigma)f + l(\sigma)\phi + i(\omega' - \frac{1}{2}vv')\frac{2}{\alpha}\phi_\alpha, \tag{7.11}$$

where

$$N(\phi, f) = F(|\phi + f|^2)(\phi + f) - F(\phi^2)\phi - F(\phi^2)f \tag{7.12}$$
$$-F'(\phi^2)\phi^2(f + \bar{f}),$$

$$l(\sigma) = \frac{1}{2}v'y + ic'\partial_y + \left(\frac{1}{2}bv' - \gamma'\right). \tag{7.13}$$

Consider the derivative of splitting condition in form (7.8) with respect to t and substitute expression (7.11) for f_t in the obtained relation. The result can be written down as follows:

$$(A_0 + A_1)\lambda = G, \tag{7.14}$$

where

$$\lambda = (\gamma' - \frac{1}{2}bv', \omega' - \frac{1}{2}vv', c', v'),\ A_0 = \{im(u_i, u_j)\}_{i,j=1}^4, \tag{7.15}$$

$$(A_1\lambda)_j = -re(l(\sigma)f, u_j) - \frac{2}{\alpha}(\omega' - \frac{1}{2}vv')im(f, u_{j\alpha}),\ G = re(N, u_j). \tag{7.16}$$

Obtain the explicit expression for the matrix A_0:

$$A_0 = \begin{pmatrix} 0 & e & 0 & 0 \\ -e & 0 & 0 & 0 \\ 0 & 0 & 0 & n \\ 0 & 0 & -n & 0 \end{pmatrix}, n = -\frac{1}{4}\|\phi\|_2^2, e = \frac{4}{\alpha}\frac{dn}{d\alpha}. \tag{7.17}$$

Under assumptions $T_2), T_3)$

$$\det A_0(\alpha_0 \neq 0, \tag{7.18}$$

see (3.7). If $\alpha(t)$ is close to α_0 and $f(t)$ is sufficiently small (actually we are going to prove it), equation (7.14) can be used to estimate λ. Substituting λ from (7.14) to the right side of (7.11) one obtains the system:

$$\sigma_t = G_1(\sigma, f), if_t = L(\alpha)f + N_1(\sigma, f). \tag{7.19}$$

Equation (7.14) is not a complete equivalent of conditions (7.3)=(7.6)=(7.8). To get the equivalence one has to add to equation (7.14) condition (7.3)= (7.6)=(7.8) at the time-moment $t = 0$:

$$\langle \vec{\chi}_0, \sigma_3 \vec{w}_\sigma(\cdot|\sigma_0) \rangle = 0. \tag{7.20}$$

Generally this condition is not satisfied by the given decomposition (5.1) of the initial data ψ_0. But if χ_0 is sufficiently small it is possible to reconstruct decomposition (5.1) of the initial data ψ_0 in order to satisfy to condition (7.20)

In fact, one has to solve the equation:

$$\langle \vec{\psi}_0 - vecw(\cdot|\sigma_1), \sigma_3 \vec{w}_\sigma(\sigma_1)\rangle = 0 \tag{7.21}$$

with respect to σ_1. Here ψ_0 should be given by (5.1) with sufficiently small χ_0, see (5.2). The local solvability of (7.21) is guaranteed by the nondegeneration of the corresponding Jacobi matrix:

$$- \langle \vec{w}_{\sigma_i}(\cdot|\sigma_0), \sigma_3 \vec{w}_{\sigma_j}(\cdot|\sigma_0)\rangle = -2iA_0(\alpha_0). \tag{7.22}$$

So one can assume that decomposition (5.1) obeys condition (7.20).

Since $\psi \in C(\mathbf{R} \to H^1)$ a little more general constructions show that condition (7.3) has to fulfil on some small time-interval. Some estimates which will be given in next sections, will show also that at the end of this time- interval the solution has the structure (5.1) with the small second term. It gives us the possibility to continue the constructions and to solve equation (7.3) for all $t \in [0, t_1]$.

8 Reduction to a spectral problem

Now one can describe the main line of the following constructions.

1)System (7.19) will be investigated on a large finite interval $t \in [0, t_1]$. In the end one will be able to consider the limit $t_1 \to \infty$.

2) On the interval $[0, t_1]$ one can pick out the leading term of system (7.19) in the form:

$$\sigma_t = 0, if_t = L(\alpha)f. \tag{8.1}$$

The first equation should be completed by more stable final data: $\sigma(t_1) = \sigma_1$, with the undefinite for the moment values:

$$\sigma_1 = \sigma(t_1), \sigma_1 = (\beta_1, \omega_1, b_1, v_1),$$

$$\omega_1 = \frac{1}{4}(v_1^2 - \alpha_1^2), b_1 = v_1 t_1 + c_1, \beta_1 = \omega_1 t_1 + \gamma_1.$$

Naturally now one has to put $L(\alpha) = L(\alpha_1)$. After that the second equation oppositely should be completed by the known initial data.

3)Rewrite full equation (7.11) in order to get the operator $L(\alpha_1)$ as the main term of the of the right side. Introduce the new function g:

$$\chi = exp(i\Phi_1)g(z,t), \Phi_1 = -\omega_1 t - \gamma_1 + \frac{1}{2}v_1 x, z = x - v_1 t - c_1. \tag{8.2}$$

It obeys the equation:

$$ig_t = L(\alpha_1)g + D(\sigma, g), \tag{8.3}$$

and D is given by the formulas

$$D = D_0 + D_1 + D_2 + D_3 + D_4, \tag{8.4}$$

$$D_0 = \exp(-i\Delta)\left[l(\sigma)\phi(y|\alpha) + i\frac{2}{\alpha}(\omega' - \frac{1}{2}vv')\phi_\alpha(y|\alpha)\right],$$

$$\Delta = \Phi_1 - \Phi,$$

$$D_1 = \left[F(\phi^2(y|\alpha) + F'(\phi^2(y|\alpha))\phi^2(y|\alpha)\right] g -$$
$$\left[F(\phi^2(z|\alpha_1)) + F'(\phi^2(z|\alpha_1)\phi^2(z|\alpha_1)\right] g,$$

$$D_2 = F'(\phi^2(y|\alpha))\phi^2(y|\alpha)[\exp(-2i\Delta) - 1]\bar{g},$$

$$D_3 = [F'(\phi^2(y|\alpha))\phi^2(y|\alpha) - F'(\phi^2(z|\alpha_1))\phi^2(z|\alpha_1)]\bar{g},$$

$$D_4 = \exp(-i\Delta)N(\phi(y|\alpha), \exp(i\Delta)g).$$

In order to investigate the long-time behavior of the solution of the second equation (8.1) and its full form (8.3) one has to separate the contributions of the discrete spectrum and of the continuous spectrum of the operator $L(\alpha_1)$, more precisely, of the operator $H(\alpha_1)$. Consider the representation

$$\vec{g} = \vec{k} + \vec{h}, \tag{8.5}$$

where $\vec{k}$ and $\vec{h}$ are the indicated contributions. One can use condition (7.6) to express the component $\vec{k}$ in terms $\vec{h}$. Since

$$\vec{k} = \sum_i \kappa_i \vec{\xi}_i(z|\alpha_1), \tag{8.6}$$

condition (7.6) leads to the relation:

$$\sum_i \kappa_i \langle \Lambda \vec{\xi}_i(z|\alpha_1), \sigma_3 \vec{\xi}_j(y|\alpha)\rangle + \langle \Lambda \vec{h}, \sigma_3 \vec{\xi}_j(y|\alpha)\rangle = 0, \tag{8.7}$$

where

$$\Lambda = \begin{pmatrix} e^{i\Delta} & 0 \\ 0 & e^{-i\Delta} \end{pmatrix}. \tag{8.8}$$

The main term of equation (8.7) is again defined by the matrix A_0:

$$\langle \vec{\xi}_i(z|\alpha_1), \sigma_3 \vec{\xi}_j(y|\alpha_1)\rangle \sim -2iA_0(\alpha_1). \tag{8.9}$$

At last for $\vec{h}$ one can write down the following integral representation (equation):

$$\vec{h} = \exp(-iH_1 t)\vec{h}_0 - i\int_0^t \exp[-iH_1(t-\tau)]P_1\vec{D}d\tau. \tag{8.10}$$

Here P_1 is the spectral projection operator on the subspace of the continuos spectrum of H_1 and

(8.11) $$\vec{h}_0 = P_1\vec{g}_0, g_0(z) = \exp\left[i\gamma_1 - i\frac{1}{2}v_1(z+c_1)\right]\chi_0(z+c_1).$$

The final form of the equations which are used in order to investigate the dynamical system on the interval $t \in [0, t_1]$ is given by relations (7.14),(8.7),(8.10).

9 Linear evolution

Consider the operator $H = H(\alpha)$ with some fixed α and assume that H satisfies conditions $T_2), T_3)$ (with α instead of α_0 in them). Let $U(t) = \exp(-iHt)$ be the corresponding evolution operator and P be the spectral projection operator on the subspace of the continuous spectrum of H. Equation (8.11) shows that one has to have some estimates of the evolution $U(t)P$. Such estimates will be presented in this section. They are enough transparent and can be proved by means of simple (but unfortunately not short) computations which use the spectral resolution of H. So let $\vec{h} = P\vec{h}$, then

(9.1) $$\|U(t)\vec{h}\|_\infty \le ct^{-1/2}[\|\vec{h}\|_2 + NR(\vec{h})];$$

(9.2) $$\|U(t)\vec{h}\|_\infty \le c(1+t)^{-1/2}[\|\vec{h}\|_{H^1} + NR(\vec{h})$$

(9.3) $$\|\varrho U(t)\vec{h}\|_2 \le c(1+t)^{-3/2}[\|\vec{h}\|_2 + NR(\vec{h})].$$

Here

$$NR(\vec{h}) \text{ can be equal } \|(1+x^2)\vec{h}\|_1 \text{ or } \|(1+x^2)\vec{h}\|_2,$$

$$\varrho(x) = (1+|x|)^{-\kappa}, \kappa > 3,5.$$

10 Estimates of nonlinear terms

All nonlinear terms of euation (8.10) can be estimated with the following set o:

$$M_0(t) = |\alpha^2 - \alpha_0^2|, M_1(t) = |d(t)|, d = y - z,$$

$$M_2(t) = \|\vec{\kappa}\|, \vec{\kappa} = (\kappa_1, \kappa_2, \kappa_3, \kappa_4), M_3(t) = \|\varrho(z)\vec{h}(z,t)\|_2, M_4 = \|\vec{h}(z,t)\|_\infty,$$

$$\mathbf{M}_0(t) = \sup_{\tau\le t} M_0(\tau), bfM_1(t) = \sup_{\tau\le t} M_1(\tau),$$

$$\mathbf{M}_2(t) = \sup_{\tau\le t}(1+\tau)^{3/2}M_2(\tau), \mathbf{M}_3(t) = \sup_{\tau\le t}(1+\tau)^{3/2}M_3(\tau),$$

$$\mathbf{M}_4(t) = \sup_{\tau \le t}(1+\tau)^{1/2} M_4(\tau).$$

At last

$$\mathbf{M}_j = \mathbf{M}_j(t_1).$$

These definitions and relation (7.14) lead more or less directly to the inequalities:

(10.1) $$\|\lambda\| \le W(\mathbf{M})(\mathbf{M}_2+\mathbf{M}_3)^2(1+t)^{-3}, t < t_1.$$

Here $W(\mathbf{M})$ is a function of $\mathbf{M}_0, \mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3, \mathbf{M}_4$, which is a bounded function on a finite vicinity of the point $\mathbf{M}_j = 0$ and can acquire infinite values outside of some larger vicinity. It is possible to present an explicit expression for W but this expression is useless for our purpose. ¿From (10.1) one can obtain:

(10.2) $$\mathbf{M}_0, \mathbf{M}_1 \le W(\mathbf{M})(\mathbf{M}_2+\mathbf{M}_3)^2.$$

Inequalities (10.1) together with the relation (8.7) generate also the estimate

(10.3) $$\mathbf{M}_2 \le W(\mathbf{M})(\mathbf{M}_2+\mathbf{M}_3)^3.$$

Now pick out from D_4 all terms containing at least one power of ϕ and denote their sum by D_{II}, the remainder will be denoted by D_{III}. Finally, let $D_I = D_1 + D_2 + D_3$.

Direct computations permit to prove the following estimates:

(10.4) $$\|(1+z^2)P_1(D_0+D_I+D_{II})\|_2 \le$$
$$W(\mathbf{M})(\mathbf{M}_2+\mathbf{M}_3+\mathbf{M}_4)^2(1+t)^{-3/2}.$$

In order to obtain a similar estimate for D_{III} one has to use additionally some information on solutions of nonlinear equation (1.1), more precisely one has to use conservation law (4.3) and estimate (4.5). As result one has obtain:

(10.5) $$\|P_1 D_{III}\|_2 + \|(1+z^2)P_1 D_{III}\|_1 \le W(\mathbf{M})\mathbf{M}_4^{2p-1}(1+t)^{-3/2}.$$

Just here it is important to assume that $4 \le p$.

11 Final estimates

Using equation (8.10) and combining estimates (9.1-3),(10.4-5) one can obtain finally:

(11.1) $$\mathbf{M}_3, \mathbf{M}_4 \le W(\mathbf{M})\left[N + (\mathbf{M}_2+\mathbf{M}_3)^2 + \mathbf{M}_4^2 + \mathbf{M}_4^{2p-1}\right],$$

where

$$N = \|(1+x^2)\chi_0\|_2 + \|\chi_0'\|_2.$$

The first term N is originated from the first free term of the right side of equation (8.10). It is controlled by the second variants of estimates (9.2-3). Other terms in brackets are originated from the integral term of equation (8.10). They are controlled by estimates (10.4-5) and by both variants of (9.1),(9.3).

Now one has obtained a closed set of inequalities (10.2-3),(11.1) and can try to solve it. Formulas (10.3),(11.1) give the system:

$$\mathbf{M}_2 + \mathbf{M}_3, \mathbf{M}_4 \leq \tag{11.2}$$
$$W(\mathbf{M})\left[N + (\mathbf{M}_2 + \mathbf{M}_3)^2 + (\mathbf{M}_2 + \mathbf{M}_3)^3 + \mathbf{M}_4^2 + \mathbf{M}_4^{2p-1}\right].$$

If N is sufficiently small, the system shows that the pair $\mathbf{M}_2 + \mathbf{M}_3, \mathbf{M}_4$ can belong either to a small vicinity of the point $(0,0)$ or to some domain whose distance from $(0,0)$ is limited from below uniformly with respect to N. It is clear that only the first possibility can be realized. Therefore all the functions $\mathbf{M}_0, \mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3, \mathbf{M}_4$ are sufficiently small:

$$\mathbf{M}_j(t) \leq \mu(N)N, \tag{11.3}$$

here $\mu(N)$ is a bounded function defined for small N. Since all constants in the estimates do not depend on t_1 the same estimates are true for $\mathbf{M}_j(t)$ uniformly in $t \in \mathbf{R}_+$:

$$\mathbf{M}_j(t) \leq \mu(N)N. \tag{11.4}$$

12 The limiting soliton

Return to (10.1) again. Estimates (11.4) show now that

$$\|\lambda\| \leq \mu(N)N^2(1+t)^{-3}. \tag{12.1}$$

It implies that all variables γ, ω, c, v have limits $\gamma_\infty, \omega_\infty, c_\infty, v_\infty$ as $t \to \infty$. So one can introduce the limiting trajectory $\sigma_+(t)$:

$$\beta_+(t) = \omega_+ t + \gamma_+, \omega_+ = \omega_\infty, \gamma_+ = \gamma_\infty + \int_0^\infty (\omega(\tau) - \omega_\infty)d\tau, \tag{12.2}$$

$$b_+(t) = v_+ t + c_+, v_+ = v_\infty, c_+ = c_\infty + \int_0^\infty (v(\tau) - v_\infty)d\tau. \tag{12.3}$$

It is clear that

$$\sigma(t) - \sigma_+(t) = O(t^{-1}), \tag{12.4}$$

as $t \to \infty$.Now the *limiting soliton* $w(x|\sigma_+(t))$ arises naturally and

$$w(x|\sigma(t)) - w(x|\sigma_+(t)) = O(t^{-1}) \tag{12.5}$$

in the space $\mathbf{L}_2 \cap \mathbf{L}_\infty$.

13 Dispersion reminder

The second term χ of the total solution $\psi = w(x|\sigma(t)) + \chi$ can be studied asymptotically if one uses the same representantion of χ as in section 8,but with ∞ instead of t_1 in transformation (8.2):

(13.1)
$$\chi = exp(i\Phi_\infty)g(z,t),$$
$$\Phi_\infty = -\beta_+(t) - \frac{1}{2}v_+x, z = x - b(t).$$

Now the operators H_1 and P_1 should be replaced by the naturally defined operators H_+ and P_+ and all construction of section 8-11 can be duplicated.

Particularly one again can separate the contributions of the discrete and the continuous spectra of H_+:

(13.2)
$$\vec{g} = \vec{k} + \vec{h}.$$

From

(13.3)
$$M_2(t) \leq \mu(N)N(1+t)^{-3/2},$$

see (11.4),one can obtain at once the estimate:

(13.4)
$$\vec{k} = O(t^{-3/2}),$$

in the space $\mathbf{L}_2 \cap \mathbf{L}_\infty$.

Reprezentation (8.10) for $\vec{h}$ acquires the form:

(13.5)
$$\vec{h} = exp(-iH_+t)P_+\vec{h}_0 - i\int_0^t exp[-iH_+(t-\tau)]P_+\vec{D}d\tau,$$

with the respectively transformed D.

Introduce the representation

(13.6)
$$\vec{h} = exp(-iH_+t)\vec{h}_\infty + \vec{R},$$

(13.7)
$$\vec{h}_\infty = P_+(\vec{h}_0 + \vec{h}_1), \vec{h}_1 = -i\int_0^\infty exp(iH_+\tau)\vec{D}d\tau,$$

(13.8)
$$\vec{R} = -i\int_t^\infty exp[-iH_+(t-\tau)]P_+\vec{D}d\tau.$$

Here $\vec{h}_\infty \in \mathbf{L}_2 \cap \mathbf{L}_\infty : \vec{h}_0 \in \mathbf{L}_2 \cap \mathbf{L}_\infty$ since $\vec{h}_0 \in H^1; \vec{h} \in \mathbf{L}_2 \cap \mathbf{L}_\infty$ in accordance with (9.1), (10.4-5). Inequalities (10.4-5) imply immediately that:

(13.9)
$$\vec{R} = O(t^{-1/2})$$

in $\mathbf{L}_2$-norm,

(13.10)
$$\vec{R} = O(t^{-1})$$

in $\mathbf{L}_\infty$-norm. So one can formulate the following result:

(13.11)
$$\psi = w(x|\sigma_+(t)) + \\ + \exp(i\Phi_\infty)\left[\exp(-iH_+t)\vec{h}_\infty\right]_1(z,t) + R,$$

where R admits estimates (13.9-10). The brackets $[\vec{v}]_1$ are used in order to indicate the first component of $\mathbf{C}^2$ - vector $\vec{v}$.

14 Scattering

In the *dispersive term* $\exp(i\Phi_\infty)\exp(-iH_+t)\vec{h}_\infty$ the element $\vec{h}_\infty$ belongs to the subspace of the continuous spectrum of the operator H_∞. So its behavior as $t \to \infty$ is *scattering behavior* (in $\mathbf{L}_2$ - norm):

(14.1)
$$\exp(-iH_+t)\vec{h}_\infty = \exp(-iH_0t)\vec{h}_+ + o(1),$$

where $\vec{h}_+ \in \mathbf{L}_2$ and is related to $\vec{h}_\infty$ in terms of the corresponding *wave operator* W_+:

(14.2)
$$\vec{h}_\infty = W_+\vec{h}_+.$$

It is not essential that the operator H_∞ is not self-adjoint in our case since its spectral resolution has the same structure as for a self-adjoint operator. We are not going to discuss here the properties of $\vec{h}_+$ and the reminder in more detail. Only note that

(14.3)
$$\exp(i\Phi_\infty[\exp(-iH_0t)\vec{h}_+]_1(z) = [\exp(-il_0t)f_+](x),$$

and

(14.4)
$$l_0 = -\partial_x^2, f_+(x) = \exp(-i\gamma_+ - i\frac{1}{2}v_+x)h_+(x - c_+).$$

Introduce representation (14.3) in formula (13.11) and write down the *final result*:

(14.5)
$$\psi = w(\cdot|\sigma_+(t)) + \exp(-il_0t)f_+ + o(1).$$

From the first author (V.B.):
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References

[Be-Li] Berestycki, H. and Lions, P.L., *Nonlinear scalar field equations.I. Existence of a ground state,* Arch. Rat. Mech. Anal. **82** (1982), 313-345.

[Ca-Li] Cazenave,T. and Lions,P.L., *Orbital stability of standing waves for somenonlinear Schroendinger equations,* Comm.Math.Phys. **85** (1982), 549-561.

[G-V] Ginibre,J. and Velo,G., *On a class of nonlinear equations. I,II,* J Funct. Anal.**32**(1979),1-71.

[He] Henry,D., *Geometrical theory of semilinear parabolic equations,* Springer(1981)

[K] Kato,T., *On nonlinear Schroedinger equation,* Ann.Inst. Henri Poincare, Physique Theorique **46** (1987),113-129.

[Sh-Str] Shatah,J. and Strauss,W., *Instability of nonlinear bound states,* Comm. Math. Phys.**55**(1977),149-162.

[Sof-We] Soffer, A. and Weinstein, M.I., *Multichannel nonlinear scattering for nonintegrable equations,* Comm. Math. Phys.

[Str1] Strauss,W.A., *Dispersion of low energy waves for two conservative equations,* Arch. Rat. Mech. Anal. **55** (1974), 86-92.

[Str2] Strauss, W.A., *Existence of solitary waves in higher dimensions,* Comm. Math. Phys. **55** (1977), 149-162.

[We1] Weinstein,M.I., *Modulational stability of ground states of nonlinear Shroedinger equations,* SIAM J.Math.Anal.**16**(1985), 472-491.

[We2] Weinstein,M.I., *Lyapunov stability of ground states or dispersive evolution equation,* Comm. Pure Appl. Math. **39**(1981),51-68

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On the spectrum of gauge-periodic elliptic operators

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On the Spectrum of Gauge-Periodic Elliptic Operators

Jochen Brüning and Toshikazu Sunada

1. Introduction

This note presents an extension of the results in [1] concerning the spectrum of symmetric elliptic operators on complete noncompact Riemannian manifolds. Thus consider a complete Riemannian manifold, M, of dimension m, with a properly discontinuous action of a discrete group, Γ, of isometries; we assume that the orbit space is compact. Moreover, let $E \to M$ be a hermitian vector bundle with a unitary representation

$$U : \Gamma \to L^2(E)\,. \tag{1.1a}$$

More precisely, we assume that Γ acts unitarily on E, via γ_*, and put

$$U_\gamma f(p) := \gamma_* f(\gamma^{-1}(p))\,. \tag{1.1b}$$

Thus each U_γ maps $C_0^\infty(E)$ to itself. Finally, let D be a symmetric elliptic differential operator on $C_0^\infty(E)$. In [1] we have assumed that D is, in addition, periodic in the sense that it commutes with all U_γ on $C_0^\infty(E)$. Now we bring in a second unitary representation, the *gauge*,

$$\begin{aligned} &V : \Gamma \to C^\infty(\operatorname{End} E)\,,\\ &V_\gamma \mid E_p \text{ is unitary for all } \gamma \in \Gamma,\ p \in M, \end{aligned} \tag{1.2}$$

which induces a unitary representation on $L^2(E)$. This representation will also be denoted by V. In general,

$$W_\gamma := V_\gamma U_\gamma \tag{1.3}$$

will not define a representation any more, since $[V_{\gamma_1}, U_{\gamma_2}]$ maybe nonzero. But frequently we have a good substitute namely

$$U_{\gamma_1} V_{\gamma_2} = X(\gamma_1, \gamma_2) V_{\gamma_2} U_{\gamma_1}\,, \tag{1.4a}$$

where

$$X(\gamma_1,\gamma_2) \text{ is in } C^\infty(\operatorname{End} E), \text{ unitary on each fiber, and a character of } \Gamma \text{ in each variable separately.} \tag{1.4b}$$

Moreover, we want that

$$X(\gamma,\gamma) = 1 \quad \text{for all } \gamma \in \Gamma\,. \tag{1.4c}$$

The operator D is called *gauge-periodic* if

$$[W_\gamma, D] = 0 \quad \text{on } C_0^\infty(E)\,. \tag{1.5}$$

The periodic case is obviously contained with V, X trivial. An interesting example with nontrivial gauge is provided by the Schrödinger operator with constant magnetic field in $\mathbb{R}^2$. This will be our main application which we deal with in greater detail below.

Assuming (1.5) we associate a C^*-algebra with D as follows. Fix a fundamental domain, $\mathcal{D}$, for Γ and introduce the isometry

$$\begin{aligned} &\Phi : L^2(E) \to L^2(\Gamma, L^2(E \mid \mathcal{D}))\,,\\ &\Phi f(\gamma) := r_{\mathcal{D}} \circ W_\gamma(f)\,, \end{aligned} \tag{1.6}$$

where $r_{\mathcal{D}}$ denotes restriction $L^2(E) \to L^2(E \mid \mathcal{D}) =: H$. Let R_γ, L_γ be right translation by γ and left translation by γ^{-1} in $L^2(\Gamma)$, respectively, and define the unitary operator X_γ in $L^2(\Gamma)$ for $\gamma \in \Gamma$ by

$$X_\gamma \sigma(\delta) := X(\delta,\gamma)\sigma(\delta)\,. \tag{1.7}$$

Then it is easy to compute that

$$\tilde{R}_\gamma := \Phi W_\gamma \Phi^{-1} = X_\gamma R_\gamma \otimes I\,. \tag{1.8}$$

Since X is a bicharacter, it is also readily seen that

$$[X_{\gamma_1} L_{\gamma_1} \otimes I, \tilde{R}_{\gamma_2}] = 0 \quad \text{for all } \gamma_1,\gamma_2 \in \Gamma\,. \tag{1.9}$$

We will see that this is satisfied in our main example (and probably in many other cases). Then we abbreviate $\tilde{L}_\gamma =: X_\gamma L_\gamma$ and introduce the C^*-algebra $\mathcal{C}_W(\Gamma)$ which is generated by $(\tilde{L}_\gamma)_{\gamma\in\Gamma}$ in $\mathcal{L}(L^2(\Gamma))$. With $\mathcal{K} = \mathcal{K}(H)$, the ideal of compact operators on $H = L^2(E \mid \mathcal{D})$, we introduce, as in [1],

$$\mathcal{C}_W(\Gamma,\mathcal{K}) := \mathcal{C}_W(\Gamma) \otimes \mathcal{K}\,. \tag{1.10}$$

On this algebra we can again define a natural trace tr_Γ (to be described in Sec. 3), such that all spectral projections of D have a finite trace. We say that $\mathcal{C}_W(\Gamma, \mathcal{K})$ has the *Kadison property* if there is a constant $C > 0$ such that

$$\mathrm{tr}_\Gamma P \geq C\,, \tag{1.11}$$

for all nonzero orthogonal projections $P \in \mathcal{C}_W(\Gamma, \mathcal{K})$. The largest constant in (1.11) will be called the *Kadison constant* of $\mathcal{C}_W(\Gamma, \mathcal{K})$, to be denoted $C_W(\Gamma)$.

We can show that D has a unique self-adjoint extension, $\bar{D}$, with spectral resolution

$$\bar{D} = \int_{-\infty}^{+\infty} \lambda dE_\lambda\,.$$

Quite analogously to [1] we then obtain

Theorem 1 *If $\lambda_1 > \lambda_2 \in \mathbb{R} \backslash \mathrm{spec}\, \bar{D}$ then $E_{\lambda_1} - E_{\lambda_2} \in \mathcal{C}_W(\Gamma, \mathcal{K})$. If $\mathcal{C}_W(\Gamma)$ has the Kadison property then the spectrum of $\bar{D}$ has band structure in the sense that the intersection of the resolvent set with any compact interval of real numbers has finitely many components.*

As noted in [1], the proof of Theorem 1 gives some quantitive information which we exploit in connection with the magnetic Schrödinger operator in $\mathbb{R}^2$. Recall that this operator is defined on $C_0^\infty(\mathbb{R}^2)$ by

$$D_A := \sum_{i=1}^{2} \Big(\frac{1}{\sqrt{-1}} \frac{\partial}{\partial x_i} + a_i\Big)^2 + v\,, \tag{1.12}$$

where $a_i, v \in C^\infty(\mathbb{R}^2)$. The magnetic field is assumed to be constant,

$$b(x) := \Big(\frac{\partial a_2}{\partial x_1} - \frac{\partial a_1}{\partial x_2}\Big)(x) \equiv b(0) =: b\,,$$

and we assume moreover that v is $\mathbb{Z}^2$-periodic. b is also equal to the magnetic flux over a unit cell,

$$b = \int_{0 \leq x_1, x_2 \leq 1} b(x_1, x_2) dx_1 dx_2 =: 2\pi\theta\,. \tag{1.13}$$

This operator fits into our framework as follows. Since the magnetic field is constant we may assume that

$$a_1(x) = bx_2/2\,, \quad a_2(x) = -bx_1/2\,.$$

With ω the standard symplectic form in $\mathbb{R}^2$, we define for $z \in \mathbb{Z}^2$

$$\begin{aligned} U_z f(x) &:= f(x-z)\,, \\ V_z f(x) &:= e^{\sqrt{-1}\, b/2\, \omega(x,z)} f(x)\,. \end{aligned} \tag{1.14}$$

Then it follows that

$$X(z_1, z_2) = e^{\sqrt{-1}\, b/2\, \omega(z_1,z_2)} \tag{1.15}$$

and

$$\tilde{L}_{z_1} \tilde{L}_{z_2} = e^{\sqrt{-1}\, b\, \omega(z_2,z_1)} \tilde{L}_{z_2} \tilde{L}_{z_1}\,. \tag{1.16}$$

Now we regard the quantity b as a parameter restricted by $|b| \le C_1$, say. It is known that the precise band structure of spec $\bar{D}_A$ in a given interval $[\lambda_1, \lambda_2]$ depends rather subtly on the arithmetic nature of θ in (1.13). We will prove

Theorem 2 *Assume that $\theta = p/q \in \mathbb{Q}$ with $(p,q) = 1$, and that $\lambda_1 > \lambda_2 \in \mathbb{R} \setminus$ spec $\bar{D}_A$. There is a constant C depending only on C_1, λ_1, λ_2, and v such that*

$$G(D_A, \lambda_1, \lambda_2) := \sharp\{ \text{ gaps in spec } \bar{D}_A \cap [\lambda_2, \lambda_1]\}$$

satisfies the estimate

$$G(D_A, \lambda_1, \lambda_2) \le C(C_1, \lambda_1, \lambda_2, v)\, q\,. \tag{1.17}$$

The proof of this result uses the fact that the Kadison constant of $\mathcal{C}_W(\Gamma)$ satisfies $C_W(\Gamma) \ge q^{-1}$. This degeneration then allows the possible development of Cantor structures if θ approaches irrational numbers. It has been shown in [3] that, for suitable v, G also has a similar lower bound. Crucial for this result was a thorough study of Harper's equation, a discrete approximation to D_A. Using only the structure of the rotation algebras (which are brought in by (1.16)) it has been shown in [2] that the maximum number of gaps is realized by Harper's operator. One might thus hope that our approach, which links all gauge-periodic operators with the rotation algebra, opens a way to bypass the discrete approximation and to establish directly that "sufficiently complicated" operators in the rational rotation algebra will indeed have the maximum number of gaps. Of course, this need not be so for every operator as illustrated by the case $v = 0$. Since $C_W(\Gamma) = 0$ for irrational θ, we also see that for a vanishing Kadison constant no general conclusion concerning the structure of the spectrum is possible.

We are indebted to Victor Guillemin and Johannes Sjöstrand for some enlightening discussions.

2. Parametrix construction

We follow essentially the outline of [1, Sec. 2]. Since Γ acts properly discontinuously the sets

$$\Gamma(K) := \{\gamma \in \Gamma \mid K \cap \gamma K \neq \emptyset\} \tag{2.1}$$

are finite for all compact $K \subset M$. It follows that for any sequence $(u_\gamma)_{\gamma\in\Gamma} \subset L^2(E)$ with supp $u_\gamma \subset \gamma K$ for some compact K and all $\gamma, u := \sum\limits_{\gamma\in\Gamma} u_\gamma$ is well defined. Moreover, we find the norm estimate

$$\|u\|^2_{L^2(E)} \le \sharp\Gamma(K) \sum_{\gamma\in\Gamma} \|u_\gamma\|^2_{L^2(E)} \,. \tag{2.2}$$

In particular, the convergence of the right hand side implies $u \in L^2(E)$.

On the other hand, if $\psi_1, \psi_2 \in C_0^\infty(M)$ and $B \in \mathcal{L}(L^2(E))$ and if we put, for $u \in L^2(E))$,

$$B_\gamma u := W_\gamma \psi_1 B \psi_2 W_\gamma^* u =: \psi_{1\gamma} W_\gamma B W_\gamma^* \psi_{2\gamma} u \,, \tag{2.3}$$

then we can easily prove the estimate

$$\sum_\gamma \|B_\gamma u\|^2_{L^2(E)} \le (\sup_M \psi_1^2)(\sup_M \psi_2^2)\sharp\Gamma(\bar{\mathcal{D}} \cup \text{supp } \psi_1 \cup \text{supp } \psi_2)\|B\|^2\|u\|^2_{L^2(E)} \,. \tag{2.4}$$

Now consider a gauge-periodic operator D with domain $C_0^\infty(E)$ in $L^2(E)$. To show that D is essentially self-adjoint we consider $u \in L^2(E)$ with

$$D^* u = \sqrt{-1} u \,.$$

Since $u \in H^\rho_{\text{loc}}(E)$, $\rho := \operatorname{ord} D$, by elliptic regularity we have $\psi_\gamma u \in H_0^\rho(E)$ for $\psi \in C_0^\infty(M)$. Now pick ψ such that

$$\sum_{\gamma\in\Gamma} \psi_\gamma = 1 \,. \tag{2.5}$$

Then we compute

$$\begin{aligned} 0 &= (u, (D^* - \sqrt{-1})u) \\ &= \sum_{\gamma,\gamma'} (\psi_\gamma u, D\psi_{\gamma'} u) + \sqrt{-1}\|u\|^2 \\ &= \overline{\sum_{\gamma,\gamma'} (\psi_\gamma u, D\psi_{\gamma'} u)} + \sqrt{-1}\|u\|^2 \,, \end{aligned}$$

which implies $u = 0$, as desired.

We identify D with its closure in $L^2(E)$. Assuming next $D \geq 0$ and $\rho > m$ we construct a local paramatrix for the heat operator $\partial_t + D$ as in [1, Lemma 1]. Using the same notation, we define the global fundamental solution by

$$\mathcal{F}_t u := \sum_{\gamma \in \Gamma} W_\gamma \varphi F_t \psi W_\gamma^* u\,, \tag{2.6}$$

and the remainder term by

$$\mathcal{R}_t u := \sum_{\gamma \in \Gamma} W_\gamma (\partial_t + D) \varphi F_t \psi W_\gamma^* u\,, \tag{2.7}$$

where ψ satisfies (2.5) and $\varphi \in C_0^\infty(M)$ equals 1 near supp ψ. Going through the proof of [1, Lemma 2] we obtain the analogous result (using (2.2) and (2.4)) i.e.

Lemma 1 *Fix $T > 0$.*
1) Uniformly in $t \in (0, T]$, we have

$$\|\mathcal{F}_t\|_{L^2(E)} + \|\mathcal{R}_t\|_{L^2(E)} \leq C_2\,.$$

2) For $u \in L^2(E)$, the functions $\mathcal{F}_t u$ and $\mathcal{R}_t u$ are continuous in $(0, T]$ with

$$\lim_{t \to 0} \mathcal{F}_t u = u\,.$$

3) $\mathcal{F} u$ is differentiable in $(0, T]$, has values in $\mathcal{D}(D)$, and satisfies the equation

$$(\partial_t + D) \mathcal{F}_t u = \mathcal{R}_t u\,.$$

As in loc. cit. we can now derive the Neumann series

$$\exp(-tD) = \sum_{j=0}^{\infty} (-1)^j (\mathcal{F} *^j \mathcal{R})_t\,, \tag{2.8}$$

where

$$(\mathcal{F} *^0 \mathcal{R})_t := \mathcal{F}_t\,, \quad (\mathcal{F} *^{j+1} \mathcal{R})_t = \int_0^t (\mathcal{F} *^j \mathcal{R})_{t-u} \mathcal{R}_u du\,. \tag{2.9}$$

The kernel estimates in [1, Lemma 1] then lead, as before, to the following result.

Lemma 2 $\exp(-tD)$ *has a smooth kernel (with respect to the given L^2-structures),*

$$K_t(p,q) \in E_p \otimes E_q^*\,, \quad t > 0\,,\ (p,q) \in M \times M\,.$$

This kernel satisfies the estimate

$$|K_t(p,q)|_{E_p \otimes E_q^*} \leq C_3 t^{-m/\rho} \exp(-C_4 d_M(p,q)^{\rho/(\rho-1)} t^{-1/(\rho-1)})\,, \tag{2.10}$$

uniformly in $(0,T] \times M \times M$; here d_M denotes the Riemannian distance.

Moreover, as $t \searrow 0$ we have the asymptotic relation

$$\operatorname{tr}_{E_p} K_t(p,p) \sim t^{-m/\rho} A(p)\,, \tag{2.11}$$

with an explicitly computable function $A(p)$ (cf. [1, (0.1)]).

3. C^*-algebras

Following the outline of [1] further, we have to introduce the trace tr_Γ on $\mathcal{C}_W(\Gamma,\mathcal{K})$, defined in (1.10). To do so we introduce the commutant of $(\tilde{\mathcal{R}}_\gamma)_{\gamma\in\Gamma}$,

$$\mathcal{M}_W(\Gamma) := \{A \in \mathcal{L}(L^2(\Gamma,H)) \mid [A,\tilde{\mathcal{R}}_\gamma] = 0 \text{ for } \gamma \in \Gamma\}\,. \tag{3.1}$$

Then we define the Fourier coefficients of $A \in \mathcal{M}_W(\Gamma)$ by

$$\hat{A}(\gamma)(v) := \tilde{\mathcal{R}}_\gamma A(\delta_1^v)(1)\,, \tag{3.2}$$

where $\gamma \in \Gamma$, $v \in H$ (such that $\hat{A}(\gamma) \in \mathcal{L}(H)$), and $\delta_1^v \in L^2(\Gamma,H)$ is given by

$$\delta_1^v(\gamma) = \begin{cases} v\,, & \gamma = 1\,, \\ 0 & \text{otherwise.} \end{cases} \tag{3.3}$$

The following properties are easily checked.

Lemma 3 *1) For $\gamma \in \Gamma$, $K \in \mathcal{K}(H)$ we have*

$$\widehat{\tilde{L}_\gamma \otimes K}(\gamma') = \begin{cases} K\,, & \gamma = \gamma'\,. \\ 0 & \textit{otherwise.} \end{cases}$$

2) For $A \in \mathcal{M}_W(\Gamma)$ and $\tau \in L^2(\Gamma,H)$, $\gamma \in \Gamma$,

$$A\tau(\gamma) = \sum_{\gamma'\in\Gamma} X(\gamma',\gamma)\hat{A}(\gamma\gamma'^{-1})(\tau(\gamma'))\,.$$

3) For $A \in \mathcal{M}_W(\Gamma)$, $\gamma \in \Gamma$

$$\widehat{A^*}(\gamma) = (\hat{A}(\gamma^{-1}))^* .$$

4) For $A, B \in \mathcal{M}_W(\Gamma)$, $\gamma \in \Gamma$

$$\widehat{AB}(\gamma) = \sum_{\gamma'} X(\gamma', \gamma)\hat{A}(\gamma\gamma'^{-1})\hat{B}(\gamma') ,$$

in particular

$$\widehat{A^*A}(1) = \sum_{\gamma} \hat{A}(\gamma)^*\hat{A}(\gamma) .$$

5) For $A \in \mathcal{M}_W(\Gamma)$ we have

$$\|A\| \leq \sum_{\gamma \in \Gamma} \|\hat{A}(\gamma)\| .$$

Proof Properties 1) through 4) follow by straightforward computations. 5) follows from the arguments in [1, Lemma 3]. □

Thus we arrive at the crucial

Lemma 4 *If D is a gauge-periodic symmetric elliptic differential operator in $L^2(E)$, of even order $\rho > m$, then*

$$e^{-D} \in \mathcal{C}_W(\Gamma, \mathcal{K}) .$$

Proof We have $e^{-D} \in \mathcal{M}_W(\Gamma)$ by assumption, and it is easily computed that for $v \in H = L^2(E \mid \mathcal{D})$, $p \in \mathcal{D}$, and $A := \Phi e^{-D} \Phi^{-1}$ one has

$$\hat{A}(\gamma)(v)(p) = \int_{\mathcal{D}} e^{-D}(p, \gamma q)\gamma_* v(q) d\,\mathrm{vol}_M(q) . \tag{3.4}$$

Thus all Fourier coefficients are compact.

In Γ we introduce the minimal word length with respect to a fixed finite set of generators; this defines a translation invariant metric, d_Γ, on $\Gamma \times \Gamma$. Then there is a constant, C_5, such that

$$d_\Gamma(\gamma_1, \gamma_2) \leq C_5 (\inf_{p,q \in \mathcal{D}} d_M(\gamma_1 p, \gamma_2 q) + 1) . \tag{3.5}$$

Now we put $r(\gamma) := d_\Gamma(\gamma, 1)$ and observe that

$$\sharp\{\gamma \in \Gamma \mid r(\gamma) \leq R\} \leq C_6 e^{C_7 R} .$$

Then the estimate (2.10) implies that

$$\sum_{\gamma \in \Gamma} \|\hat{A}(\gamma)\| < \infty .$$

Combining this with Lemma 3, 1) and 5), we reach the desired conclusion. □

It remains to define tr_Γ. We put, for $A \in \mathcal{M}_W(\Gamma)^+ :=$ the positive part of $\mathcal{M}_W(\Gamma)$,

$$\mathrm{tr}_\Gamma A := \mathrm{tr}_H \hat{A}(1) . \tag{3.6}$$

It follows from Lemma 3, 4) that tr_Γ is a faithful trace on $\mathcal{M}_W(\Gamma)$, hence on $\mathcal{C}_W(\Gamma, \mathcal{K})$. Now if $\lambda_1 > \lambda_2$ are real numbers, and D is a gauge-periodic symmetric elliptic operator with spectral resolution $D = \int_{-\infty}^{+\infty} \lambda dE_\lambda$, then $E_{\lambda_1} - E_{\lambda_2}$ is an integral operator with smooth kernel [4]. It follows as in (3.4) that

$$\mathrm{tr}_\Gamma(E_{\lambda_1} - E_{\lambda_2}) = \int_{\mathcal{D}} \mathrm{tr}_{E_p}(E_{\lambda_1} - E_{\lambda_2})(p,p) d\,\mathrm{vol}_M(p) . \tag{3.7}$$

Thus we arrive at

Lemma 5 *For any gauge-periodic symmetric elliptic operator D and real numbers $\lambda_1 > \lambda_2$ we have an estimate*

$$0 \leq \mathrm{tr}_\Gamma(E_{\lambda_1} - E_{\lambda_2}) \leq C(\lambda_1, \lambda_2, D) . \tag{3.8}$$

The dependence on D is only through the coefficients and their derivatives in an arbitrary neighborhood of $\bar{\mathcal{D}}$.

4. Proof of Theorem 1 and Theorem 2

The proof of Theorem 1 now follows from Lemmas 4 and 5, precisely as the proof of [1, Theorem 1].

Proof of Theorem 2 Fix $\lambda_1 > \lambda_2$ not in spec D_A, and restrict the magnetic field to $|b| \leq C_1$. Then we obtain from Lemma 5

$$\mathrm{tr}_\Gamma(E_{\lambda_1} - E_{\lambda_2}) \leq C(\lambda_1, \lambda_2, C_1) . \tag{3.9}$$

The theorem will thus be proved if we can show that

$$C_W(\Gamma) \geq 1/q , \tag{3.10}$$

if $b = 2\pi\theta$ and $\theta = p/q$, $(p,q) = 1$. To prove (3.10) we introduce the (universal) rotation algebra $\mathcal{A}_\theta$, with generators u, v satisfying

$$vu = e^{2\pi\sqrt{-1}\,\theta} uv =: \mu\, uv . \tag{3.11}$$

Recall that $\mathcal{A}_\theta$ admits a canonical action of $T^2 = S^1 \times S^1 \ni (w_1, w_2) =: w \mapsto \alpha_w \in \operatorname{Aut} \mathcal{A}_\theta$ such that $\alpha_w u = w_1 u$, $\alpha_w v = w_2 v$. We will also need a distinguished irreducible representation,

$$\begin{aligned}
&\pi : \mathcal{A}_\theta \to M(q, \mathbf{C}), \\
&\pi(u) = \operatorname{diag}(1, \mu, \ldots, \mu^{q-1}),\ \pi(v) \text{ cyclic permutation of} \\
&\text{the standard basis.}
\end{aligned} \tag{3.12}$$

Finally, denote by $\varphi : \mathcal{A}_\theta \times \mathcal{K} \to \mathcal{C}_W(\Gamma)$ the representation sending $u \otimes K$ to $\tilde{L}_{e_1} \otimes K$ and $v \otimes K$ to $\tilde{L}_{e_2} \otimes K$. Then we claim that for all $A \in \mathcal{A}_\theta \otimes K$ with $\operatorname{tr}_\Gamma \varphi(A)$ finite we have

$$\operatorname{tr}_\Gamma \varphi(A) = q^{-1} \int_{T^2} \operatorname{tr}_{\mathbf{C}^q \otimes H} (\pi \otimes I \circ \alpha_w \otimes I)(A) dw\,, \tag{3.13}$$

where dw is normalized Haar measure on T^2. To prove (3.13) we only have to observe that

$$\widehat{\varphi(A)}(0,0) = \int_{T^2} (\alpha_w \otimes I)(A) dw\,.$$

Since φ is an isomorphism, (3.13) implies (3.10) and the proof is complete. $\square$

References

[1] J. Brüning and T. Sunada: *On the spectrum of periodic elliptic operators.* Nagoya Math. J. **126** (1992), 159-171

[2] M.-D. Choi, G. Elliott and N. Yui: *Gauss polynomials and the rotation algebra.* Invent. Math. **99** (1990), 225–246

[3] B. Helffer and J. Sjöstrand: *Analyse semi-classique pour l' équation de Harper.* Suppl. Bull. Soc. Math. France, Mémoire **34** (1988)

[4] L. Hörmander: *The spectral function of an elliptic operator.* Acta Math. **121** (1968), 193–218

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Graded C^*-algebras and many-body perturbation theory : II. The Mourre estimate

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Graded C^*-Algebras and Many-Body Perturbation Theory: II. The Mourre Estimate

Anne Boutet de Monvel-Berthier and Vladimir Georgescu [1]

1. Introduction

We have introduced in [BG 1,2] the notion of graded C^*-algebra with the purpose of obtaining a natural framework for the description and study of hamiltonians with a many-channel structure. If H is a self-adjoint operator in a Hilbert space $\mathscr{H}$, the expression "H has a many-channel structure" is not mathematically well defined, although in examples of physical interest the meaning is rather obvious. Spectral theory alone is not enough in order to decide whether H is a many-channel hamiltonian or not. Usually the distinction is acquired with the help of scattering theory through the introduction of the channel wave operators. However, there are results (like the HVZ theorem which describes the essential spectrum of a N-body hamiltonian in terms of the spectra of the subsystems) which are outside the scope of scattering theory but should belong to a general theory of "many-channel hamiltonians". Our proposal in [BG 1,2] was to define the many-channel character of a self-adjoint operator H by its affiliation to a C^*-algebra provided with a graduation which allows one to describe a "subsystem structure" for the system whose hamiltonian is H. From our point of view, the main object associated to the physical system is a graded C^*-algebra, the possible dynamics are given by self-adjoint operators H affiliated to it, and we are interested in assertions independent of the explicit form of H.

Our purpose here is to show that the Mourre estimate fits very nicely in such a framework. Given two self-adjoint operators H, A such that the commutator [H,A] is a continuous sesquilinear form on D(H), we associate to them a function $\rho:\mathbb{R}\to]-\infty,+\infty]$ in terms of which the property of A of being locally conjugated to H is easily described. If the action of the unitary group associated to A is compatible in some sense with the grading of the C^*-algebra and if this algebra has a property which we call reducibility, then the ρ-function associated to H can be estimated in terms of the ρ-functions associated to "sub-hamiltonians". Our arguments are inspired from those of Froese and Herbst [FH], but the main point here is that the explicit form of H is never used, but only its affiliation to the algebra. In particular, in the N-body case H could be of the form described in

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[1] Lecture delivered by V. Georgescu

Proposition 7 of [BG 2] (see also section 2 below; this class is more general than the class of dispersive hamiltonians of [D2] and [G]) or it could be a hamiltonian with hard core interactions (this situation is treated in a joint work with A.Soffer, paper in preparation). We shall explicitely calculate the ρ-function (and so get the result of [PSS] and [FH]) for Agmon hamiltonians using theorem 3.4 which gives the ρ-function of an operator $H = H_1 \otimes 1 + 1 \otimes H_2$ in terms of those of H_j assuming that A is similarly decomposable. Theorems 3.4 and 4.4 are, technically speaking the main results of this paper, the applications to hamiltonians affiliated to the N-body C^*-graded algebra, being only an example (in this context theorem 2.1 being important)

In the rest of this section we shall recall the framework introduced in [BG1,2]. Some more specific properties of what we call the N-body C^*-graded algebra are studied in section 2. In section 3 we introduce in a more general setting the ρ-functions (which are more systematically studied in [ABG 2]) and prove the first important result, formula (3.8). Finally, in section 4 we define the reducible algebras and show how a Mourre estimate is proved for hamiltonians affiliated to such algebras.

We recall now the definition of a C^*-graded algebra as introduced in [BG1,2]. Let $\mathscr{A}$ be a C^*-algebra and $\mathscr{L}$ a finite lattice, i.e. a finite partially ordered set such that the upper bound $Y \vee Z$ and the lower bound $Y \wedge Z$ of each pair $Y, Z \in \mathscr{L}$ exists. We shall denote $\mathbf{O}$ (resp. X) the least (resp. the biggest) element of $\mathscr{L}$. We say that $\mathscr{A}$ *is a* $\mathscr{L}$*-graded* C^**-algebra* if a family $\{\mathscr{A}(Y)\}_{Y \in \mathscr{L}}$ of C^*-subalgebras of $\mathscr{A}$ is given such that

(i) $\mathscr{A} = \Sigma\{\mathscr{A}(Y) \mid Y \in \mathscr{L}\}$, the sum being direct (as linear spaces);

(ii) $\mathscr{A}(Y)\mathscr{A}(Z) \subset \mathscr{A}(Y \vee Z)$ for all $Y, Z \in \mathscr{L}$.

One can introduce such a notion for infinite $\mathscr{L}$ also (then $\Sigma\{\mathscr{A}(Y) \mid Y \in \mathscr{L}\}$ is only dense in $\mathscr{A}$) and an interesting example of such an object will appear in the next section.

We can put in evidence a *filtration* of $\mathscr{A}$ by a family $\{\mathscr{A}_Y\}_{Y \in \mathscr{L}}$ of C^*-subalgebras by defining $\mathscr{A}_Y = \Sigma\{\mathscr{A}(Z) \mid Z \leq Y\}$. Then $\mathscr{A}_Y \subset \mathscr{A}_Z$ if $Y \leq Z$ and $\mathscr{A}_X = \mathscr{A}$. If we denote $\mathscr{L}(Y) = \{Z \in \mathscr{L} \mid Z \leq Y\}$, then $\mathscr{L}(Y)$ is a finite lattice also and $\mathscr{A}_Y$ is a $\mathscr{L}(Y)$-graded C^*-algebra in a canonical way. Finally, observe that $\mathscr{A}(X)$ is a $*$-ideal in $\mathscr{A}$ (so $\mathscr{A}(Y)$ is a $*$-ideal in $\mathscr{A}_Y$), and if we denote $\mathscr{B}_Y = \Sigma\{\mathscr{A}(Z) \mid Z \not\leq Y\}$, then $\{\mathscr{B}_Y\}_{Y \in \mathscr{L}}$ is a decreasing family of closed $*$-ideals in $\mathscr{A}$ such that $\mathscr{A} = \mathscr{A}_Y + \mathscr{B}_Y$ (algebraic direct sum) for all $Y \in \mathscr{L}$.

For each $Y \in \mathscr{L}$ we shall denote $\mathscr{P}(Y)$, $\mathscr{P}_Y$ the projection operators of $\mathscr{A}$ onto $\mathscr{A}(Y)$, resp. $\mathscr{A}_Y$, associated to the direct sum decompositions $\mathscr{A} = \Sigma\{\mathscr{A}(Y) \mid Y \in \mathscr{L}\}$

resp. $\mathcal{A}=\mathcal{A}_Y+\mathcal{B}_Y$. More precisely, if $S\in\mathcal{A}$, then one can write it in a unique way as a sum $S=\Sigma\{S(Y)\mid Y\in\mathcal{L}\}$ with $S(Y)\in\mathcal{A}(Y)$. Then $\mathcal{P}(Y)(S)=S(Y)$. Obviously $\mathcal{P}_Y=\Sigma\{\mathcal{P}(Z)\mid Z\leq Y\}$, which is equivalent to $\mathcal{P}(Y)=\Sigma\{\mathcal{P}_Z\,\mu(Z,Y)\mid Z\leq Y\}$, where $\mu:\mathcal{L}\times\mathcal{L}\to\mathbb{Z}$ is the Möbius function of $\mathcal{L}$. Clearly each $\mathcal{P}(Y):\mathcal{A}\to\mathcal{A}$ is a linear, continuous projection (i.e.$\mathcal{P}(Y)^2=\mathcal{P}(Y)$) which commutes with the involution. But the main point is that $\mathcal{P}_Y:\mathcal{A}\to\mathcal{A}$ *is a linear, continuous projection which is also a* $*$*-homomorphism of* $\mathcal{A}$ *onto* $\mathcal{A}_Y$. In particular, if $S\in\mathcal{A}$ is a normal element and f is a complex continuous function on the spectrum of S (which vanishes at zero if $\mathcal{A}$ has not unit) then $\mathcal{P}_Y(f(S))=f(\mathcal{P}_Y(S))$. Observe that $\mathcal{B}_Y=\ker\mathcal{P}_Y$, which gives a new proof of the fact that $\mathcal{B}_Y$ is a closed $*$-ideal in $\mathcal{A}$.

Let $\mathcal{A}$ be an arbitrary C^*-algebra realised on a Hilbert space $\mathcal{H}$ (i.e. $\mathcal{A}$ is a C^*-subalgebra of $B(\mathcal{H})$, the space of bounded linear operators in $\mathcal{H}$) and H a self-adjoint operator in $\mathcal{H}$. Denote $C_\infty(\mathbb{R})$ the abelian C^*-algebra of complex continuous functions on $\mathbb{R}$ which tend to zero at infinity (with the sup norm). Then $(\lambda-H)^{-1}\in\mathcal{A}$ for some complex λ if and only if $f(H)\in\mathcal{A}$ for all $f\in C_\infty(\mathbb{R})$. If this is fulfilled, we shall say that H *is affiliated to* $\mathcal{A}$. In some applications it is useful to work with *self-adjoint but non-densely defined operators in* $\mathcal{H}$. By this we mean that a closed subspace $\mathcal{K}$ of $\mathcal{H}$ and a self-adjoint densely defined operator H in $\mathcal{K}$ are given (so $\mathcal{K}$ is the closure of the domain of H in $\mathcal{H}$; think, formally, that $H=\infty$ on $\mathcal{H}\ominus\mathcal{K}$). Let then $R(\lambda)=(\lambda-H)^{-1}$ on $\mathcal{K}$ and $R(\lambda)=0$ on $\mathcal{H}\ominus\mathcal{K}$, for $\lambda\in\mathbb{C}\setminus\mathbb{R}$. Clearly, the family $\{R(\lambda)\mid\lambda\in\mathbb{C}\setminus\mathbb{R}\}$ of bounded operators in $\mathcal{H}$ is a pseudo-resolvent, i.e. $R(\lambda)^*=R(\lambda^*)$ and $R(\lambda_1)-R(\lambda_2)=(\lambda_2-\lambda_1)R(\lambda_1)R(\lambda_2)$. In fact, as shown in [HP], there is a bijective correspondence between (not necessarily densely defined) self-adjoint operators in $\mathcal{H}$ and pseudo-resolvents on $\mathcal{H}$ (or spectral measures E such that $E(\mathbb{R})\neq 1$). Using Stone-Weierstrass theorem, it is trivial to establish a bijective correspondence between pseudo-resolvents and $*$-homomorphisms $\phi:C_\infty(\mathbb{R})\to B(\mathcal{H})$ (put $R(\lambda)=\phi(r_\lambda)$ where $r_\lambda(x)=(\lambda-x)^{-1}$). Clearly $\phi(f)|_{\mathcal{K}}=f(H)$ and $\phi(f)|_{\mathcal{H}\ominus\mathcal{K}}=0$.

As a conclusion of this discussion, if $\mathcal{A}$ is an arbitrary C^*-algebra, a $*$-homomorphism $\phi:C_\infty(\mathbb{R})\to\mathcal{A}$ will be called *self-adjoint operator affiliated to* $\mathcal{A}$. As above, to give ϕ is equivalent to giving a pseudo-resolvent $\{R(\lambda)\mid\lambda\in\mathbb{C}\setminus\mathbb{R}\}$ with $R(\lambda)\in\mathcal{A}$. We shall use in such a case a symbol H and denote $\phi(f)=f(H)$ for $f\in C_\infty(\mathbb{R})$ and $R(\lambda)=(\lambda-H)^{-1}$. When $\mathcal{A}$ is realised in a Hilbert space $\mathcal{H}$, then H is realised as a (non-densely defined in general) self-adjoint operator in $\mathscr{H}$. If $\mathscr{A}_1$ is another C^*-algebra and $\mathscr{P}:\mathscr{A}\to\mathscr{A}_1$ is a $*$-homomorphism then $\mathscr{P}\phi:C_\infty(\mathbb{R})\to\mathscr{A}_1$ is a $*$-homomorphism which defines a self-adjoint operator H_1 affiliated to $\mathscr{A}_1$. We shall denote $H_1=\mathscr{P}(H)$.

Let us go back now to our $\mathscr{L}$-graded C^*-algebra $\mathscr{A}$. For each self-adjoint operator H affiliated to $\mathscr{A}$ and each $Y\in\mathscr{L}$ we may consider the self-adjoint operator H_Y affiliated to $\mathscr{A}_Y$ defined by $H_Y=\mathscr{P}_Y(H)$ (i.e. $f(H_Y)=\mathscr{P}_Y(f(H))$ for all $f\in C_\infty(\mathbb{R})$). Observe that $H_X=H$. If H is just an element of $\mathscr{A}$, then $H_Y=\mathscr{P}_Y(H)$ is just the projection of H onto $\mathscr{A}_Y$. If $\mathscr{A}$ is realised on a Hilbert space $\mathscr{H}$ and H is the hamiltonian of a system (i.e. e^{-iHt} describes the time evolution of the system), then the H_Y's will be called sub-hamiltonians (they describe the evolution of the system when parts of the interaction have been suppressed). Observe that each H_Y (and $H=H_X$) has its own domain $D(H_Y)$ which is not dense in $\mathscr{H}$ in general. In the many-body case with hard-core interactions, D(H) is not dense, $D(H_{\mathbf{O}})$ is dense and $D(H_Y)$ for $Y\neq\mathbf{O}$, X is sometimes dense and sometimes not. If H_Y is densely defined for all Y, we shall say that the densely defined self-adjoint operator H in $\mathscr{H}$ is $\mathscr{L}$-affiliated to $\mathscr{A}$. Such operators are easy to construct using the following criterion. Let $H_{\mathbf{O}}=H(\mathbf{O})$ by a densely defined self-adjoint operator in $\mathscr{H}$ affiliated to $\mathscr{A}_{\mathbf{O}}=\mathscr{A}(\mathbf{O})$. For each $Y\neq\mathbf{O}$, let H(Y) be a symmetric, $H_{\mathbf{O}}$-bounded operator in $\mathscr{H}$ with relative bound zero and such that $H(Y)(H_{\mathbf{O}}+i)^{-1}\in\mathscr{A}(Y)$. Then $H=\Sigma\{H(Y)\,|\,Y\in\mathscr{L}\}$ is self-adjoint and $\mathscr{L}$-affiliated to $\mathscr{A}$. Moreover, for all $Y\in\mathscr{L}$, we have $H_Y=\mathscr{P}_Y(H)=\Sigma\{H(Z)\,|\,Z\leq Y\}$. If $H_{\mathbf{O}}$ is bounded below, then it is enough that H(Y) be $H_{\mathbf{O}}$-form bounded with relative bound zero and for c large enough $(H_{\mathbf{O}}+c)^{-1/2}H(Y)(H_{\mathbf{O}}+c)^{-1/2}\in\mathscr{A}(Y)$.

We stop here this accumulation of definitions. In [BG 2] these notions are used in the spectral theory of N-body systems. For example, we show that the Weinberg-Van Winter equation and the HVZ theorem are very natural in this framework (both the statements and the proofs).

2. The N-body Algebra

In this section we shall describe some important properties of a graded C^*-algebra canonically associated to an Euclidean space (in place of the usual N-body formalism, we prefer to work in the geometrical setting first considered by Agmon, Froese and Herbst and systematically developed in [ABG 1]).

Let E be an Euclidean space (finite dimensional real Hilbert space). We provide it with the unique translation invariant Borel measure such that the volume of a unit cube is $(2\pi)^{-(\dim E)/2}$. Then $\mathscr{H}(E)$ is the Hilbert space $L^2(E)$ and the Fourier transform $(\mathscr{F} f)(x)=\int_E e^{-i(x|y)}f(y)dy$ induces a unitary operator in $\mathscr{H}(E)$. Denote $\mathbf{B}(E)=B(\mathscr{H}(E))$. If $E=\mathbf{O}\equiv\{0\}$ then $\mathscr{H}(\mathbf{O})=\mathbb{C}$ and $\mathscr{F}=1$. For any Borel function $f:E\to\mathbb{C}$ we denote $f(Q)$ the operator of multiplication by f and $f(P)=\mathscr{F}^*f(Q)\mathscr{F}$. Then $\mathbf{K}(E)$ will be the C^*-algebra of compact operators on $\mathscr{H}(E)$ and $\mathbf{T}(E)$ the C^*-algebra of operators of the form $f(P)$ with $f:E\to\mathbb{C}$ continuous and convergent to zero at infinity (i.e. $f\in C_\infty(E)$). By convention $\mathbf{K}(\mathbf{O})=\mathbf{T}(\mathbf{O})=\mathbb{C}$.

If E,F are Euclidean spaces and $G=E\oplus F$ is their euclidean direct sum, then there is a canonical isomorphism of $\mathscr{H}(E)\otimes\mathscr{H}(F)$ (Hilbert tensor product) with $\mathscr{H}(G)$. For $S\in\mathbf{B}(E)$, $T\in\mathbf{B}(F)$ we write $S\otimes_E^G T$ for the operator in $\mathbf{B}(G)$ corresponding to $S\otimes T$ by the preceding isomorphism. Finally, if $\mathscr{M}\subset\mathbf{B}(E)$, $\mathscr{N}\subset\mathbf{B}(F)$ are $*$-subalgebras, then we denote $\mathscr{M}\hat{\otimes}_E^G\mathscr{N}$ the C^*-algebra on $\mathscr{H}(G)$ obtained as the norm-closure of the linear space generated by the operators of the form $S\otimes_E^G T$ with $S\in\mathscr{M}, T\in\mathscr{N}$.

Now let us fix an Euclidean space X and denote $\Pi(X)$ the set of all subspaces of X provided with the natural order relation (inclusion). Then $\Pi(X)$ is a complete lattice with $\mathbf{O}$, resp. X, as least, resp. biggest, element. For $Y,Z\in\Pi(X)$ we have $Y\vee Z=Y+Z$ and $Y\wedge Z=Y\cap Z$. Let $Y\in\Pi(X)$ and $Y^\perp\in\Pi(X)$ its orthogonal. Then $Y,Y^\perp$ are Euclidean spaces, $X=Y\oplus Y^\perp$ and we abbreviate $\otimes_Y^X=\otimes_Y$. We shall be interested in the C^*-subalgebras of $\mathbf{B}(X)$ defined by

$$(2.1)\qquad \mathscr{T}(Y)=\mathbf{K}(Y)\hat{\otimes}_Y\mathbf{T}(Y^\perp).$$

The family $\{\mathscr{T}(Y)|\ Y\in\Pi(X)\}$ has the following properties:

(i) The algebraic sum $\Sigma\{\mathscr{T}(Y)\,|\,Y\in\Pi(X)\}$ is direct i.e. each element S in the linear subspace of $\mathbf{B}(X)$ generated by $\cup\{\mathscr{T}(Y)\,|\,Y\in\Pi(X)\}$ can be *uniquely* written as a sum $S=\Sigma\{S(Y)\,|\,Y\in\Pi(X)\}$ with $S(Y)\in\mathscr{T}(Y)$ and $S(Y)\neq 0$ only for a finite number of Y's.

(ii) For all $Y,Z\in\Pi(X)$ we have: $\mathscr{T}(Y)\mathscr{T}(Z)\subset\mathscr{T}(Y+Z)$.

For proofs of the first, resp. second, assertion, see [BG 2], resp. [ABG 1].

In particular, the $*$-subalgebra $\Sigma\{\mathscr{T}(Y)\,|\,Y\in\Pi(X)\}$ of $\mathbf{B}(X)$ is $\Pi(X)$-graded in a natural sense. It is obviously not norm-closed, and *we shall denote* $\mathscr{T}$ *its closure.* This is the graded C^*-algebra canonically associated to X we were talking about at the beginning of this section.

For the N-body problem only subalgebras of $\mathscr{T}$ of the following type are needed. Let $\mathscr{L}\subset\Pi(X)$ be a finite family of subspaces of X such that $\mathbf{O},X\in\mathscr{L}$ and $Y+Z\in\mathscr{L}$ if $Y,Z\in\mathscr{L}$ (so $\mathscr{L}$ is *not* a sub-lattice of $\Pi(X)$, because $Y\cap Z\notin\mathscr{L}$ in general; however, $\mathscr{L}$ is a lattice for the order relation induced by $\Pi(X)$). Denote:

(2.2) $\quad \mathscr{A}=\Sigma\,\{\mathscr{T}(Y)\,|\,Y\in\mathscr{L}\}.$

Then $\mathscr{A}$ is a C^*-subalgebra of $\mathscr{T}$ which is also a $\mathscr{L}$-graded C^*-algebra (in the notation we do not mention the dependence on $\mathscr{L}$, which is considered fixed from now on). Let us mention that the projection $\mathscr{P}_Y$ of $\mathscr{T}$ onto the subalgebra $\mathscr{A}_Y=\Sigma\{\mathscr{T}(Z)\,|\,Z\in\mathscr{L},Z\subset Y\}$ can be explicitely described as follows. Assume $Y\neq X$ and denote Y^+ the set of elements of $Y^\perp$ which do not belong to any $Z^\perp$ with $Z\in\mathscr{L}$, $Z\not\subset Y$. Then Y^+ is a dense cone in $Y^\perp$ and for any $\omega\in Y^+$ we have $\mathscr{P}_Y(S)=\text{s-lim}_{\lambda\to\infty}e^{-i\lambda(P,\omega)}Se^{i\lambda(P,\omega)}$ for all $S\in\mathscr{A}$.

Let us explain in what sense the choice of $\mathscr{L}$ corresponds to the N-body problem. Define, inductively, $\mathscr{L}_1=\mathscr{L}$, $\mathscr{L}^1=\{X\}$; $\mathscr{L}_2=\mathscr{L}_1\backslash\mathscr{L}^1$, $\mathscr{L}^2$=the set of maximal elements of $\mathscr{L}_2$; $\mathscr{L}_3=\mathscr{L}_2\backslash\mathscr{L}^2$, $\mathscr{L}^3$=the set of maximal elements of $\mathscr{L}_3$; etc.... Then, N is the integer defined by $\mathscr{L}_N=\{\mathbf{O}\}$. For example, the two-body problem corresponds to $\mathscr{L}=\{\mathbf{O},X\}$ and the characteristic C^*-algebra is $\mathscr{A}=\mathbf{T}(X)+\mathbf{K}(X)$ (direct sum). The (generalized) three-body problem is described by $\mathscr{L}=\{\mathbf{O},Y_1,...,Y_n,X\}$ where Y_j are subspaces such that $\mathbf{O}\neq Y_j\neq X$ and $Y_i+Y_j=X$ if $i\neq j$ (hence $Y_i\not\subset Y_j$ for $i\neq j$; observe that one could have $Y_i\cap Y_j\neq\mathbf{O}$, but $Y_i\wedge Y_j=\mathbf{O}$ in $\mathscr{L}$). The characteristic C^*-algebra in such a case is $\mathscr{A}=\mathbf{T}(X)+\mathscr{T}(Y_1)+...+\mathscr{T}(Y_n)+\mathbf{K}(X)$ (direct sum) and if $S_i\in\mathscr{T}(Y_i)$ then $S_iS_j\in\mathbf{K}(X)$ if $i\neq j$. The complications which appear for $N\geq4$ are due to the "nested" structure of $\mathscr{L}$.

A large class of (densely defined) self-adjoint operators $\mathscr{L}$-affiliated to the algebra $\mathscr{A}$ is described in Proposition 7 of [BG 2]. Very roughly, they are of the form $H=h(P)+\Sigma\{V_Y(Q_Y,P)\,|\,Y\in\mathscr{L},Y\neq\mathbf{O}\}$ where $h:X\to\mathbb{R}$ is a continuous function divergent at infinity and Q_Y is the projection on Y of Q, so that $\mathscr{F}V_Y\mathscr{F}^*$ is, in the representation $\mathscr{H}(X)\cong L^2(Y^\perp,\mathscr{H}(Y))$, the operator of multiplication by an operator-valued function.

In the rest of this section we shall isolate some properties of the algebra $\mathscr{T}$ related to the *"geometric"* methods introduced by Simon [S] in the N-body problem and further refined in [PSS] and [FH].

THEOREM 2.1: *Let* $\chi: X \to \mathbb{C}$ *be continuous and homogeneous of degre zero outside the unit sphere* (i.e. $\chi(x)=\chi(x/|x|)$ *if* $|x|\geq 1$). *Then* $[S,\chi(Q)]$ *is a compact operator for each* $S \in \mathscr{T}$. *If* $S \in \mathscr{T}(Z)$ *for some* $Z \in \Pi(X)$ *and* $\chi(e)=0$ *for* $e \in Z^{\perp}$, $|e|=1$, *then both* $S\chi(Q)$ *and* $\chi(Q)S$ *are compact operators.*

Proof: Observe first that for each $M<\infty$ there is $c>0$ such that if $|y| \leq M$:

$$(2.3) \qquad |\chi(x+y)-\chi(x)| = \left|\chi\left(\tfrac{x+y}{|x+y|}\right)-\chi\left(\tfrac{x}{|x|}\right)\right| \leq w\left(\tfrac{c}{|x|}\right)$$

for x large enough, where w is the modulus of continuity of the restriction of χ to the unit sphere. It is clearly enough to prove the theorem for S of the form $K\otimes_Z T$ with $K\in \mathbf{K}(Z)$ and $T \in \mathbf{T}(Z^{\perp})$. Let $\chi_0(x) = \chi(\pi_Z^{\perp}(x))$ where $\pi_Z^{\perp}$ is the orthogonal projection of X onto $Z^{\perp}$. Then $\chi_0(Q)=1\otimes_Z \Phi$ where Φ is the operator of multiplication by $\chi|_{Z^{\perp}}$ in $\mathscr{H}(Z^{\perp})$. From (2.3) and a result of Cordes [C] it follows that $[T,\Phi]$ is compact in $\mathscr{H}(Z^{\perp})$. So $[S,\chi_0(Q)]=K\otimes_Z[T,\Phi]$ is compact in $\mathscr{H}(X)$.

Writing $[S,\chi(Q)]=[S,\chi(Q)-\chi_0(Q)]+[S,\chi_0(Q)]$ and observing that $\chi(x)-\chi_0(x)=0$ if $x\in Z^{\perp}$, it follows that it is enough to prove the second part of the proposition for bounded uniformly continuous functions $\chi:X\to\mathbb{C}$ such that $|\chi(z+z')| \to 0$ as $|z'|\to \infty$, $z'\in Z^{\perp}$, uniformly in z when z runs over any compact subset of Z (use (2.3) to show that this is fulfilled by $\chi-\chi_0$ or by the initial χ if $\chi(e)=0$ for $e\in Z^{\perp}$, $|e|=1$). Let us show for example that $S\chi(Q)=(1\otimes_Z T)(K\otimes_Z 1\cdot\chi(Q))$ is compact. In the representation $\mathscr{H}(X)\cong L^2(Z^{\perp};\mathscr{H}(Z))$, the operator $K\otimes_Z 1\cdot\chi(Q)$ becomes the operator of multiplication by the function $z'\mapsto K\psi(z')\in \mathbf{B}(Z)$ where $(\psi(z')u)(z)=\chi(z+z')u(z)$. Since χ is bounded and uniformly continuous, $\psi: Z^{\perp}\to\mathbf{B}(Z)$ is bounded and norm-continuous. The last condition we put on χ is equivalent to $\text{s-lim}_{|z'|\to\infty}\psi(z')=0$. Since K is compact in $\mathscr{H}(Z)$ we get $\|K\psi(z')\|_{\mathbf{B}(Z)}\to 0$ as $|z'|\to\infty$. It is standard now to show that $K\otimes_Z 1\cdot\chi(Q)$ is the norm-limit in $\mathbf{B}(X)$ of operators of the form $\sum K_j\otimes_Z\Phi_j$ where $K_j\in\mathbf{K}(Z)$ and Φ_j is the operator of multiplication by a C_0^{∞} function in $\mathscr{H}(Z^{\perp})$. Since $(1\otimes_Z T)(K_j\otimes_Z\Phi_j)=K_j\otimes_Z(T\Phi_j)$ and $T\Phi_j\in\mathbf{K}(Z^{\perp})$, the proof is finished. ■

Remark: The fact that $[S,\chi(Q)]$ is compact for $S\in\mathscr{T}$ shows that $\mathscr{T}$ is a non-trivial subalgebra (and a rather small one) of $\mathbf{B}(X)$.

Let us go back to the N-body algebra $\mathscr{A}$ associated to some semi-lattice $\mathscr{L}\subset\Pi(X)$ as in (2.2). Let $Y\in\mathscr{L}$, $Y\neq X$. Following [FH] and [ABG 1], we shall call a function $\chi_Y:X\to\mathbb{R}$ *Y-reducing*, if it is continuous, homogeneous of degree zero outside the unit sphere and if $\chi_Y(e) = 0$ for all e such that $|e|=1$ and $e \in Z^\perp$ for some $Z \in \mathscr{L}$ with $Z\not\subset Y$. Recall that $\mathscr{B}_Y=\Sigma\{\mathscr{T}(Z) \mid Z\in \mathscr{L}, Z\not\subset Y\}$ is a norm-closed $*$-ideal in $\mathscr{A}$ and $\mathscr{A} = \mathscr{A}_Y+\mathscr{B}_Y$ direct sum. It follows from theorem 2.1 that for a Y-reducing function χ_Y we have (remark that $\mathscr{A}(X) = \mathbf{K}(X)$):

(i) $[S,\chi_Y(Q)] \in \mathscr{A}(X)$ for all $S \in \mathscr{A}$;

(ii) $S\chi_Y(Q)$ and $\chi_Y(Q)S$ belong to $\mathscr{A}(X)$ for all $S \in \mathscr{B}_Y$.

A family $\{\chi_Y\}_{Y\in\mathscr{L}}$ of functions $\chi_Y:X\to\mathbb{R}$ is called $\mathscr{L}$-reducing if $\chi_X=0$, each χ_Y is Y-reducing for $Y\neq X$ and $\Sigma\{\chi_Y^2 \mid Y\in\mathscr{L}\}=1$ on X. It is easy (see [ABG 1]), to construct such families having the supplementary properties:

(iii) $\chi_Y=0$ if Y is not a maximal element in $\mathscr{L}\setminus\{X\}$ (i.e. $\chi_Y\neq 0$ only for $Y\in\mathscr{L}^2$);

(iv) $\chi_Y \in C^\infty(X)$ and $\chi_Y(x)=0$ on a neighbourhood on the unit sphere of the set $\cup\{S_X\cap Z^\perp \mid Z \in \mathscr{L},\ Z\not\subset Y\}$.

Let us make a final remark concerning the structure of the algebra $\mathscr{T}$. It is convenient now to indicate explicitly the dependence on the space X by denoting $\mathscr{T}(Y)=\mathscr{T}^X(Y)$, $\mathscr{T}=\mathscr{T}^X$. Let $\mathscr{T}^X_Y$ be the norm-closure of $\Sigma\{\mathscr{T}^X(Z) \mid Z \in \Pi(X), Z\subset Y\}$ and $\mathscr{S}^X_Y$ the norm-closure of $\Sigma\{\mathscr{T}^X(Z) \mid Z\in \Pi(X),\ Z\not\subset Y\}$. So $\mathscr{T}^X_Y$ is a C^*-subalgebra of $\mathscr{T}^X$, $\mathscr{S}^X_Y$ is a norm-closed $*$-ideal and $\mathscr{T}^X_X = \mathscr{T}^X$. We would like to point out the following relations: for $Z,Y \in \Pi(X)$ such that $Z\subset Y$ we have

$$\mathscr{T}^X(Z)=\mathscr{T}^Y(Z)\hat{\otimes}_Y\mathbf{T}(Y^\perp). \tag{2.4}$$

In fact, if we denote $E=Y\cap Z^\perp$, then $Y=Z\oplus E$ and $Z^\perp=E\oplus Y^\perp$. It is clear that $\mathbf{T}(Z^\perp)=\mathbf{T}(E)\hat{\otimes}^{Z^\perp}_E\mathbf{T}(Y^\perp)$ so we get:

$$\mathscr{T}^X(Z)=\mathbf{K}(Z)\hat{\otimes}^X_Z(\mathbf{T}(E)\hat{\otimes}^{Z^\perp}_E\mathbf{T}(Y^\perp))=(\mathbf{K}(Z)\hat{\otimes}^Y_Z\mathbf{T}(E))\hat{\otimes}^X_Y\mathbf{T}(Y^\perp)=$$
$$=\mathscr{T}^Y(Z)\hat{\otimes}^X_Y\mathbf{T}(Y^\perp).$$

From (2.4) we also obtain:

$$\mathscr{T}^X_Y=\mathscr{T}^Y\hat{\otimes}_Y\mathbf{T}(Y^\perp). \tag{2.5}$$

Here we may specialize to the N-body algebra $\mathcal{A} \equiv \mathcal{A}^X$ associated to $\mathcal{L}$ with the convention that $\mathcal{A}_Y$ is constructed using $\mathcal{L}(Y)$. So:

(2.6) $\qquad \mathcal{A}_Y^X = \mathcal{A}_Y \hat{\otimes}_Y T(Y^\perp).$

To $\mathcal{A}_Y$, if $Y \neq 0$, we may associate a family $\{\chi_Z^Y\}_{Z \in \mathcal{L}(Y)}$ (with $\chi_Z^Y \neq 0$ only if $Z <\!\bullet Y$, i.e. Y covers Z) with $\chi_Z^Y : Y \to \mathbb{R}$ and then we may extend $\chi_{ZY} = \chi_Z^Y \otimes_Y 1$ (i.e. $\chi_{ZY} : X \to \mathbb{R}$ is given by $\chi_{ZY}(x) = \chi_Z^Y(\pi_Y(x))$. Observe that for each fixed $Y \in \mathcal{L} \setminus \{0\}$ we shall have $\Sigma\{\chi_{ZY}^2 \mid Z \in \mathcal{L}, Z <\!\bullet Y\} = 1$.

3. General Considerations on the Mourre Estimate

In this section we shall quit the graded C^*-algebra setting in order to present certain notions and results related to Mourre theory in the framework introduced in [ABG 1,2] and [BGM]. We do this step hopping that so we shall put in a better light the proof of the Mourre estimate for hamiltonians with a many channel structure.

Let $\mathcal{H}$ be a (complex, separable) Hilbert space and A a self-adjoint operator in $\mathcal{H}$. Denote $W_\alpha = e^{iA\alpha}$ the unitary group in $\mathcal{H}$ generated by A. We shall say that *a closed operator* T *in* $\mathcal{H}$ *is of class* $C^1(A)$, and we shall write $T \in C^1(A)$, if its domain D(T) is invariant under the group W and if for all $u \in D(T)$ the function $\alpha \mapsto \langle W_\alpha u | T W_\alpha u \rangle$ is of class C^1. In this case we denote [T,A] the sesquilinear form on D(T) given by $\langle u | i[T,A] u \rangle = \frac{d}{d\alpha} \langle W_\alpha | T W_\alpha \rangle |_{\alpha=0}$. Let $\mathcal{G} = D(T)$ equipped with the graph-norm. Then [T,A] is a continuous sesquilinear form on $\mathcal{G}$ and it is often useful to think of it as a continuous linear operator from $\mathcal{G}$ to its adjoint space $\mathcal{G}^*$. It is shown in [ABG 1] that, if $\mathcal{G}$ is invariant under W, then $T \in C^1(A)$ if and only if the sesquilinear forms $\left[T, \frac{1}{\alpha} W_\alpha\right]$ on $\mathcal{G}$ converge weakly when $\alpha \to 0$ and in this case:

(3.1) $\qquad i[T,A] = \text{s-}\lim_{\alpha \to 0} \left[T, \frac{1}{\alpha} W_\alpha\right],$

the strong limit being in $B(\mathcal{G}, \mathcal{G}^*)$. If the limit exists in norm in this space, then we write $T \in C_n^1(A)$; this is equivalent to the norm-derivability of $\alpha \mapsto W_\alpha^* T W_\alpha \in B(\mathcal{G}, \mathcal{G}^*)$. For bounded T we identify $B(\mathcal{G}, \mathcal{G}^*) = B(\mathcal{H})$.

We shall now associate to each self-adjoint operator H in $\mathscr{H}$ of class $C^1(A)$ two functions $\hat{\rho} \equiv \hat{\rho}_H^A$ and $\rho = \rho_H^A$ defined on $\mathbb{R}$ with values in $]-\infty,+\infty]$, according to the following rule. Denote $E(\lambda;\varepsilon)=E((\lambda-\varepsilon,\lambda+\varepsilon))$ for $\lambda \in \mathbb{R}$ and $\varepsilon>0$. Then

(3.2) $$\hat{\rho}_H^A(\lambda) = \sup\{a \in \mathbb{R} \mid \text{there is } \varepsilon>0 \text{ and a compact operator K such that } E(\lambda;\varepsilon)[iH,A]E(\lambda;\varepsilon) \geq aE(\lambda;\varepsilon)+K\},$$

(3.3) $$\rho_H^A(\lambda) = \sup\{a \in \mathbb{R} \mid \exists\varepsilon>0 \text{ such that } E(\lambda;\varepsilon)[iH,A]E(\lambda;\varepsilon) \geq aE(\lambda;\varepsilon)\}.$$

Another way of defining ρ_H^A is as follows. For $\varepsilon>0$, let

$$\rho_\varepsilon(\lambda) = \inf\{\langle u \mid [iH,A]u\rangle \mid u=E(\lambda;\varepsilon)u,\ \|u\|=1\}$$

(with the convention $\inf \emptyset=\infty$).Then $\rho_\varepsilon(\lambda)\to\rho(\lambda)$ as $\varepsilon\to+0$. Let us also mention the following fact. If $\lambda_0 \in \mathbb{R}$, then the spectral measure of the operator $H-\lambda_0$ is $S \longmapsto E(S+\lambda_0)$ ($S\subset\mathbb{R}$ Borel set). Hence we get $\rho_{H-\lambda_0}^A(\lambda)=\rho_H^A(\lambda+\lambda_0)$ and similarly for $\hat{\rho}$.

A systematic study of the functions ρ and $\hat{\rho}$ is presented in [ABG 2], from which we quote now some results. It is easy to show that ρ and $\hat{\rho}$ are lower semicontinuous (l.s.c.) functions, $\hat{\rho}(\lambda)<\infty$ if and only if $\lambda\in\sigma_{ess}(H)$ and $\hat{\rho}(\lambda)<\infty$ if and only if $\lambda\in\sigma(H)$. From the virial theorem we get that, if $\hat{\rho}(\lambda)>0$, then λ has a neighbourhood in which there is at most a finite number of eigenvalues (counting multiplicities). A deeper consequence of this theorem is the following result (implicitly contained in [FH] and explicitly isolated and proved in [ABG 2]).

PROPOSITION 3.1: *If λ is an eigenvalue of* H *and* $\rho(\lambda)>0$, *then* $\rho(\lambda)=0$. *Otherwise,* $\hat{\rho}(\lambda)=\rho(\lambda)$.

The next result is easy, but very useful in applications.

PROPOSITION 3.2: *Let $\Lambda\subset\mathbb{R}$ be a compact set and $\theta: \Lambda\to\mathbb{R}$ an upper semicontinuous function (u.s.c.) such that* $\theta(\lambda)<\rho(\lambda)$ *for all $\lambda\in\Lambda$. Then there is* $\varepsilon>0$ *such that for all $\lambda\in\Lambda$:*

(3.4) $$E(\lambda;\varepsilon)[iH,A]E(\lambda;\varepsilon) \geq \theta(\lambda)E(\lambda;\varepsilon).$$

Functions θ as in the last proposition play a role in the proof of the propagation theorems (see [D1] and [T]) but we shall need them in the proof of the theorem below. They are very easy to construct, as the next example shows (this explains corollary 4.3 from [D1]). For any $\nu>0$, let

(3.5) $$\theta_\nu(\lambda) = \inf_{|\mu-\lambda|<\nu} \rho(\mu)-\nu.$$

Then $\theta_v:\mathbb{R}\to]-\infty,+\infty]$ is upper semicontinuous, $\theta_{v_1}(\lambda)<\theta_{v_2}(\lambda)$ if $v_2<v_1$ and $\theta_{v_1}(\lambda)\neq\infty$, and $\lim_{v\to 0}\theta_v(\lambda)=\rho(\lambda)$ for all $\lambda\in\mathbb{R}$. Moreover, $\theta_v(\lambda)<\infty$ if $\mathrm{dist}(\lambda,\sigma(H))<v$. This choice is useful in abstract considerations, but a better one can be made in the case of Agmon hamiltonians. Let us mention that

$$\rho_v(\lambda)\leq \inf_{|\mu-\lambda|<v}\rho(\mu)\leq\rho(\lambda)$$

with ρ_v defined after (3.3).

We can introduce now the main concept of Mourre theory.

DEFINITION: *Let* H *be a self-adjoint operator in the Hilbert space* $\mathcal{H}$. *We shall say that a self-adjoint operator* A is conjugated to H at some point $\lambda\in\mathbb{R}$ *if* $H\in C^1(A)$ *and* $\hat{\rho}_H^A(\lambda)>0$.

In the graded C^*-algebra setting it is better to work only with bounded operators. So it is useful to be able to express the preceding property in terms of the resolvent of H.

PROPOSITION 3.3: *Let* H *and* A *be self-adjoint operators,* λ_0 *a complex number outside the spectrum of* H *and* $R=(\lambda_0-H)^{-1}$. *Assume that* $e^{iA\alpha}$ *leaves invariant the domain of* H. *Then* $H\in C^1(A)$ (resp. $H\in C_n^1(A)$) *if and only if* $R\in C^1(A)$ (resp. $R\in C_n^1(A)$). *In this case*

$$[R,A]=R[H,A]R. \tag{3.6}$$

Assume, moreover, that $\lambda_0\in\mathbb{R}$ *(so H has to have a spectral gap). Then, for all real* $\lambda\neq\lambda_0$, *we shall have*

$$\hat{\rho}_R^A((\lambda_0-\lambda)^{-1})=(\lambda_0-\lambda)^{-2}\hat{\rho}_H^A(\lambda). \tag{3.7}$$

In particular, A *is conjugated to* H *at some* $\lambda\in\mathbb{R}\setminus\{\lambda_0\}$ *if and only if it is conjugated to* R *at* $(\lambda_0-\lambda)^{-1}$.

Proof: Since $W_\alpha=e^{iA\alpha}$ leaves invariant the domain of H, it is easy to show that $[R,1/\alpha W_\alpha]=R[H,1/\alpha W_\alpha]R$. Denote $\mathcal{G}$ the domain of H (assumed dense without loss of generality) provided with the graph norm; then $\mathcal{G}\subset\mathcal{H}$ continuously and densely and, after identification of $\mathcal{H}$ with its adjoint space $\mathcal{H}^*$ using Riesz lemma, we get $\mathcal{G}\subset\mathcal{H}\subset\mathcal{G}^*$. Using (3.1) and the fact that R is an isomorphism of $\mathcal{H}$ onto $\mathcal{G}$ and of $\mathcal{G}^*$ onto $\mathcal{H}$, we see that $[R,1/\alpha W_\alpha]$ is weakly convergent in $B(\mathcal{H})$ (i.e. R is of class $C^1(A)$) if and only if $H\in C^1(A)$ and then (3.6) is true.

In order to prove (3.7), we may assume $\lambda_0=0$. Let $\varphi:\mathbb{R}\setminus\{0\}\to\mathbb{R}\setminus\{0\}$ be the diffeomorphism $\varphi(\lambda)=-\lambda^{-1}$. Then the spectral measure of R is $E_R(S) = E(\varphi(S))$. Using (3.6) we get for $\lambda>0$ (for example) and $0<\varepsilon<\lambda$:

$$E_R(\lambda;\varepsilon)[iR,A]E_R(\lambda;\varepsilon) = H^{-1}E(I_\varepsilon)[iH,A]E(I_\varepsilon)H^{-1},$$

where we have denoted $I_\varepsilon=(-(\lambda-\varepsilon)^{-1},-(\lambda+\varepsilon)^{-1})$. For each $a<\hat{\rho}_H^A(-\lambda^{-1})$ there are $\varepsilon_0>0$ and a compact operator K such that

$$E(-\lambda^{-1};\varepsilon_0)[iH,A]E(-\lambda^{-1};\varepsilon_0) \geq aE(-\lambda^{-1};\varepsilon_0)+K.$$

If ε is small enough, I_ε is a neighbourhood of $-\lambda^{-1}$ contained in $(-\lambda^{-1}-\varepsilon_0,-\lambda^{-1}+\varepsilon_0)$, hence $E(I_\varepsilon)[iH,A]E(I_\varepsilon) \geq aE(I_\varepsilon)+E(I_\varepsilon)KE(I_\varepsilon)$. We get

$$\begin{aligned} H^{-1}E(I_\varepsilon)[iH,A]E(I_\varepsilon)H^{-1} &\geq aH^{-2}E(I_\varepsilon)+H^{-1}E(I_\varepsilon)KE(I_\varepsilon)H^{-1} \geq \\ &\geq a(\lambda-\varepsilon)^2E(I_\varepsilon)+H^{-1}E(I_\varepsilon)KE(I_\varepsilon)H^{-1}. \end{aligned}$$

Since the last term here is compact, we obtain $\hat{\rho}_R^A(\lambda)\geq\lambda^2\hat{\rho}_H^A(-\lambda^{-1})$. For the reverse inequality one has to start from $E(\lambda;\varepsilon)[iH,A]E(\lambda;\varepsilon) = HE(\lambda;\varepsilon)[iR,A]E(\lambda;\varepsilon)H$. ■

Remark: The preceding proposition is not true if D(H) is not assumed invariant under $e^{iA\alpha}$. For N-body hamiltonians with hard-core interactions, if A is the generator of dilations, then R is of class $C^1(A)$ but D(H) is not invariant under $e^{iA\alpha}$.

We pass now to the main result of this section, namely the calculation of the ρ-function for an operator H of the form $H^1\otimes 1+1\otimes H^2$ assuming that A admits a similar decomposition. Assume that two self-adjoint *bounded from below* operators H^1, H^2 are given in Hilbert spaces $\mathcal{H}_1$, $\mathcal{H}_2$. We denote $\mathcal{G}^j=D(H^j)$ provided with the graph norm, so that $\mathcal{G}^j$ is a Hilbert space continuously embedded in $\mathcal{H}_j$. Let $\mathcal{H}=\mathcal{H}_1\otimes\mathcal{H}_2$, $\mathcal{G}_1=\mathcal{G}^1\otimes\mathcal{H}_2$ and $\mathcal{G}_2=\mathcal{H}_1\otimes\mathcal{G}^2$ (Hilbert tensor products). It is known that there are continuous embeddings $\mathcal{G}_1\subset\mathcal{H}$ and $\mathcal{G}_2\subset\mathcal{H}$, $\mathcal{G}_1$ (resp. $\mathcal{G}_2$) being the domain of the self-adjoint operator $H_1= H^1\otimes 1$ (resp. $H_2=1\otimes H^2$) in $\mathcal{H}$. Moreover, the operator $H=H_1+H_2$ is self-adjoint on the domain $\mathcal{G}=\mathcal{G}_1\cap\mathcal{G}_2$ and its spectrum is given by $\sigma(H)=\sigma(H^1)+\sigma(H^2)$ (these assertions depend on the boundedness from below of the operators, see section 2.1 in [ABG 1]). Consider now a self-adjoint operator A^j in $\mathcal{H}_j$ such that H^j is of class $C^1(A^j)$. Recall that the self-adjoint operator $A=A^1\otimes 1+1\otimes A^2\equiv A_1+A_2$ can be defined by the property $e^{iA\alpha}=e^{iA^1\alpha}\otimes e^{iA^2\alpha}$ for all $\alpha\in\mathbb{R}$. It is then obvious that $D(H)=\mathcal{G}$ is invariant under $e^{iA\alpha}$. By hypothesis,

$B^j=[iH^j,A^j]$ is a continuous sesquilinear form on $\mathcal{G}^j$. It is well-known that B^1 will extend to a continuous sesquilinear form $B_1=B^1\otimes 1$ on $\mathcal{G}_1$ and similarly B^2 to $B_2=1\otimes B^2$ on $\mathcal{G}_2$. Now it is easy to show that H_j is of class $C^1(A_j)$ and of class $C^1(A)$ and $[iH_j,A_j]=[iH_j,A]=B_j$ (use $e^{-iA\alpha}H_1e^{+iA\alpha}=e^{-iA_1\alpha}H_1e^{+iA_1\alpha}=(e^{-iA^1\alpha}H^1e^{+iA^1\alpha})\otimes 1$). Since $\mathcal{G}=\mathcal{G}_1\cap\mathcal{G}_2$ (with the intersection topology), the sesquilinear form $B=B_1+B_2$ is continuous on $\mathcal{G}$. It follows that H is of class $C^1(A)$ and $[iH,A]=B$.

These arguments prove the first part of the next theorem:

THEOREM 3.4: *Let* H^1, H^2 *be two self-adjoint, bounded from below operators in the Hilbert spaces* $\mathcal{H}_1$, $\mathcal{H}_2$ *.Assume that* A^j *is a self-adjoint operator in* $\mathcal{H}_j$ *such that* H^j *is of class* $C^1(A^j)$. *Let* $H=H^1\otimes 1+1\otimes H^2$ *and* $A=A^1\otimes 1+1\otimes A^2$, *self-adjoint operators in* $\mathcal{H}=\mathcal{H}_1\otimes\mathcal{H}_2$. *Then* H *is of class* $C^1(A)$ *and for all* $\lambda\in\mathbb{R}$:

$$\rho_H^A(\lambda) = \inf_{\lambda=\lambda_1+\lambda_2} [\, \rho_{H^1}^{A^1}(\lambda_1)+ \rho_{H^2}^{A^2}(\lambda_2)] \tag{3.8}$$

Proof: (i) We have to prove only the preceding formula. Denote $\rho=\rho_H^A$, $\rho_j=\rho_{H^j}^{A^j}$. Since $\sigma(H)=\sigma(H^1)+\sigma(H^2)$, (3.8) is obvious if $\lambda\notin\sigma(H)$, both members being equal to $+\infty$. Moreover, by adding to H^j a constant and taking into account that $\rho_{H-\lambda_0}^A(\lambda)=\rho_H^A(\lambda+\lambda_0)$, we can assume $H^j\geq 0$, so that H is positive too. Hence, when we prove (3.9), we may assume without loss of generality that $\lambda\in\sigma(H)$, $\lambda\geq 0$ and we may consider only decompositions $\lambda=\lambda_1+\lambda_2$ with $\lambda_j\in\sigma(H_j)$, so that $\lambda_j\geq 0$.

(ii) Let us first prove that the function $f(\lambda)$ defined by the r.h.s. of (3.8) on $\mathbb{R}_+=[0,+\infty[$ is l.s.c. (then its extension by $+\infty$ for $\lambda<0$ will be l.s.c. on $\mathbb{R}$). Let $f_j=\rho_j|_{\mathbb{R}_+}$ and $F(\lambda_1,\lambda_2)=f_1(\lambda_1)+f_2(\lambda_2)$. Then $F:\mathbb{R}_+^2\to]-\infty,\infty]$ is l.s.c.. For $\lambda\geq 0$ denote $I_\lambda=\{(\lambda_1,\lambda_2)\mid\lambda_j\geq 0 \text{ and } \lambda_1+\lambda_2=\lambda\}$. I_λ is a compact subset of $\mathbb{R}_+^2$ and $f(\lambda)=\inf\{F(\lambda_1,\lambda_2)\mid(\lambda_1,\lambda_2)\in I_\lambda\}$. Assume $f(\lambda)>a$; we have to show that $f(\mu)>a$ for μ in a neighbourhood of λ. We have $F(\lambda_1,\lambda_2)>a$ for all $(\lambda_1,\lambda_2)\in I_\lambda$, hence each such (λ_1,λ_2) has a neighbourhood $U(\lambda_1,\lambda_2)$ in $\mathbb{R}_+^2$ on which F is strictly greater than a. I_λ being compact, it may be covered by a finite set $U_1,\dots,U_n$ of such neighbourhoods. Then $U=U_1\cup U_2\cup\dots\cup U_n$ is a neighbourhood of I_λ. Since I_λ is compact, U will contain a set of the form $I_\lambda(\varepsilon)=\{(\lambda_1,\lambda_2)\in\mathbb{R}_+^2\mid\lambda-\varepsilon\leq\lambda_1+\lambda_2\leq\lambda+\varepsilon\}$. So $F(\lambda_1,\lambda_2)>a$ on $I_\lambda(\varepsilon)$. Since F attains its lower bound on compacts, we shall have $f(\mu)>a$ for $\lambda-\varepsilon\leq\mu\leq\lambda+\varepsilon$.

(iii) For each $\nu>0$ we denote θ_ν^j the function $\mathbb{R}\rightarrow]-\infty,+\infty]$ associated to ρ_j according to the rule (3.5). Then θ_ν^j is u.s.c. and is finite on the open neighbourhood $\{\mu\in\mathbb{R} \mid \mathrm{dist}(\mu;\sigma(H^j))<\nu\}$ of $\sigma(H^j)$. On this set we also have $\theta_\nu^j(\mu)<\rho_j(\mu)$.

Let us fix some arbitrary $\lambda\in\sigma(H)$ (so $\lambda\geq 0$) and some (small) numbers $\nu>\nu'>0$. The set of all $\mu\leq\lambda$ such $\mathrm{dist}(\mu;\sigma(H^j))\leq\nu'$ is a compact and the restriction of θ_ν^j to it is a finite-valued u.s.c. function such that $\theta_\nu^j(\mu)<\rho_j(\mu)$. According to Proposition 3.2, there is $\varepsilon\in(0,\nu')$ such that for all $\mu\leq\lambda$ with $\mathrm{dist}(\mu;\sigma(H^j))\leq\nu'$:

$$E^j(\mu;\varepsilon)B^jE^j(\mu;\varepsilon)\geq\theta_\nu^j(\mu)E^j(\mu;\varepsilon). \tag{3.9}$$

Here E^j is the spectral measure of H^j. But, if $\mathrm{dist}(\mu;\sigma(H^j))>\nu'$, then $E^j(\mu;\varepsilon)=0$, because we assumed $\varepsilon<\nu'$. Hence (3.9) is valid for all $\mu\leq\lambda$ if we give an arbitrary finite value to $\theta_\nu^j(\mu)$ for $\mathrm{dist}(\mu;\sigma(H^j))>\nu'$.

It will be convenient to define $\theta_\nu^j(\mu)$ for $\mu\leq\lambda$ and $\mathrm{dist}(\mu;\sigma(H^j))>\nu'$ as equal to a finite constant bigger than $\sup\left\{\theta_\nu^j(\tau) \mid \tau\leq\lambda,\ \mathrm{dist}(\tau;\sigma(H^j))\leq\nu'\right\}$ (observe that the function θ_ν^j being u.s.c. is bounded from above on this compact set). We shall, however, keep the same notation for this new function.

(iv) Let us work in a spectral representation of the operator H^2. Then there is a measure space S_2 and a Borel function $\omega_2:S_2\rightarrow\mathbb{R}_+$ such that $\mathscr{H}_2\cong L^2(S_2)$ and H^2 is the operator of multiplication by ω_2. We then identify $\mathscr{H}_1\otimes\mathscr{H}_2\cong L^2(S_2;\mathscr{H}_1)$ so that H becomes the operator of multiplication by the operator-valued function $s\longmapsto H^1+\omega_2(s)$. From (3.9) we get for all $s\in S_2$:

$$E^1(\lambda-\omega_2(s);\varepsilon)B^1E^1(\lambda-\omega_2(s);\varepsilon)\geq\theta_\nu^1(\lambda-\omega_2(s))E^1(\lambda-\omega_2(s);\varepsilon). \tag{3.10}$$

If f is a bounded Borel function, then $f(H)$ is in $L^2(S_2;\mathscr{H}_1)$ the operator of multiplication by the operator-valued function $s\longmapsto f(H^1+\omega_2(s))$. Hence, if E is the spectral measure of H, then $E(\lambda;\varepsilon)$ is just the operator of multiplication by $s\longmapsto E^1(\lambda-\omega_2(s);\varepsilon)$ (take f equal to the characteristic function of $(\lambda-\varepsilon,\lambda+\varepsilon)$). So (3.10) is equivalent to

$$E(\lambda;\varepsilon)B_1E(\lambda;\varepsilon)\geq[1\otimes\theta_\nu^1(\lambda-H^2)]E(\lambda;\varepsilon). \tag{3.11}$$

Observe that $1\otimes\theta_\nu^1(\lambda-H^2)=\theta_\nu^1(\lambda-H_2)$. Writing an estimate similar to (3.11) with H^1 and H^2 interchanged, we obtain ($B=B_1+B_2$):

$$E(\lambda;\varepsilon)BE(\lambda;\varepsilon)\geq[\theta_\nu^1(\lambda-H_2)+\theta_\nu^2(\lambda-H_1)]E(\lambda;\varepsilon). \tag{3.12}$$

(v) We have to find the lower bound of the operator $\theta^1_\nu(\lambda-H_2)+\theta^2_\nu(\lambda-H_1)$ on the subspace $E(\lambda;\varepsilon)\mathscr{H}$. Let us work in a spectral representation of both H^1 and H^2, so that $\mathscr{H}\cong L^2(S_1\times S_2)$, H_j is the operator of multiplication by $(s_1,s_2)\mapsto\omega_j(s_j)$ and H is $(s_1,s_2)\mapsto\omega_1(s_1)+\omega_2(s_2)$. Hence $\theta^1_\nu(\lambda-H_2)+\theta^2_\nu(\lambda-H_1)$ is the operator of multiplication by $\theta^1_\nu(\lambda-\omega_2(s_2))+\theta^2_\nu(\lambda-\omega_1(s_1))$ and the subspace $E(\lambda;\varepsilon)\mathscr{H}$ is the set of functions in $\mathscr{H}$ which are zero outside the set $\{(s_1,s_2)\mid\lambda-\varepsilon<\omega_1(s_1)+\omega_2(s_2)<\lambda+\varepsilon\}$. In conclusion:

$$[\theta^1_\nu(\lambda-H_2)+\theta^2_\nu(\lambda-H_1)]E(\lambda;\varepsilon)\geq$$

$$\geq[\inf\{\theta^1_\nu(\lambda-\tau_2)+\theta^2_\nu(\lambda-\tau_1)\mid\lambda-\varepsilon<\tau_1+\tau_2<\lambda+\varepsilon,\ \tau_j\in\sigma(H_j)\}]\,E(\lambda;\varepsilon).$$

Let us consider the inf in the r.h.s. and replace the variables τ_1, τ_2 by $\lambda_1=\lambda-\tau_2$, $\lambda_2=\lambda-\tau_1$. Then we must have $\lambda_1\leq\lambda$, $\lambda_2\leq\lambda$, $|\lambda_1+\lambda_2-\lambda|<\varepsilon$, and we are interested in $\inf(\theta^1_\nu(\lambda_1)+\theta^2_\nu(\lambda_2))$. Taking into account the way θ^j_ν has been chosen in (iii), we may also assume $\mathrm{dist}(\lambda_j,\sigma(H^j))\leq\nu'$. But then clearly this infimum is minorated by

$$\inf\Big\{\inf_{|\mu_1-\lambda_1|<\nu}\rho_1(\mu_1)+\inf_{|\mu_2-\lambda_2|<\nu}\rho_2(\mu_2)-2\nu\ \Big|\ \lambda_1,\lambda_2\leq\lambda,\ |\lambda_1+\lambda_2-\lambda|<\varepsilon\Big\}.$$

The numbers μ_1, μ_2 which appear here satisfy $\mu_j\leq\lambda_j+\nu$ and $|\mu_1+\mu_2-\lambda|<\varepsilon+2\nu$. Hence we can bound by below the above quantity by:

$$\inf\{\rho_1(\mu_1)+\rho_2(\mu_2)-2\nu\mid\mu_1,\mu_2\leq\lambda+\nu,\ |\mu_1+\mu_2-\lambda|<\varepsilon+2\nu\}\geq$$

$$\geq\inf\{\rho_1(\mu_1)+\rho_2(\mu_2)-2\nu\mid|\mu_1+\mu_2-\lambda|<\varepsilon+2\nu\}=$$

$$=\inf_{|\mu-\lambda|<\varepsilon+2\nu}\ \inf_{\mu=\mu_1+\mu_2}[\rho_1(\mu_1)+\rho_2(\mu_2)]-2\nu=$$

$$=\inf_{|\mu-\lambda|<\varepsilon+2\nu}f(\mu)-2\nu\geq\inf_{|\mu-\lambda|<3\nu}f(\mu)-2\nu:=\theta_\nu.$$

From (3.12) we obtain then: $E(\lambda;\varepsilon)BE(\lambda;\varepsilon)\geq\theta_\nu E(\lambda;\varepsilon)$. So $\rho(\lambda)\geq\theta_\nu$. Since $\nu>0$ is arbitrary and $\theta_\nu\to f(\lambda)$ as $\nu\to+0$ due to the lower semicontinuity of f, we get $\rho(\lambda)\geq f(\lambda)$.

(vi) It remains to be shown that the equality is in fact realised in $\rho(\lambda)\geq f(\lambda)$. Of course, only the case $\lambda\in\sigma(H)$ is non trivial. By the lower semi-continuity of F and the compactness of I_λ (see (ii)) it follows that there are $\lambda_1\in\sigma(H^1)$ and $\lambda_2\in\sigma(H^2)$ such that $\lambda=\lambda_1+\lambda_2$ and $f(\lambda)=\rho_1(\lambda_1)+\rho_2(\lambda_2)$. By the definition of $\rho_j(\lambda_j)$ (see the remark after (3.3)) there is a sequence $\{u^j_n\}_{n\in\mathbb{N}}$ (j=1,2) such that $u^j_n=E^j(\lambda_j;\frac{1}{n})u^j_n$,

$\|u_n^j\|=1$ and $<u_n \mid B^j u_n^j> \to \rho_j(\lambda_j)$. Let $u_n=u_n^1\otimes u_n^2$. Then $\|u_n\|=1$ and $E(\lambda;\frac{2}{n})u_n=u_n$. Moreover

$$<u_n \mid Bu_n> = <u_n^1 \mid B^1u_n^1> + <u_n^2 \mid B^2u_n^2> \to \rho_1(\lambda_1)+\rho_2(\lambda_2).$$

This finishes the proof. ■

Remark: Assume that H^2 has a purely continuous spectrum. Then $\rho_{H^2}^{A^2} = \hat{\rho}_{H^2}^{A^2}$, H has also a purely continuous spectrum and

$$(3.13) \qquad \hat{\rho}_H^A(\lambda) = \rho_H^A(\lambda) = \inf_{\lambda=\lambda_1+\lambda_2} [\rho_{H^1}^{A^1}(\lambda_1) + \rho_{H^2}^{A^2}(\lambda_2)].$$

As an example, let us see how the theorem should be used for the case of Agmon hamiltonians (cf. [ABG 1]). Let $Y \in \mathscr{L}\setminus\{X\}$ and $H_Y = H^Y\otimes_Y 1 + 1\otimes_Y \Delta^{Y^\perp}$. We take $A=A^Y\otimes_Y 1+1\otimes_Y A^{Y^\perp}$ where A is the generator of the dilation group normalised such that $[i\Delta,A]=\Delta$. Obviously, for $X\neq 0$:

$$\rho_\Delta^A(\lambda) = \begin{cases} +\infty & \text{if } \lambda<0 \\ \lambda & \text{if } \lambda\geq 0. \end{cases}$$

Let $\rho^Y=\rho_{H^Y}^{A^Y}$ and $\rho_Y=\rho_{H_Y}^A$. For $Y\neq X$ we have $\rho_Y=\hat{\rho}_Y := \hat{\rho}_{H_Y}^A$ by Proposition 3.1. In conclusion:

$$(3.14) \qquad \hat{\rho}_Y(\lambda) = \inf_{\mu\geq 0} [\rho^Y(\lambda-\mu)+\mu] \text{ for all } Y \in \mathscr{L}\setminus\{X\} \text{ and } \lambda \in \mathbb{R}.$$

4. Reducible Graded C*-Algebras

In this section we shall introduce a class of graded C*-algebras so that the ρ-function of a hamiltonian affiliated to such an algebra can be easily estimated in terms of the ρ-functions of sub-hamiltonians if the action of the conjugate operator is compatible with the graduation. The definition below is motivated by Theorem 2.1 and the existence of $\mathscr{L}$-reducing families (mentioned after the proof of theorem 2.1) for the N-body algebra.

Let us consider a finite lattice $\mathscr{L}$ and a $\mathscr{L}$-graded C*-algebra $\mathscr{A}$. Recall that for each $Y \in \mathscr{L}$ we have a canonical decomposition $\mathscr{A}=\mathscr{A}_Y+\mathscr{B}_Y$ such that $\mathscr{A}_Y$ is a C*-subalgebra of $\mathscr{A}$, $\mathscr{B}_Y$ is a closed $*$-ideal, $\mathscr{A}_Y\cap\mathscr{B}_Y=\{0\}$ and the projection $\mathscr{P}_Y:\mathscr{A}\to\mathscr{A}_Y$ is a $*$-homomorphism. Moreover, $\mathscr{A}_Y\subset\mathscr{A}_Z$ if $Y\leq Z$ and $\mathscr{A}_X=\mathscr{A}$. In this section we shall furthermore assume that $\mathscr{A}$ is realised on a (separable) Hilbert space $\mathscr{H}$ (i.e. $\mathscr{A} \subset B(\mathscr{H})$ is a C^*-subalgebra).

DEFINITION: *A family* $\{J_Y\}_{Y\in\mathscr{L}}$ *of bounded, symmetric operators in* $\mathscr{H}$ *is called* $\mathscr{A}$-reducing *if:*

(a) $J_X=0$ *and* $\Sigma\{J_Y^2 \mid Y\in\mathscr{L}\}=1$;

(b) *for each* $S\in\mathscr{A}$ *and* $Y\in\mathscr{L}$, *we have* $[S,J_Y]\in\mathscr{A}(X)$;

(c) *if* $Y\in\mathscr{L}$ *and* $S\in\mathscr{B}_Y$, *then* SJ_Y *and* J_YS *belong to* $\mathscr{A}(X)$.

If such a family exits, we shall say that $\mathscr{A}$ *is a reducible* $\mathscr{L}$*-graded* C^**-algebra.* Recall that $\mathscr{A}_Y$ is canonically a $\mathscr{L}(Y)$-graded C^*-algebra; if each $\mathscr{A}_Y$ is reducible , we shall say that $\mathscr{A}$ *is completely reducible.*

In connection with this definition, recall that $\mathscr{A}(X)$ is also a closed $*$-ideal in $\mathscr{A}$ (and $\mathscr{A}(Y)$ in $\mathscr{A}_Y$), hence at (c) we could have required only $SJ_Y\in\mathscr{A}(X)$. If $\mathscr{L}=\{\mathbf{O},X\}$, then $\mathscr{A}$ is (completely) reducible: it is enough to take $J_O=1$, $J_X=0$. The remarks which end section 2 prove that the N-body algebra is completely reducible (take $J_Y=\chi_Y(Q)$).

For two operators $S,T\in\mathscr{A}$ we shall write $S \sim T$ if $S-T\in\mathscr{A}(X)$. Since $\mathscr{A}(X)$ is a closed $*$-ideal, this relation is equivalent with equality in the quotient $\mathscr{A}/\mathscr{A}(X)$ C^*-algebra, so it is compatible with the algebraic operations and with continuous functional calculus for normal elements. This can also be seen from the fact that $S\sim T$ if and only if $\mathscr{P}_Y(S)=\mathscr{P}_Y(T)$ for all $Y\neq X$ (and if and only if $\mathscr{P}(Y)(S)=\mathscr{P}(Y)(T)$ for all $Y\neq X$).

PROPOSITION 4.1: *Let* $\{J_Y\}_{Y\in\mathscr{L}}$ *be an* $\mathscr{A}$*-reducing family. For each* $S\in\mathscr{A}$ *and* $Y\in\mathscr{L}$ *denote* $S_Y=\mathscr{P}_Y(S)$. *Then for* $S^1,\dots,S^n\in\mathscr{A}$ *we have*

$$S^1S^2\dots S^n \sim \Sigma_Y\, J_YS_Y^1S_Y^2\dots S_Y^nJ_Y. \tag{4.1}$$

Proof: Since $\mathscr{P}_Y$ is a homomorphism, we have $(S^1S^2\dots S^n)_Y=S_Y^1S_Y^2\dots S_Y^n$, so we may assume that there is only one factor. Then, using $[S,J_Y]\in\mathscr{A}(X)$ and $(S-S_Y)J_Y\in\mathscr{A}(X)$ (because $S-S_Y\in\mathscr{B}_Y$) we get

$$S=\Sigma_Y\, SJ_Y^2=\Sigma_Y\,([S,J_Y]J_Y+J_Y(S-S_Y)J_Y+J_YS_YJ_Y)\sim\Sigma_YJ_YS_YJ_Y. \blacksquare$$

COROLLARY 4.2: *If* H *is a self-adjoint operator affiliated to* $\mathscr{A}$, $\varphi\in C_\infty(\mathbb{R})$ *and* $S\in\mathscr{A}$, *then*

(4.2) $\qquad \varphi(H) \sim \Sigma_Y J_Y\varphi(H_Y)J_Y,$

(4.3) $\qquad \varphi(H)S\varphi(H) \sim \Sigma_Y J_Y\varphi(H_Y)S_Y\varphi(H_Y)J_Y.$

Remark: In the N-body case considered in section 2 we have $\mathscr{A}(X)=\mathbf{K}(X)$. Taking into account theorem 2.1, if H is a self-adjoint operator in $\mathscr{H}(X)$ affiliated to $\mathscr{T}$, $\varphi\in C_\infty(\mathbb{R})$ and $\chi:X\rightarrow\mathbb{C}$ is continuous and homogeneous of degree zero for $|x|\geq 1$, we shall have $[\varphi(H),\chi(Q)]\in\mathbf{K}(X)$. If H is affiliated to the algebra $\mathscr{A}$ described by (2.2) and $\chi=\chi_Y$ is Y-reducing, then we also have $\chi_Y(Q)(\varphi(H)-\varphi(H_Y))\in\mathbf{K}(X)$. These assertions are generalisations of some of the results from section 2.6 of [ABG 1].

We arrive, finally, to what we call "Mourre theory in a graded C*algebra setting". From now on we assume that a densely defined, self-adjoint operator A in $\mathscr{H}$ is given such that the group of automorphisms associated to $W_\alpha=e^{iA\alpha}$ leaves $\mathscr{A}$ invariant and its action is compatible with the grading, i.e.

(4.4) $\qquad W_\alpha^*\mathscr{A}(Y)W_\alpha\subset\mathscr{A}(Y)$ for all $Y\in\mathscr{L}$ and $\alpha\in\mathbb{R}$.

If we denote $\{\mathscr{W}_\alpha\}$ the group of automorphisms of $B(\mathscr{H})$ given by $\mathscr{W}_\alpha(S)=W_\alpha^*SW_\alpha$, then the preceding requirements are fulfilled if and only if $\mathscr{W}_\alpha(\mathscr{A})=\mathscr{A}$ and $\mathscr{W}_\alpha\mathscr{P}(Y)=\mathscr{P}(Y)\mathscr{W}_\alpha$ for all $Y\in\mathscr{L}$, $\alpha\in\mathbb{R}$ (the second condition being equivalent to $\mathscr{W}_\alpha\mathscr{P}_Y=\mathscr{P}_Y\mathscr{W}_\alpha$ for all Y,α).

Let us remark that if we consider the algebra $\mathscr{T}$ of section 2.2 and if W_α is the dilation group, then these conditions are fulfilled (so for $\mathscr{A}$ given by (2.2) also). Moreover, in this case $\{\mathscr{W}_\alpha\}_{\alpha\in\mathbb{R}}$ induces a *norm-continuous* group of automorphisms of $\mathscr{T}$ (in particular, its generator, which is formally $[\cdot,iA]$, is norm-densely defined).

We will be interested in the spectral analysis of a self-adjoint operator H affiliated to $\mathscr{A}$ by the conjugate operator method. Proposition 3.3 shows that, if H has a spectral gap (i.e. $\exists\lambda_0\in\mathbb{R}\setminus\sigma(H)$; in fact we shall be interested only in H bounded from below), then it is better to study $R=(\lambda_0-H)^{-1}$, which is bounded, self-adjoint and belongs to $\mathscr{A}$. In particular, we shall not have to put any condition of invariance under W_α of D(H), which could be non-dense (in hard-core case for example). So, for the moment we consider an arbitrary self-adjoint operator $R\in\mathscr{A}$.

PROPOSITION 4.3: *Let* $R\in\mathscr{A}$ *and denote* $R(Y)=\mathscr{P}(Y)(R)$, $R_Y=\mathscr{P}_Y(R)$.*Then* $R\in C^1_n(A)$ *if and only if* $R(Y)\in C^1_n(A)$ *for all* $Y\in\mathscr{L}$ *and also if and only if* $R_Y\in C^1_n(A)$ $(\forall Y\in\mathscr{L})$. *In this case we shall have*

$[iR,A]\in\mathscr{A}$ *and* $\mathscr{P}(Y)([iR,A])=[iR(Y),A]$, $\mathscr{P}_Y([iR,A]=[iR_Y,A]$ *for all* $Y\in\mathscr{L}$.

The proof is trivial because $\mathscr{A}$, $\mathscr{A}(Y)$, $\mathscr{A}_Y$ are norm-closed and $\mathscr{P}(Y)$, $\mathscr{P}_Y$ commute with $\mathscr{W}_\alpha$. The problem which we would like to study now is the relation between $\hat{\rho}^A_R$ and $\hat{\rho}^A_{R_Y}$ with $Y\neq X$. Since A is fixed in this section, we shall leave it out in the notations of the $\hat{\rho}$-functions.

As an example, let us consider the "two-body" case $\mathscr{L}=\{\mathbf{O},X\}$. Let $R\in\mathscr{A}$ self-adjoint with $R\in C^1_n(A)$. Then $R=R_\mathbf{O}+R(X)$ with $R_\mathbf{O}\in\mathscr{A}_\mathbf{O}=\mathscr{A}(\mathbf{O})$ and $R(X)\in\mathscr{A}(X)$ (which is $\mathbf{K}(X)$ in the N-body case). If $R\in C^1_n(A)$, then according to proposition 4.3

$$[iR,A] = [iR_\mathbf{O},A] + [iR(X),A] \sim [iR_\mathbf{O},A]$$

(because $[iR(X),A]=\mathscr{P}(X)([iR,A])\in\mathscr{A}(X)$). If $\varphi:\mathbb{R}\to\mathbb{C}$ is continuous (and $\varphi(0)=0$ if $\mathscr{A}$ has not a unit) then $\varphi(R)=\mathscr{P}_\mathbf{O}(\varphi(R))+\mathscr{P}(X)(\varphi(R))=\varphi(R_\mathbf{O})+\mathscr{P}(X)(\varphi(R))\sim\varphi(R_\mathbf{O})$. Hence $\varphi(R)[iR,A]\varphi(R)\sim\varphi(R_\mathbf{O})[iR_\mathbf{O},A]\varphi(R_\mathbf{O})$ and $\varphi^2(R)\sim\varphi^2(R_\mathbf{O})$ if $\varphi\in C^\infty_0(\mathbb{R})$ (and $\varphi(0)=0$ if $\mathscr{A}$ has not unit). If $\mathscr{A}(X)$ contains only compact operators, it is easy to get from this that $\hat{\rho}_R(\lambda)=\hat{\rho}_{R_0}(\lambda)$ for all λ ($\neq 0$ if $\mathscr{A}$ has not unit) . In particular, A is conjugated to R at λ ($\neq 0$ if $\mathscr{A}$ has not unit) if and only if it is conjugated to $R_\mathbf{O}$ at λ.

Recall that if $\mathscr{L}=\{\mathbf{O},X\}$, then $\mathscr{A}$ is automatically reducible. Let us go back now to a general $\mathscr{A}$, but assume it reducible. Let $\{J_Y\}$ be an $\mathscr{A}$-reducible family. Consider a self-adjoint element $R\in\mathscr{A}$ of class $C^1_n(A)$ and a continuous function $\varphi:\mathbb{R}\to\mathbb{R}$ which vanishes at zero if $\mathscr{A}$ has not a unit. Then $\varphi(R)\in\mathscr{A}$ and $\mathscr{P}_Y(\varphi(R))=\varphi(R_Y)$. Let us take $S=[iR,A]$ in (4.3). Then corollary 4.2 and proposition 4.3 give:

(4.5) $\quad \varphi(R)[iR,A]\varphi(R)\sim\Sigma_Y J_Y\varphi(R_Y)[iR_Y,A]\varphi(R_Y)J_Y,$

(4.6) $\quad \varphi^2(R)\sim\Sigma_Y J_Y\varphi^2(R_Y)J_Y.$

Let us write $S \lesssim T$ for $S,T \in \mathscr{A}$, if we have this inequality modulo $\mathscr{A}(X)$ (i.e. $\exists K \in \mathscr{A}(X)$ such that $S \leq T+K$). It follows from (4.5), (4.6) that we have $\varphi(R)[iR,A]\varphi(R) \gtrsim a\varphi^2(R)$ for some $a \in \mathbb{R}$ if and only if

$$(4.7) \qquad \Sigma_Y J_Y[\varphi(R_Y)[iR_Y,A]\varphi(R_Y) - a\varphi^2(R_Y)]J_Y \gtrsim 0.$$

In conclusion, the following result has been proved (observe that $J_X = \mathbf{O}$):

THEOREM 4.4: *Let* $\mathscr{A}$ *be a reducible* $\mathscr{L}$*-graded* C^**-algebra such that* $\mathscr{A}(X)$ *contains only compact operators. Let* A *be a densely defined self-adjoint operator in* $\mathscr{H}$ *such that* $e^{-iA\alpha}\mathscr{A}(Y)e^{iA\alpha} \subset \mathscr{A}(Y)$ *for all* $Y \in \mathscr{L}$ *and* $\alpha \in \mathbb{R}$. *Consider a self-adjoint operator* $R \in \mathscr{A}$ *of class* $C^1_n(A)$. *Then for all* $\lambda \in \mathbb{R} \setminus \{0\}$ *we have*

$$(4.8) \qquad \hat{\rho}^A_R(\lambda) \geq \min\left\{\hat{\rho}^A_{R_Y}(\lambda) \mid Y \in \mathscr{L} \setminus \{X\}\right\}.$$

In particular, if A *is conjugated at some* $\lambda \neq 0$ *to all* R_Y *with* $Y < X$, *then* A *is also conjugated at* λ *to* R.

Remarks:

(a) If $\mathscr{A}$ has unit, the condition $\lambda \neq 0$ is not necessary.

(b) Only $J_Y \neq 0$ really appear in (4.7); hence in (4.8) the minimum has to be taken only over these Y's. For example, if there is an $\mathscr{A}$-reducing family $\{J_Y\}$ with $J_Y \neq 0$ only for $Y \in \mathscr{L}^2$ (as in the N-body situation considered in section 2), then:

$$(4.9) \qquad \hat{\rho}^A_R(\lambda) \geq \min\left\{\hat{\rho}^A_{R_Y}(\lambda) \mid Y \in \mathscr{L}^2\right\}.$$

In the next corollary we use the obvious fact that if $\lambda_0 \notin \sigma(H)$ then $\lambda_0 \notin \sigma(H_Y)$ for any $Y \in \mathscr{L}$ (because $\mathscr{P}_Y$ are $*$-homomorphisms).

COROLLARY 4.5: *Assume that* H *is a self-adjoint unbounded operator in* $\mathscr{H}$ *which has a spectral gap and which is affiliated to* $\mathscr{A}$. *Moreover, assume that the domain of* H_Y *is invariant under* $e^{iA\alpha}$ *(all* $Y \in \mathscr{L}$, $\alpha \in \mathbb{R}$*). If* H *is of class* $C^1_n(A)$, *then each* H_Y *is of class* $C^1_n(A)$ *and*

$$(4.10) \quad \hat{\rho}^A_H \geq \min\left\{\hat{\rho}^A_{H_Y} \mid Y \in \mathscr{L} \setminus \{X\}\right\}.$$

(*Remark* (b) *above applies here too*). *In particular, if* A *is conjugated to each* H_Y *with* $Y < X$ *at some* $\lambda \in \mathbb{R}$, *then* H *is conjugated to* H *at* λ.

Combining theorem 3.4 (more precisely fromula (3.14)) with corollary 4.5 one easily gets the results of [PSS], [FH] and [ABG 1] for N-body or Agmon hamiltonians (much more general situations may be considered, as we shall show in a later publication). In fact (3.14) shows by induction over Y that $\hat{\rho}_Y \geq 0$ for all Y. Hence, using again (3.14) and proposition 3.1 we see that for Y<X we have $\hat{\rho}_Y(\lambda)=0$ only if $\hat{\rho}^Y(\lambda)=0$ or if $\hat{\rho}^Y(\lambda)>0$ but λ is an eigenvalue of H^Y. So we get by induction that $\hat{\rho}_Y(\lambda)>0$ if λ is not a threshold or eigenvalue of H^Y. Then (4.10) implies $\hat{\rho}_X(\lambda)>0$ if λ is not a threshold of H.

REFERENCES

[ABG1] Amrein W.O., Boutet de Monvel-Berthier A. and Georgescu V., *Notes on the* N-*Body Problem, I*, Preprint Université de Genève, UGVA-DPT 1988/11-598.

[ABG2] Amrein W.O., Boutet de Monvel-Berthier A. and Georgescu V., *Notes on the* N-*Body Problem, II*, Preprint Université de Genève, UGVA-DPT 1991/04-718, p.164-424.

[BG1] Boutet de Monvel-Berthier A. and Georgescu V., *Graded C*-Algebras and Many-Body Perturbation Theory.* I. *The N-Body Problem,* C.R.Acad.Sci. Paris, **312**, Série I, p.477-482, 1991.

[BG2] Boutet de Monvel-Berthier A. and Georgescu V., *Graded C*-Algebras in the N-Body Problem,* J.Math.Phys., **32**, n°11 (1991), p.3101-3110.

[BGM] Boutet de Monvel-Berthier A., Georgescu V. and Mantoiu M., *Locally Smooth Operators and the Limiting Absorption Principle for N-Body Hamiltonians,* Rev. in Math. Phys. (1992), to appear — preprint Universität Bielefeld, BIBOS, n°433/1990, p.1-101].

[C] Cordes H.O., *On the Compactness of Commutators of Multiplications and Convolutions, and Boundedness of Pseudo-Differential Operators,* J.Funct.Analysis, **18** (2) (1975), p.115-132.

[D1] Derezinski J., *A New Proof of the Propagation Theorem for N-Body Quantum Systems,* Comm. Math Phys. ,**122** (1989), p.203-231.

[D2] Derezinski J., *The Mourre Estimate for Dispersive N-Body Schrödinger Operators,* Preprint Virginia Polytechnic Institute, 1988.

[C] Gérard C., *The Mourre Estimate for Regular Dispersive Systems,* Ann. Inst. Henri Poincaré, **54** (1) (1991), p.59-88.

[FH] Froese R.G. and Herbst I., *A New Proof of the Mourre Estimate,* Duke Math J., **49** (1982), p.1075-1085.

[HP] Hille E. and Phillips R.S., *Functional Analysis and Semi-groups,* Amer. Math. Soc., Providence, R.I. 1957.

[PSS] Perry P., Sigal. I.M. and Simon B., *Spectral Analysis of N-Body Schrödinger Operators,* Ann. Math., **114** (1981), p.519-567.

[S] Simon B., *Geometric Methods in Multiparticle Quantum Systems,* Comm. Math. Phys., **55** (1977), p.259-274.

[T] Tamura R., *Propagation Estimates for N-body Quantum Systems,* Bull. Fac. Sci. Ibaraki Univ., **22** (1990), p.29-48.

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The homogeneous Monge-Ampère equation on a pseudoconvex domain

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The homogeneous Monge-Ampere equation on a pseudoconvex domain

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§1. Introduction

Let X be a compact complex n-dimensional manifold with a smooth strictly-pseudoconvex boundary. Without loss of generality one can assume that X sits inside an open complex manifold, Z. A smooth function, $\phi : Z \longrightarrow \mathbb{R}$, is a *defining function* of X if it has the property:

$$\phi(p) \leq 1 \Longleftrightarrow p \in X$$

and if it has no critical points on the boundary. There are an infinity of different ways of choosing such a defining function, and it is a problem of considerable interest in the theory of pseudoconvex domains to find ways of making *canonical* choices. Jack Lee proved a result in his thesis which sheds some light on this problem: Suppose all the data above are real-analytic. Let S be the boundary of X and let $\Gamma \longrightarrow S$ be the bundle of outward-pointing conormal vectors to S. Given a real-analytic section, $\mu : S \longrightarrow \Gamma$, Lee proved that there exists a unique real-analytic defining function, ϕ, which satisfies the boundary condition, $d\phi = \mu$ on S and satisfies the homogeneous Monge-Ampere equation

$$(\bar{\partial}\partial\phi)^n = 0 \tag{1.1}$$

on a neighborhood of S.* One of the aims of this paper is to give a new proof of this result. This proof is similar to a proof that Matt Stenzel and I gave of an existence theorem for Monge-Ampere with a different set of boundary conditions in $[GS]_1$. I will give a brief description of this proof below; however, first I want to describe the other main result of this paper. Let X be a compact Riemannian manifold. Suppose that X is real-analytic, and suppose that $f : X \longrightarrow \mathbb{R}$ is a real-analytic function. Several years ago Boutet de Monvel proved the following surprising result:

Theorem. *[B] The following are equivalent*

1. *f can be extended holomorphically to a Grauert tube of radius r about X.*
2. *The wave equation*

$$\frac{\partial u}{\partial t} = \sqrt{\Delta} u \ , \qquad u(x,0) = f(x)$$

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*See [L]. Subsequently Jerison and Lee [JL] showed that there is a canonical way of choosing μ as well (by solving a CR variant of the Yamabe problem).

can be solved backwards in time over the interval $-r \le t \le 0$.

In other words Boutet's result says that the problem of extending f to a small neighborhood of X inside the complexification, $X_{\mathbb{C}}$, is equivalent to solving a diffusion problem in the wrong direction! Matt Stenzel and I showed in $[GS]_2$ that this result has some interesting connections with homogeneous Monge-Ampere. In this paper I will show that there is a form of Boutet's result which is true for an *arbitrary* real-analytic pseudoconvex domain; and this, too, will involve homogeneous Monge-Ampere in a fundamental way. The statement and proof of this result will be given in §5 and I will give my new proof of Lee's theorem in §4. As in $[GS]_1$ the main step in this proof will be the complexification of a solution of a certain *real* Monge-Ampere equation which I now want to describe: Let X and Y be real n-dimensional manifolds and consider the DeRham complex on $X \times Y$. By the Künneth theorem this complex is a double complex with an exterior derivative, d_x, that only involves the X-variables and an exterior derivative, d_y, that only involves the Y-variables. In particular, given a function, $\phi = \phi(x, y)$, on $X \times Y$ one gets a two-form, $d_x d_y \phi$, and, wedging this form with itself n times, a $2n$-form, $(d_x d_y \phi)^n$. Now let S be a hypersurface in $X \times Y$ and ϕ_0 a defining function for it. Suppose that ϕ_o satisfies:

$$(d_x d_y \phi_0)^{n-1} \wedge d_x \phi_0 \wedge d_y \phi_0 \neq 0 \tag{1.2}$$

on a neighborhood of S.* I will prove in §2 that, on every sufficiently small neighborhood of S, there exists a unique function, ϕ, such that $\phi - \phi_0$ vanishes to second order on S and

$$(d_x d_y \phi)^n = 0. \tag{1.3}$$

In other words given a surface, S, with the convexity property, (1.2), the Cauchy problem for (1.3), with initial data on S, can always be solved in a neighborhood of S. The proof will involve some ideas that have come up earlier in the work of Phong and Stein, [PS], and in my own work with Sternberg ([GS], Chapter 6) on Radon integral transforms; and I will explain what Monge-Ampere has to do with this subject in §2–3.

To conclude I would like to mention a number of recent articles on homogeneous Monge-Ampere dealing with issues that I've touched on here. These are, in addition to my two articles with Stenzel cited above, the article, [EM], of Epstein-Melrose and the articles, [LS] of Lempert-Szöke, [S] of Szöke and [Lem] of Lempert. In particular, in Lempert's article, it is shown that for the Monge-Ampere problem discussed in $[GS]_1$, $[GS]_2$ the analyticity assumptions are *necessary* as well as sufficient.

§2. Double fibrations.

*This condition depends only on S not on the choice of ϕ_0. It is the analogue in this "Künneth" theory of the Levi condition.

Let X and Y be n-dimensional manifolds and S a closed $(2n-1)$-dimensional submanifold of $X \times Y$. Let π and ρ be the restrictions to S of the projection maps of $X \times Y$ onto X and Y. The triple (S, π, ρ) is called a *double fibration* if both π and ρ are fiber mappings. I will assume that the conormal bundle of S is oriented and will denote by Γ the set of its positively-oriented vectors. Composing the inclusion, $\Gamma \longrightarrow T^*(X \times Y)$, with the projections of $T^*(X \times Y)$ and T^*X and T^*Y one gets maps

$$\pi_1 : \Gamma \longrightarrow T_0^*X \quad \text{and} \quad \rho_1 : \Gamma \longrightarrow T_0^*Y \tag{2.1}$$

of Γ onto the punctured cotangent bundles of X and Y.* The data, (S, π, ρ), are said to satisfy the *Bolker* condition if π_1 and ρ_1 are diffeomorphisms, in which case the composite mapping, $\rho_1 \circ \pi_1^{-1}$ is well-defined. Composing this mapping with the involution:

$$\sigma : T_0^*Y \longrightarrow T_0^*Y \quad , \quad \sigma(y, \eta) = (y, -\eta)$$

one gets a canonical transformation

$$\gamma : T_0^*X \longrightarrow T_0^*Y \tag{2.2}$$

which I will call the *canonical transformation associated with the double fibration* (S, π, ρ).

To check that the Bolker condition is satisfied, one has to check first that π_1 and ρ_1 are diffeomorphisms locally in the neighborhood of each point of Γ, and then check that they are one-one and onto. Often the second criterion is *implied* by the first. (This is so, for instance, if both X and Y are compact.) As for the first criterion, it is easy to see that if π_1 is locally a diffeomorphism at a point of Γ, ρ_1 is as well. This criterion can also be checked rather easily by the following means. Let $\phi = \phi(x, y)$ be a defining function of S i.e. let S be the subset of $X \times Y$ defined by the equation, $\phi(x, y) = 1$; and assume $d\phi_p \neq 0$ at all points, $p \in S$. Let $d_x d_y \phi$ be the two-form

$$\sum_{i,y=1}^{n} \frac{\partial^2 \phi}{\partial x_i \partial y_i} dx_i \wedge dy_j$$

Lemma. *For π_1 and ρ_1 to be local diffeomorphisms at all points of Γ it is necessary and sufficient that the $2n$-form*

$$(d_x d_y \phi)^{n-1} \wedge d_x \phi \wedge d_y \phi \tag{2.3}$$

be non-vanishing on a neighborhood of S.

I will leave the proof of this as an easy exercise. My goal in this section is to prove that if S satisfies the Bolker condition it has a defining function which satisfies, in addition to (2.3), the homogeneous Monge-Ampere equation described in the introduction:

*Given a manifold, M, we will denote by $T_0^*(M)$ the cotangent bundle of M with its zero section deleted.

Theorem 1. *Let $\mu : S \longrightarrow \Gamma$ be a section of Γ. Then there exists a unique defining function, ϕ, of S such that*

$$(d_x d_y \phi)^n \equiv 0 \tag{2.4}$$

on a neighborhood of S, and such that, in addition, $d\phi_p = \mu_p$ at all points, $p \in S$.*

Proof. Existence: There exists a unique homogeneous function of degree one on Γ which is identically equal to one on the image of μ. Lets denote this function by H_0. Under the diffeomorphism $T_0^*X \longrightarrow \Gamma$ this pulls back to a homogeneous function of degree one, H, on T_0^*X. Since (S, π, ρ) is a double fibration the fibers, $S_y = \rho^{-1}(y)$, above points of Y are $(n-1)$-dimensional submanifolds of X. Now, with y fixed, solve the Hamilton-Jacobi equation:

$$H(d\phi) = H\left(x, \frac{\partial \phi}{\partial x_1}, \ldots, \frac{\partial \phi}{\partial x_n}\right) = 1 \tag{2.5}$$

with the initial condition $\phi = 1$ on S_y.* This solution depends parametrically on y so it is really a function, $\phi = \phi(x, y)$, of *both* the x and the y variables and is well-defined in a neighborhood, U, of S. Let's show that it satisfies the Monge-Ampere equation and the required initial conditions. That it satisfies the initial conditions is equivalent to the assertion that $H_0(d\phi) = 1$ on S and this is equivalent to the assertion that, for y fixed, the equation $H(d\phi) = 1$ holds on X. To check that ϕ satisfies Monge-Ampere, we note that because H doesn't depend on y we can differentiate the identify

$$H\left(\frac{\partial \phi}{\partial x_1}, \ldots, \frac{\partial \phi}{\partial x_n}, x\right) = 1$$

with respect to y_i getting:

$$\sum_{j=1}^{n} \frac{\partial H}{\partial \xi_j}(d_x\phi, x) \frac{\partial^2 \phi}{\partial x_j \partial y_i} = 0$$

Since $\frac{\partial H}{\partial \xi}(x, \xi) \neq 0$ when $\xi \neq 0$ this implies that

$$\det\left(\frac{\partial^2 \phi}{\partial x_i \partial y_j}\right) = 0.$$

Uniqueness: Let ϕ be a defining function of S satisfying the given initial conditions. By assumption the map

$$\pi_1 : S \times \mathbb{R}^+ \longrightarrow T_0^*X$$

---

*In local coordinates this is just the Monge-Ampere equation $\det(\frac{\partial^2 \phi}{\partial x_i \partial y_j}) = 0$.

*Let's briefly review how this is done. The equation, $H = 1$, cuts out a hypersurface in the conormal bundle of S_y. This hypersurface is an isotropic submanifold of T^*X of dimension $n-1$, so if we take its flow-out with respect to the Hamiltonian flow, $\exp t\Xi_H$, we get an n-dimensional Lagrangian submanifold, Λ, of T^*X. In the vicinity of S_y Λ is the graph of an exact one form, $d\phi$, and if we normalize ϕ to be one on S_y this determines it uniquely.

sending (x, y, s) to $(x, sd_x\phi)$ is a diffeomorphism; and, by our definition of H, it embeds S onto the hypersurface, $H = 1$. Suppose now that ϕ satisfies the Monge-Ampere equation on a neighborhood of S. This says that the map

$$p : X \times Y \longrightarrow T_0^*X, \quad p(x, y) = (x, d\phi_x), \tag{2.6}$$

is of rank $2n - 1$ in a neighborhood of S, and hence is a *fibering* of a neighborhood, U, of S onto the hypersurface, $H = 1$. In particular, for y fixed, $\phi(x, y)$ satisfies the Hamilton-Jacobi equation

$$H\left(x, \frac{\partial \phi}{\partial x}\right) = 1.$$

Moreover, since ϕ is a defining function of S, it takes the value, $\phi = 1$, on S. Therefore, if one fixes y and regards it as a function of x alone, it takes the initial value, $\phi = 1$ on S_y. Hence the uniqueness of ϕ follows from standard uniqueness results in the Hamilton-Jacobi theory. Q.E.D.

Remark. If ϕ satisfies Monge-Ampere, the function, $\psi = \phi^2$, satisfies

$$\det\left(\frac{\partial^2 \psi}{\partial x_i \partial y_j}\right) \neq 0 \tag{2.7}$$

everywhere on a neighborhood of S. To see this, note that since

$$d_x d_y \psi = 2(\phi d_x d_y \phi + d_x \phi \wedge d_y \phi),$$

Monge-Ampere implies that

$$(d_x d_y \psi)^n = n 2^n \phi^{n-1} (d_x d_y \phi)^{n-1} \wedge d_x \phi \wedge d_y \phi$$

and the expression on the right is non-zero on a neighborhood of S in view of (2.3). (Recall that $\phi = 1$ on S.) Therefore, by specifying a section, μ, of $\Gamma \longrightarrow S$ one gets, not only a solution of Monge-Ampere on a neighborhood of S, but also a *symplectic* form on that neighborhood, (i.e. $d_x d_y \psi$) and a *pseudo-Riemannian metric* of signature (n, n) :

$$\Sigma \frac{\partial^2 \psi}{\partial x_i \partial y_j} dx_i \circ dy_j. \tag{2.8}$$

§3. A dynamical interpretation at the Monge-Ampere equation (2.4).

For simplicity I will assume in this section that X, Y and S are compact. Let ϕ be a defining function of S and let S_t be the subset of $X \times Y$ defined by the equation, $\phi = 1 - t$.

(In particular, $S_0 = S$.) For t sufficiently small, S_t will also satisfy the Bolker condition and hence give rise to a canonical transformation

$$\gamma_t : T_0^*X \longrightarrow T_0^*Y.$$

I will prove below that if ϕ satisfies Monge-Ampere the canonical transformations, γ_t, are related to one another in a very simple way: As we saw in the preceding section, the initial data, $\mu : S \longrightarrow \Gamma$, determine a homogeneous function of degree one, H, on T_0^*X. Let Ξ_H be the Hamiltonian vector field corresponding to H. Because of the homogeneity of H the group of symplectomorphisms generated by Ξ_H is a one-parameter group of canonical transformations. Lets denote this one-parameter group by $\exp t\Xi_H, -\infty < t < \infty$.

Theorem 2. *The following are equivalent:*

1. *ϕ satisfies Monge-Ampere.*
2. $\gamma_t = \gamma \circ \exp t\Xi_H$.

Proof that 1 implies 2:. Suppose ϕ satisfies Monge-Ampere. For the moment lets fix $y \in Y$ and think of $\phi(x, y)$ as a function of x alone.

Lemma. *There exists a neighborhood, U, of S_y and, for every point, $x \in U$, a unique point, $x_0 \in S_y$ such that*

$$\exp t\Xi_H(x_0, \xi_0) = (x, \xi) \tag{3.1}$$

where $\xi_0 = d\phi_{x_0}$, $\xi = d\phi_x$ and $\phi(x) = 1 + t$.

Proof. Let Λ_0 be the set

$$\{(x_0, \xi_0);\ x_0 \in S_y,\ \xi_0 = d\phi_{x_0}\}.$$

For ϵ sufficiently small the map of $\Lambda_0 \times (-\epsilon, \epsilon)$ into T^*X which sends (x_0, ξ_0, t) onto $(\exp t\Xi_H)(x_0, \xi_0)$ is a diffeomorphism of $\Lambda_0 \times (-\epsilon, \epsilon)$ onto a Lagrangian submanifold, Λ, of T^*X. Moreover, Λ is also the image of a neighborhood, U of S_y in X with respect to the mapping

$$d\phi : U \longrightarrow T^*X, \quad x \longrightarrow (x, d\phi_x).*$$

Thus, if x is in U, there is a unique $x_0 \in S_y$ and a unique t on the interval $(-\epsilon, \epsilon)$ such that

$$\exp t\Xi_H(x_0, \xi_0) = (x, \xi)$$

with $\xi_0 = d\phi_{x_0}$ and $\xi = d\phi_x$. Thus all that is left to prove is that $t = \phi(x)$. This, however, follows easily from the homogeneity of H. Namely, by Euler's identity

$$H(x, \xi) = \Sigma \frac{\partial H}{\partial \xi_i}(x, \xi)\xi_i;$$

*See the footnote following the display (2.4) in§2.

so, if $\xi = d\phi_x$:

$$1 = H(x, d\phi_x) = \Sigma \frac{\partial H}{\partial \xi_i}(x,\xi)\frac{\partial \phi}{\partial x_i}. \tag{3.2}$$

Let $(x(t), \xi(t))$, $0 \le t \le \epsilon$, be the integral curve of Ξ_H starting at (x_0, ξ_0). Then by (3.2)

$$\frac{d}{dt}\phi(x(t)) = 1.$$

Hence since $\phi = 1$ at x_0, $\phi = 1 + t$ at $x(t)$. Q.E.D.

Let's now compare the canonical transformations, $\gamma_t \circ \exp(-t\Xi_H)$ and γ. Because of the homogeneity properties of γ, γ_t and H it suffices to check that they are equal at all points, (x_0, ξ_0), on the hypersurface, $H = 1$. However, each point on this hypersurface is the image under the mapping (2.6) of a point, $(x_0, y) \in S$. In other words there is a unique $y \in Y$ such that $(d_x\phi)(x_0, y) = \xi_0$. Thus, by definition

$$\gamma(x_0, \xi_0) = (y, d_y\phi(x_0, y)). \tag{3.3}$$

On the other hand, by the lemma

$$\exp(-t\Xi_H)(x_0, \xi_0) = (x, \xi)$$

with $\xi = (d_x\phi)(x, y)$ and $\phi(x, y) = 1 - t$. Thus $(x, y) \in S_t$ and, hence

$$\gamma_t(x, \xi) = (y, d_y\phi(x, y)) = \gamma_t \circ \exp(-t\Xi_H)(x_0, \xi_0).$$

Therefore, if we denote by β the projection of T_0^* onto Y, we conclude from (3.3) and (3.4) that

$$\beta \circ \gamma_t \circ \exp(-t\Xi_H) = \beta \circ \gamma,$$

and hence that the canonical transforms, γ and $\gamma_t \circ \exp(-t\Xi_H)$ are themselves the same.*

Proof that 2 implies 1:. Not only does the hypersurface S_t determine the canonical transformation, γ_t, but it is clear from the definition of γ_t that the reverse is true: The canonical transformation, γ_t, determines the hypersurface, S_t. Thus if 2 holds, ϕ has the same level surfaces as does the corresponding solution of Monge-Ampere and hence has to be *equal* to this solution. Q.E.D.

I will conclude with a few words about the "quantum picture" that goes along with the result above. Let F_t be an elliptic Fourier integral operator whose underlying canonical transformation is γ_t. then by Theorem 2

$$F_t = F_0 U(t) Q + K \tag{3.4}$$

*Fact: If $\gamma_i : T_0^*X \longrightarrow T_0^*Y$, $i = 1, 2$, are canonical transforms, then $\beta \circ \gamma_1 = \beta \circ \gamma_2$ implies $\gamma_1 = \gamma_2$. (see, for instance [AM].)

K being a smoothing operator, Q an invertible elliptic pseudodifferential operator and $U(t)$ a one-parameter unitary group of the form

$$U(t) = \exp \sqrt{-1}tP \tag{3.5}$$

where P is a pseudodifferential operator with the function, H, as its leading symbol. We will see in section 5 that for he Monge-Ampere equation on a complex manifold there is no analogue of Theorem 2 per se, but there *is* an analogue of the statements (3.4) and (3.5). In the analogue of (3.5), however, the unitary group, $\exp \sqrt{-1}tP$, gets replaced by the corresponding heat semi-group, $\exp(-tP)$.

§4. The proof of Lee's theorem.

First of all note that if one replaces real $\mathcal{C}^\infty$ data by complex holomorphic data the existence theorem of §2 is still true and can be proved, with a few small changes, in exactly the same way. More explicitly, suppose Z and W are complex n-dimensional manifolds, $S_{\mathbb{C}}$ a complex hypersurface in $Z \times W$ and $\phi_{\mathbb{C}} = \phi_{\mathbb{C}}(z,w)$ a holomorphic defining function of $S_{\mathbb{C}}$ which satisfies the complex analogue of (2.3). Then one can modify $\phi_{\mathbb{C}}$, without changing $d\phi_{\mathbb{C}}$ at points of $S_{\mathbb{C}}$, so that it also satisfies

$$\det\left(\partial^2 \phi_{\mathbb{C}} \middle| \partial z_i \partial w_j\right) = 0 \tag{4.1}$$

on a neighborhood of S. Moreover, this modified $\phi_{\mathbb{C}}$ is unique.

Now let X be a compact complex n-dimensional manifold with a real-analytic strictly pseudoconvex boundary and let Z be an open complex manifold containing it. Let S be the boundary of X and let ϕ be a real-analytic defining function of S. I will denote by W the manifold, Z, equipped with its conjugate complex structure, and by ι the diagonal imbedding of Z into $Z \times W$. It is clear that there exists an open neighborhood, U, of the image of S in $Z \times W$ and a (unique) holomorphic function, $\phi_{\mathbb{C}}$, on U such that $\iota^*\phi_{\mathbb{C}} = \phi$. Let $S_{\mathbb{C}}$ be defined by the equation, $\phi_{\mathbb{C}} = 1$. Then the Levi condition implies that $\phi_{\mathbb{C}}$ satisfies the holomorphic analogue of (2.3) at all points $\iota(p), p \in S$; and, therefore, if U is chosen small enough, this condition is satisfied at all points of $S_{\mathbb{C}}$. Therefore, by the holomorphic version of Theorem 1, one can modify $\phi_{\mathbb{C}}$, without changing the first derivatives of $\phi_{\mathbb{C}}$ along $S_{\mathbb{C}}$, so that it satisfies (4.1). This, however, implies that $d\iota^*\phi_{\mathbb{C}} = d\phi$ at points of S and, in addition,

$$\det\left(\partial^2 \iota^* \phi_{\mathbb{C}} / \partial z_i \partial \bar{z}_j\right) = 0. \tag{4.2}$$

Moreover, $\iota^*\phi_{\mathbb{C}}$ is the unique real-analytic solution of (4.2) satisfying the given initial condition. However, since the initial data are real-valued, $\overline{\iota^*\phi_{\mathbb{C}}}$ is another solution of (4.2) with these initial data; so $\iota^*\phi_{\mathbb{C}} = \overline{\iota^*\phi_{\mathbb{C}}}$: i.e. $\iota^*\phi_{\mathbb{C}}$ is itself real-valued.

§5. Homogeneous Monge-Ampere and the extendibility problem.

Let X be a compact, complex n-dimensional manifold with a real-analytic strictly pseudoconvex boundary. As above I will assume that X is sitting inside an open complex manifold, Z, and that $\phi : Z \longrightarrow \mathbb{R}$ is a real analytic defining function of X. By choosing ϵ sufficiently small one can arrange that for all t on the interval, $(-\epsilon, \epsilon)$, $\phi - t$ is the defining function for a strictly pseudoconvex domain, X_{t+1} defined by the inequality, $\phi(z) \leq 1 + t$.

The problem I want to consider below is the extendibility problem: Given $s < t$ and given a holomorphic function, f, on X_s, can one extend f to a holomorphic function on X_t? I would like an answer to this question which is similar in spirit to the result of Boutet de Monvel that I quoted in the introduction: namely f can be extended providing one can solve some kind of diffusion process, with f as initial data, backwards in time over the interval $[s-t, 0]$. I will show that one can find a characterization of extendibility, in these terms, if ϕ satisfies homogeneous Monge-Ampere.* First of all, however, let me formulate the extendibility problem in a way that only involves the behavior of ϕ on the annulus

$$Z_\epsilon = \{z \in Z,\ 1 - \epsilon < \phi(z) < 1 + \epsilon\}$$

Let S_t be the boundary of the region, X_t, and ι_t the inclusion map of S_t into Z. Let $\mathcal{O}(X_t)$ be the space of functions which are holomorphic on $\mathrm{Int}(X_t)$ and smooth up to the boundary. Then the restriction map

$$\iota^* : \mathcal{O}(X_t) \longrightarrow \mathcal{C}^\infty(S_t)$$

is injective, and its image is the space of *Cauchy-Riemann functions* on S_t. I will denote this space by $\mathbb{CR}(S_t)$. Thus for $s < t$ one gets a diagram:

$$\text{(5.1)} \qquad \begin{array}{ccc} \mathcal{O}(X_t) & \xrightarrow{\cong} & \mathbb{C}R(S_t) \\ \big\downarrow & & \big\downarrow \\ \mathcal{O}(X_s) & \longrightarrow & \mathbb{CR}(S_s) \end{array}$$

the left hand arrow being the restriction map and $R_{s,t}$ being, by definition, the right hand arrow. Note that, for $-\epsilon < s < t < \mu < \epsilon$:

$$\text{(5.2)} \qquad R_{s,t}\ R_{t,u} = R_{s,u}.$$

It is clear that the extendibility problem is equivalent to the problem of characterizing the ranges of the mappings, $R_{s,t}$.

To formulate my main result I will have to discuss some geometric properties of the annulus, Z_ϵ, associated with the function, ϕ. I will think of the complex structure on Z as being given by a morphism, J, of the tangent bundle of Z, with $J^2 = -I$. Since $d\phi_p \neq 0$ at all points, $p \in Z_\epsilon$ the one-forms:

$$\text{(5.3)} \qquad d\phi \quad \text{and} \quad \alpha =: -d\phi \circ J$$

are non-vanishing and linearly independent everywhere. Corresponding to these one forms are a dual pair of vector fields, $\mathfrak{v}$ and $\mathfrak{w}$, which I will define by means of the following:

*And, in some sense, only if ϕ satisfies homogeneous Monge-Ampere.

Proposition. *There exists a unique vector field, $\mathfrak{w}$, on Z_ϵ with the following three properties*

$$(5.4)\qquad \begin{array}{ll} i. & \iota(\mathfrak{w})\alpha = 1 \\ ii. & \iota(\mathfrak{w})d\phi = 0 \\ iii. & \iota(\mathfrak{w})d\alpha \textit{ is the product of } d\phi \textit{ with a } \mathcal{C}^\infty \textit{ function.} \end{array}$$

Proof. To say that the hypersurfaces, $\phi = 1 + t$, are strictly pseudoconvex for $-\epsilon < t < \epsilon$ is equivalent to saying that

$$(5.5)\qquad (d\alpha)^{n-1} \wedge \alpha \wedge d\phi \neq 0$$

at all points of Z_ϵ, and the existence of a unique vector field, $\mathfrak{w}$, satisfying (5.4) can be deduced from (5.5) by elementary linear algebra. Q.E.D.

I will now define $\mathfrak{v}$ to be the vector field,

$$(5.6)\qquad \mathfrak{v} = J\mathfrak{w}.$$

From (5.3) and (5.4) one deduces

$$(5.7)\qquad \iota(\mathfrak{v})d\phi = 1 \quad \text{and} \quad \iota(\mathfrak{v})\alpha = 0.$$

Next I want to recall a standard criterion for the function, ϕ, to satisfy homogeneous Monge-Ampere:

Lemma. *ϕ satisfies homogeneous Monge-Ampere if and only if the condition, (5.4) iii., can be replaced by the stronger condition*

$$(5.8)\qquad \iota(\mathfrak{w})d\alpha = 0.$$

Proof. ϕ satisfies homogeneous Monge-Ampere if and only if the two-form, $d\alpha$, is of rank $n-1$ at all points of Z_ϵ, or in other words, if and only if there exists a nowhere vanishing vector field, $\mathfrak{w}$, satisfying (5.8). However, because of (5.5), if such a vector field exists, it can always be chosen to satisfy (5.4), i. and ii., as well. Q.E.D.

Corollary. *ϕ satisfies homogeneous Monge-Ampere if and only if $[\mathfrak{v}, \mathfrak{w}] = 0$.*

Proof. Since $\iota(\mathfrak{w})d\alpha$ is a multiple of $d\phi$ the condition (5.8) holds if and only if $d\alpha(\mathfrak{v}, \mathfrak{w}) = 0$. Note, however, that

$$(5.9)\qquad d\alpha(\mathfrak{v}, \mathfrak{w}) = D_{\mathfrak{v}}(\alpha(\mathfrak{w})) = D_{\mathfrak{w}}(\alpha(\mathfrak{v})) - \alpha([\mathfrak{v}, \mathfrak{w}]) = -\alpha([\mathfrak{v}, \mathfrak{w}]).$$

Therefore, if $[\mathfrak{v}, \mathfrak{w}] = 0$, ϕ satisfies Monge-Ampere. Conversely, suppose ϕ satisfies Monge-Ampere. Then $\iota(\mathfrak{w})d\alpha = 0$ by the Lemma. Moreover, since $d\alpha = (1/2i)\bar{\partial}\partial\phi$, $d\alpha$ is J-invariant;

so $\iota(\mathfrak{w})d\alpha = 0$. As we have just remarked, ϕ satisfies Monge-Ampere if and only if $d\alpha$ is of rank $n-1$ everywhere, in which case the annihilator of $d\alpha$ is an integrable two-dimensional subbundle of the tangent bundle of Z_ϵ. Since $\mathfrak{v}$ and $\mathfrak{w}$ are sections of the subbundle it follows from the Frobenius condition that

$$[\mathfrak{v}, \mathfrak{w}] = f_1\mathfrak{v} + f_2\mathfrak{w}$$

for appropriately chosen $\mathcal{C}^\infty$ functions, f_1 and f_2. However, by (5.9), $f_2 = 0$, and f_1 is zero in view of the identity:

$$d\phi([\mathfrak{v}, \mathfrak{w}]) = D_\mathfrak{v}(D_\mathfrak{w}\phi) - D_\mathfrak{w}D_\mathfrak{v}\phi = 0.$$

Q.E.D.

Since $\mathfrak{w} = J\mathfrak{v}$ this result can be interpreted as saying that there is a (local) action of the complex, group, $\mathbb{C}$, on Z_ϵ generated by the complex vector field, $\mathfrak{v} + \sqrt{-1}\mathfrak{w}$. This action of $\mathbb{C}$ does *not* preserve the complex structure of Z_ϵ; however, the fact that $\mathfrak{w} = J\mathfrak{v}$ implies that the orbits of $\mathbb{C}$ are one-dimensional complex submanifolds of Z_ϵ. The existence of a $\mathbb{C}$-action with this property is probably the single most important consequence of the fact that ϕ satisfies Monge-Ampere.*

From now on I will assume that ϕ satisfies homogeneous Monge-Ampere and will describe some of the implications this has for the extendibility problem. Using the results above I will derive a formula for the restriction operator

$$R_{s,u} : \mathbb{CR}(S_u) \longrightarrow \mathbb{CR}(S_s)$$

in terms of an infinite series which will, in general, *not* converge; however, I will extract from this formula a meaningful expression by the insertion of Szegö projectors, and the main theorem of this paper will say that what I get is still a good approximation to $R_{s,u}$.

Let f be in $\mathcal{O}(X_u)$ and let $t = u - s$. Since $\mathfrak{v} - \sqrt{-1}\mathfrak{w}$ is an anti-holomorphic vector field,

$$\left(D_\mathfrak{v} - \sqrt{-1}D_\mathfrak{w}\right) f = 0$$

and hence, formally,

$$f = \exp t\left(D_\mathfrak{v} - \sqrt{-1}D_\mathfrak{w}\right) f.$$

Since $D_\mathfrak{v}$ and $D_\mathfrak{w}$ commute one can formally rewrite this equation in the form,

$$f = \exp(-\sqrt{-1}tD_\mathfrak{w})(\exp t\mathfrak{v})^* f,$$

hence if g is the restriction of f to the surface, S_u, we get for $R_{s,u}g$ the following formal expression

$$R_{s,u}g = \exp\left(-\sqrt{-1}tD_\mathfrak{w}\right)(\exp t\mathfrak{v})^* g. \tag{5.10}$$

*For some of its implications see Dan Burn's article [Bu]. This $\mathbb{C}$-action also plays an important role in the articles of Lempert and Szöke mentioned in the introduction.

Let's see to what extent this formula makes sense as a representation of $R_{s,u}$. Since $\exp t\mathfrak{v}$ is a diffeomorphism of S_s onto S_u, the operator

$$(5.11) \qquad (\exp t\mathfrak{v})^* : \ \mathbb{C}\mathbb{R}(S_u) \longrightarrow \mathcal{C}^\infty(S_s)$$

makes perfectly good sense. As for the operator, $\exp(-\sqrt{-1}tD_{\mathfrak{w}})$, if we substitute for it the infinite series

$$(5.12) \qquad I + \left(-\sqrt{-1}tD_{\mathfrak{w}}\right) + \frac{1}{2!}\left(\sqrt{-1}tD_{\mathfrak{w}}\right)^2 \dots$$

each of the terms in this series is well defined as an operator on $\mathcal{C}^\infty(S_s)$ since the vector field, $\mathfrak{w}$, is tangent to S_s. Indeed, if h is a real-analytic function on S_s, then

$$(\exp tD_{\mathfrak{w}})h = (\exp t\mathfrak{w})^* h$$

and the term on the left is real analytic in t as well as in the manifold variables, so it can be analytically continued to a small neighborhood of the origin on the imaginary t-axis. Thus, $\exp(-\sqrt{-1}tD_{\mathfrak{w}})$ is well-defined as an operator, but its domain of definition is a rather small subspace of $\mathcal{C}^\infty(S_s)$.

Let me next recall the definition of the *Szegö projector* on $\mathcal{C}^\infty(S_s)$. Restricting to S_s the $(2n-1)$-form, $\alpha \wedge (d\alpha)^{n-1}$, it becomes a volume form and provides $L^2(S_s)$ with a Hilbert space structure. Let $H^2(S_s)$ be the L^2 completion of $\mathbb{C}\mathbb{R}(S_s)$ in $L^2(S_s)$ and let π_s be the orthogonal projection of $L^2(S_s)$ onto $H^2(S_s)$. This projection maps $\mathcal{C}^\infty(S_s)$ onto $\mathcal{C}^\infty(S_s) \cap H^2(S_s)$; and the latter space is $\mathbb{C}R(S_s)$; so, by restricting π_s to $\mathcal{C}^\infty(S_s)$ one gets an operator:

$$\pi_s : \ \mathcal{C}^\infty(S_s) \longrightarrow \mathbb{C}R(S_s);$$

and this is, by definition, the Szegö projector. I will now modify the right hand side of (5.12) by replacing the operator, $D_{\mathfrak{v}}$, wherever it occurs, by its Szegö cut-off: $\pi_s D_{\mathfrak{w}} \pi_s$. With this modification the right hand side of (5.12) becomes $\exp\left(-\sqrt{-1}t\pi_s D_{\mathfrak{w}}\pi_s\right)$ and since $t = u - s$, the right hand side of the formula, (5.10), for $R_{s,u}$ becomes

$$(5.13) \qquad \exp\left(-(u-s)T_s\right) F_{s,u}$$

where

$$(5.14) \qquad T_s = \pi_s \sqrt{-1} D_{\mathfrak{w}} \pi_s$$

and

$$(5.15) \qquad F_{s,u} = \pi_s (\exp(u-s)\mathfrak{v})^*.$$

For the following I will refer to [BG]:

Proposition A. *T_s is a positive first order self-adjoint elliptic Toeplitz operator. In particular it has real discrete spectrum:*

$$\lambda_0 \leq \lambda_1 \leq \lambda_2 \leq \dots,$$

with the λ_i's tending to $+\infty$ and satisfying the Weyl asymptotics:

$$N(\lambda) = \text{ volume } (S_s)\lambda^n + O(\lambda^{n-1})$$

where $N(\lambda) = \#\{\lambda_i < \lambda\}$.

For the proof of this see §1 of [BG]. The point of the proposition is that T_s has exactly the same kind of spectral behavior as a positive definite elliptic pseudodifferential operator of order one on a compact n-dimensional manifold.

As for $F_{s,u}$ one has:

Proposition B. *The operator, $F_{s,u} : \mathbb{CR}(S_u) \longrightarrow \mathbb{CR}(S_s)$ is an elliptic Fourier-Toeplitz operator of order zero with $\exp(u-s)\mathfrak{v} : S_s \longrightarrow S_u$ as its underlying canonical transformation. Moreover, for $u - s$ sufficiently small, it is invertible.*

This also follows easily from the theory of Fourier-Toeplitz operators developed in [BG] or from the more general theory of Fourier integral operators with positive phase function developed in [MS]. I won't bother to give a proof of it here.

Thanks to these two propositions, the operator, (5.13), has very nice analytic properties, and this brings up the question: To what extent is it still a good approximation to $R_{s,u}$. The main result of this paper is that it is still a good approximation in the following sense.

Theorem 4. *For u and s close to one and $u - s$ small there exists an invertible zeroth order elliptic Toeplitz operator*

$$\mathcal{Q}_{s,u} : \mathbb{CR}(S_s) \longrightarrow \mathbb{CR}(S_s)$$

which depends real-analytically on u and s and satisfies:

$$R_{s,u} = \exp(-(u-s)T_s)\mathcal{Q}_{s,u}F_{s,u}. \tag{5.16}$$

This theorem says, in particular, that for $u - s$ small the range of $R_{s,u}$ agrees with the range of $\exp(-(u-s)T_s)$ so, in particular, one obtains from Theorem 4 the following result on extendibility.

Theorem 5. *Let f be a holomorphic function on X_s, which is smooth up to the boundary. Then it extends to a holomorphic function on X_u, which is smooth up to the boundary, iff the restriction of f to the boundary of X_s is in the range of $\exp(-(u-s)T_s)$.*

§6. The proof of the extendibility theorem.

Let $u > s > 1$ and let $S_1 = S$, $\pi_1 = \pi$ and $T_1 = T$. For $u < 1 + \epsilon$ consider the operator

$$W_{s,u} = F_{1,s} R_{s,u} F_{1,u}^{-1}. \tag{6.1}$$

This operator maps $\mathbb{CR}(S)$ onto $\mathbb{CR}(S)$ and, for $s < t < u$, satisfies the semigroup property

$$W_{s,t} W_{t,u} = W_{s,u} \tag{6.2}$$

In particular

$$\frac{d}{ds} W_{s,u} = P_s W_{s,u} \tag{6.3}$$

where

$$P_s = -\left(\frac{d}{d\epsilon}\right)_+ W_{s-\epsilon,s} \quad \text{at } \epsilon = 0. \tag{6.4}$$

we will prove:

Lemma. *P_s is a first order Toeplitz operator with the same leading symbol as T.*

Proof. Given a $\mathbb{CR}$-function, $h \in \mathbb{CR}(S)$, let $g = F_{1,s}^{-1} h$ and let f be the unique element of $\mathcal{O}(X_s)$ whose restriction to S_s is g. Finally let $\iota : S \longrightarrow Z$ be the inclusion map. Then

$$\begin{aligned} W_{s-\epsilon,s} h &= F_{1,s-\epsilon} R_{s-\epsilon,s} g \\ &= \pi \iota^* \left(\exp(s-\epsilon)\mathfrak{v}\right)^* f \\ &= \pi \iota^* (\exp s\mathfrak{v})^* (\exp -\epsilon \mathfrak{v})^* f \end{aligned}$$

Thus, if we take the right hand derivative with respect to ϵ we get, at $\epsilon = 0$:

$$\left(\frac{d}{d\epsilon}\right)_+ W_{s-\epsilon,s} h = -\pi \iota^* (\exp s\mathfrak{v})^* D_{\mathfrak{v}} f.$$

Since f is holomorphic on the interior of X_s and smooth up to the boundary, and $\mathfrak{v} - \sqrt{-1}\mathfrak{w}$ is an anti-holomorphic vector field, $D_{\mathfrak{v}} f = \sqrt{-1} D_{\mathfrak{w}} f$. Moreover, since $\mathfrak{w}$ is tangent to S_s, $\sqrt{-1} D_{\mathfrak{w}} f$ is equal to $\sqrt{-1} D_{\mathfrak{w}} g$ on S_s; so the right hand side of the equation above is equal to

$$\pi (\exp s\mathfrak{v})^* (-\sqrt{-1} D_{\mathfrak{w}}) g$$

or

$$F_{1,s} (-\sqrt{-1} D_{\mathfrak{w}}) F_{1,s}^{-1} h.$$

Thus we obtain for P_s the formula

$$P_s = F_{1,s} (\sqrt{-1} D_{\mathfrak{w}}) F_{1,s}^{-1}. \tag{6.5}$$

By proposition B of §5 $F_{1,s}$ is a Fourier-Toeplitz operator whose underlying canonical transformation is $\exp(s-1)\mathfrak{v}$. Since $[\mathfrak{v}, \mathfrak{w}] = 0$

$$(6.6) \qquad (\exp t\mathfrak{v})^* D_{\mathfrak{w}} = D_{\mathfrak{w}} (\exp t\mathfrak{v})^*$$

for all t. Thus, by the composition formula for Fourier-Toeplitz operators described in [BG] §7, the operator (6.5) is a Toeplitz operator, and has the same leading symbol as the Toeplitz operator, $\pi(\sqrt{-1}D_{\mathfrak{v}})\pi$. Q.E.D.

Let $A(s) = P_s - T$. This operator is a zeroth order Toeplitz operator depending analytically on the parameter, s, and, by (6.3), it satisfies the operator equation

$$\frac{d}{ds} W_{s,u} = TW_{s,u} + A(s)W_{s,u}.$$

With u fixed, let $s = u - t$, and let $W(t) = W_{u-t,u}$ and $B(t) = -A(u-t)$. Then the equation above can be rewritten in the form

$$(6.7) \qquad \frac{d}{dt} W(t) = -TW(t) + B(t)W(t),$$

on the interval $0 \leq t \leq u-1$, with $W(0) = I$. Formally one can solve this equation by "variation of constants": i.e. setting

$$(6.8) \qquad B^{\#}(t) = (\exp tT) B(t) \exp(-tT),$$

one can express the solution of (6.7) in the form:

$$(6.9) \qquad W(t) = \exp(-tT) Q(t),$$

where $Q(t)$ is the solution of the operator equation,

$$(6.10) \qquad \frac{dQ(t)}{dt} = B^{\#}(t) Q(t) \quad \text{with} \quad Q(0) = I.$$

To make sense of this formal solution we must first make sense of (6.8), and this we will do as follows: Since $B(t)$ depends real-analytically on t, it extends to a holomorphic function of t on a small neighborhood of the origin in the complex t-plane. Thus in particular $B(\sqrt{-1}t)$ is well defined, by analytic continuation, for real values of t close to zero. Now notice that when we replace t by $\sqrt{-1}t$ in (6.8), (6.8) becomes:

$$(6.11) \qquad B^{\#}(\sqrt{-1}t) = \exp\sqrt{-1}tT \; B(\sqrt{-1}t) \exp(-\sqrt{-1}tT).$$

Since $\exp\sqrt{-1}tT$ is an elliptic zeroth order Fourier-Toeplitz operator, it follows from Egorov's theorem that (6.11) is a zeroth order Toeplitz operator, also depending in a real analytic fashion on t. Thus we can again, for $|t|$ small, replace t by $-\sqrt{-1}t$ in (6.11), and we end up with a well-defined zeroth order Toeplitz operator which is, formally, the operator (6.8). This we will now *define* to be the operator, $B^{\#}(t)$. With this definition of $B^{\#}(t)$ the equation (6.8) holds in the sense that for all $a > t$

$$\exp(-aT)B^{\#}(t) = \exp(t-a)TB(t)\exp(-tT). \tag{6.12}$$

Plugging this Toeplitz operator, $B^{\#}(t)$, that we have just defined, into (6.10) and solving for $\mathcal{Q}(t)$ we end up with a putative solution, $W(t) = \exp(-tT)\mathcal{Q}(t)$, to the equation, (6.7). To show, by means of (6.12), that this is an actual solution is not hard. We leave details to the reader.*

Inserting (6.10) into (6.1) and remembering that $\mathcal{Q}(t)$ depends analytically on the parameter, μ, as well as on t we get

$$\exp-(u-s)Q_u(u-s) = F_{1,s}R_{s,u}F_{1,s}^{-1}$$

or, in particular, setting $s = 1$,

$$R_{1,u} = \exp(-(u-1)T)Q_u(u-1)F_{1,u}$$

for $1 < u < \epsilon$. This proves Theorem 4 for $s = 1$; and the theorem, for arbitrary s, can be deduced from this special case by replacing ϕ, in the discussion above, by $\phi - (s-1)$.

BIBLIOGRAPHY

[AM] R. Abraham and J. Marsden,, *Foundations of Mechanics*, Benjamin, Reading, MA, 1978.

[B] L. Boutet de Monvel, *Convergence dans le domaine complex des séries de fonctions propres*, C.R. Acad. Sc. Paris (Serie A) **t.285** (1978), 855–856.

[BG] L. Boutet de Monvel and V. Guillemin, *The spectral theory of Toeplitz operators*, Ann. of Math. Studies no. 99, Princeton U. Press Princeton, N.J., 1981.

[Bu] D. Burns, *Curvature of Monge-Ampere foliations and parabolic manifolds*, Ann. of Math. **115** (1982), 349–373.

[EM] C. Epstein and R. Melrose, *Shrinking tubes and the $\bar{\partial}$-Neumann problem*, preprint (1990).

[GS$_1$] V. Guillemin, *Grauert tubes and the homogeneous Monge-Ampere equation I*, J. of Diff. Geom. (to appear).

[GS$_2$] ———, *Grauert tubes and the homogeneous Monge-Ampere equation II*, preprint (1990).

[GS] V. Guillemin and S. Sternberg, *Geometric Asymptotics*, AMS Math. Surveys no. 14, Providence, R.I., 1978.

[JL] D. Jerison and J. Lee, *The Yamabe problem on CR manifolds*, J. Diff. Geom. **25** (1987), 167–197.

[L] J. Lee, *Higher asymptotics of the complex Monge-Ampere equation and geometry of CR-manifolds*, Ph.D thesis M.I.T. (1982).

[Lem] L. Lempert, *Complex structures on the tangent bundle of a Riemannian manifold*, preprint (1990).

*The argument I've just sketched is due to Boutet de Monvel. See [B].

[LS] L. Lempert and R. Szöke, *Global solutions of the homogeneous complex Monge-Ampere equation and complex structures on the tangent bundle of a Riemannian manifold*, preprint (1990).

[MS] A. Melin and J. Sjöstrand, *Fourier integral operators with complex-valued phase functions*, Lecture Notes, Springer Verlag **459**, 120–223.

[S] R. Szöke, *Complex structures on tangent bundles of Riemannian manifolds*, preprint (1990).

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Classification and normal forms for quantum mechanical eigenvalue cossings

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Classification and Normal Forms for Quantum Mechanical Eigenvalue Crossings

George A. Hagedorn

In the study of molecular dynamics, it is often useful to consider the quantum mechanics of the electrons with the nuclei in fixed positions. When this is done, the positions of the nuclei are described by a nuclear configuration vector $X \in \mathbb{R}^n$, and the Hamiltonian for the electrons is a self-adjoint operator-valued function $h(X)$ of the nuclear configurations. A discrete eigenvalue $E(X)$ of $h(X)$ is called an electron energy level.

Electron energy levels play a major role in the time–dependent Born–Oppenheimer approximation [1,2]. In this approximation the electrons propagate adiabatically and the nuclei obey a semiclassical approximation. In this context, adiabatic means that if the electrons are initially in an eigenstate associated with a level $E(X)$, then at a later time, they will be again be found in an eigenstate associated with $E(X)$. The eigenvalue $E(X)$ also acts an effective potential for the semiclassical propagation of the nuclei.

This approximation breaks down when the electron energy level $E(X)$ crosses any other part of the spectrum of $h(X)$, and the simplest such breakdown occurs when $E(X)$ crosses another eigenvalue of $h(X)$. In this paper we describe the first step in the study of what happens when a Born–Oppenheimer state encounters such a crossing. This first step is the classification of generic minimal degeneracy quantum eigenvalue crossings and determination of normal forms for $h(X)$ near each type of crossing. The various different types of crossings arise from different symmetry situations. We prove below that eleven distinct situations can occur.

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Throughout the paper we assume $h(X)$ is a C^2 function of $X \in \mathbb{R}^n$ in the sense that its resolvent is C^2. In the various different situations, we assume the dimension n of the nuclear configuration space is large enough so that the appropriate type of crossing can occur generically. We show below that in each generic crossing situation, the two eigenvalues coincide on a submanifold Γ of some specific codimension. If n is less than this codimension, then that type of crossing generically does not occur.

We let G denote the symmetry group of $h(X)$. That is, G is the group of all unitary and antiunitary operators that are X–independent in some representation of the electronic Hilbert space, and that commute with all the operators $h(X)$. We let H denote the subgroup of unitary elements of G, and note that antiunitary elements of G reverse time.

Since the product of unitary and antiunitary operators is antiunitary, there are clearly two cases: Either $G = H$ or H is a subgroup of G of index 2.

When $G = H$, standard group representation theory applies, and each distinct eigenvalue of $h(X)$ is associated with a unique representation of G. Minimal multiplicity eigenvalues correspond to 1–dimensional representations, and if two simple eigenvalues $E_{\mathcal{A}}(X)$ and $E_{\mathcal{B}}(X)$ cross, then there are two possiblilities:

Type A Crossings: The two irreducible representations of G that correspond to $E_{\mathcal{A}}(X)$ and $E_{\mathcal{B}}(X)$ are not unitarily equivalent to one another.

Type B Crossings: The two irreducible representations of G that correspond to $E_{\mathcal{A}}(X)$ and $E_{\mathcal{B}}(X)$ are unitarily equivalent to one another.

When H is a subgroup of index 2, standard group representation theory does not apply. Instead of representations, the basic objects of interest are called corepresentations. A general theory of corepresentations was first developed by Wigner [6]. A more modern, non–basis–dependent treatment can be found in [5]. This general theory shows that any corepresentation can be decomposed as a direct sum of irreducible corepresentations. Furthermore, there are three distinct types of irreducible corepresentations which are called Types *I, II, and III.*

To describe these three types, we first note that G can be decomposed as $G = H \cup \mathcal{K}H$, where $\mathcal{K}$ is an arbitrary, but fixed, antiunitary element of G. Then, if U is an irreducible corepresentation of G, we let U_H denote the restriction of U to H. Then the three types are described as follows [5]:

Type I Corepresentations: U_H is an irreducible representation.

Type II Corepresentations: U_H decomposes into a direct sum of two equivalent irreducible representations, $U_H = D \oplus D$. Furthermore, U may be cast in the form
$U(h) = \begin{pmatrix} D(h) & 0 \\ 0 & D(h) \end{pmatrix}$, $U(\mathcal{K}) = \begin{pmatrix} 0 & -K \\ K & 0 \end{pmatrix}$, and $U(\mathcal{K}h) = U(\mathcal{K})\,U(h)$, for all $h \in H$. Here K is an antiunitary operator that satisfies $K^2 = -D(\mathcal{K}^2)$ and $K\,D(\mathcal{K}^{-1}h\mathcal{K})\,K^{-1} = D(h)$ for all $h \in H$.

Type III Corepresentations: U_H decomposes into a direct sum of two inequivalent irreducible representations, $U_H = D \oplus C$. Furthermore, U may be cast in the form
$U(h) = \begin{pmatrix} D(h) & 0 \\ 0 & C(h) \end{pmatrix}$, $U(a) = \begin{pmatrix} 0 & D(\mathcal{K}^2)K^{-1} \\ K & 0 \end{pmatrix}$, and $U(\mathcal{K}h) = U(\mathcal{K})\,U(h)$, for all $h \in H$. Here $K : \mathcal{H}_D \to \mathcal{H}_C$ is an antiunitary operator that satisfies $K\,D(\mathcal{K}^{-1}h\mathcal{K})\,K^{-1} = C(h)$ for all $h \in H$.

When $G \neq H$, each distinct eigenvalue of $h(X)$ is associated with a unique corepresentation of G. From the structure theory outlined above, it is clear that minimal multiplicity eigenvalues associated with Type I corepresentations have multiplicity 1. Minimal multiplicity eigenvalues associated with Type II or Type III corepresentations have multiplicity 2. In the minimal multiplicity situations, the antiunitary operators K that occur in Type II corepresentations map a one dimensional space to itself. A simple calculation shows that such operators satisfy $K^2 = 1$. Thus, in the minimal multiplicity situation, K is a conjugation, and $D(\mathcal{K}^2) = -1$.

This structure theory of corepresentations shows that if two minimal multiplicity eigenvalues $E_{\mathcal{A}}(X)$ and $E_{\mathcal{B}}(X)$ cross, then there are nine possiblilities:

Type C Crossings: The two irreducible corepresentations of G that correspond to $E_{\mathcal{A}}(X)$ and $E_{\mathcal{B}}(X)$ are both of Type I, but are not unitarily equivalent to one another. Both eigenvalues have multiplicity 1 away from the crossing.

Type D Crossings: The two irreducible corepresentations of G that correspond to $E_{\mathcal{A}}(X)$ and $E_{\mathcal{B}}(X)$ are both of Type *II*, but are not unitarily equivalent to one another. Both eigenvalues have multiplicity 2 away from the crossing.

Type E Crossings: The two irreducible corepresentations of G that correspond to $E_{\mathcal{A}}(X)$ and $E_{\mathcal{B}}(X)$ are both of Type *III*, but are not unitarily equivalent to one another. Both eigenvalues have multiplicity 2 away from the crossing.

Type F Crossings: The two irreducible corepresentations of G that correspond to $E_{\mathcal{A}}(X)$ and $E_{\mathcal{B}}(X)$ are of Types *I* and *II*. Away from the crossing, the eigenvalue associated with the Type *I* corepresentation has multiplicity 1 and the other eigenvalue has multiplicity 2 away from the crossing.

Type G Crossings: The two irreducible corepresentations of G that correspond to $E_{\mathcal{A}}(X)$ and $E_{\mathcal{B}}(X)$ are of Types *I* and *III*. Away from the crossing, the eigenvalue associated with the Type *I* corepresentation has simple multiplicity and the other eigenvalue has multiplicity 2.

Type H Crossings: The two irreducible corepresentations of G that correspond to $E_{\mathcal{A}}(X)$ and $E_{\mathcal{B}}(X)$ are of Types *II* and *III*. Both eigenvalues have multiplicity 2 away from the crossing.

Type I Crossings: The two irreducible corepresentations of G that correspond to $E_{\mathcal{A}}(X)$ and $E_{\mathcal{B}}(X)$ are both of Type *I* and are unitarily equivalent to one another. Both eigenvalues are multiplicity 1 away from the crossing.

Type J Crossings: The two irreducible corepresentations of G that correspond to $E_{\mathcal{A}}(X)$ and $E_{\mathcal{B}}(X)$ are both of Type *II* and are unitarily equivalent to one another. Both eigenvalues are multiplicity 2 away from the crossing.

Type K Crossings: The two irreducible corepresentations of G that correspond to $E_{\mathcal{A}}(X)$ and $E_{\mathcal{B}}(X)$ are both of Type *III* and are unitarily equivalent to one another. Both eigenvalues are multiplicity 2 away from the crossing.

REMARK: One can easily find simple quantum systems that provide examples of the various types of crossings.

We now turn to the detailed structure of the electron Hamiltonian function

$h(X)$ near a generic crossing of each type. In our applications [3,4] we assume that the nuclear wave packets propagate non-tangentially through the manifold Γ, where $E_{\mathcal{A}}(X) = E_{\mathcal{B}}(X)$. As these packets propagate through the crossing, their mean momentum is approximately given by a fixed vector η_0. This vector determines a special direction in the nuclear configuration space that is not tangent to Γ. In some cases, the normal forms we derive for $h(X)$ depend on this special direction.

STRUCTURE OF CROSSINGS OF TYPES A AND C. Suppose two eigenvalues $E_{\mathcal{A}}(X)$ and $E_{\mathcal{B}}(X)$ of a C^2 electron Hamiltonian function $h(X)$ have a crossing of Type A or Type C at $X = 0$. By properly labeling the eigenvalues, we may assume that $E_{\mathcal{A}}(X)$ corresponds to one irreducible representation or corepresentation U_1 of G for all X, and that $E_{\mathcal{B}}(X)$ corresponds to U_2 for all X. Since $h(X)$ commutes with the action of G, it follows that $h(X)$ commutes with the orthogonal projections P_1 and P_2 onto the mutually orthogonal carrier subspaces associated with U_1 and U_2, respectively.

For X in a neighborhood of the origin, one can write the spectral projection $P(X)$ for $h(X)$ associated with both the eigenvalues $E_{\mathcal{A}}(X)$ and $E_{\mathcal{B}}(X)$ as

$$P(X) \;=\; \frac{1}{2\pi i}\int_C (z - h(X))^{-1}\, dz,$$

where C is a contour that encloses $E_{\mathcal{A}}(X)$ and $E_{\mathcal{B}}(X)$ but no other parts of the spectrum of $h(X)$. From this it follows that $P(X)$ is a C^2, rank 2 operator valued function of X near $X = 0$ that commutes with P_1 and P_2. Since U_1 and U_2 are inequivalent, it follows that $P_{\mathcal{A}}(X) = P_1\, P(X)$ and $P_{\mathcal{B}}(X) = P_2\, P(X)$ are C^2, rank one orthogonal projections that project onto mutually orthogonal subspaces.

For Type A crossings, we arbitrarily choose $\Phi_{\mathcal{A}}(0)$ and $\Phi_{\mathcal{B}}(0)$ to be unit vectors in the ranges of $P_{\mathcal{A}}(0)$ and $P_{\mathcal{B}}(0)$, respectively. We then define

$$\Phi_{\mathcal{A}}(X) \;=\; \frac{P_{\mathcal{A}}(X)\Phi_{\mathcal{A}}(0)}{\sqrt{\langle \Phi_{\mathcal{A}}(0),\, P_{\mathcal{A}}(X)\Phi_{\mathcal{A}}(0)\rangle}}$$

and

$$\Phi_{\mathcal{B}}(X) \;=\; \frac{P_{\mathcal{B}}(X)\Phi_{\mathcal{B}}(0)}{\sqrt{\langle \Phi_{\mathcal{B}}(0),\, P_{\mathcal{B}}(X)\Phi_{\mathcal{B}}(0)\rangle}}.$$

By standard perturbation theory, these unit–vector valued functions are C^2 in a neighborhood of the origin and belong to the ranges of $P_{\mathcal{A}}(X)$ and $P_{\mathcal{B}}(X)$, respectively, for each X. Furthermore, $\Phi_{\mathcal{A}}(X)$ and $\Phi_{\mathcal{B}}(X)$ are eigenvectors of $h(X)$ that correspond to $E_{\mathcal{A}}(X)$ and $E_{\mathcal{B}}(X)$, respectively. Standard arguments also show that $E_{\mathcal{A}}(\cdot)$ and $E_{\mathcal{B}}(\cdot)$ are C^2 functions in a neighborhood of the origin.

For Type C crossings, we perform the same construction, but impose an additional constraint. By decomposing $G = H \cup \mathcal{K}H$, we have selected a special antiunitary element $\mathcal{K}$ of G. A simple calculation shows that we may choose the phases of the vectors $\Phi_{\mathcal{A}}(0)$ and $\Phi_{\mathcal{B}}(0)$ so that $\mathcal{K}\,\Phi_{\mathcal{A}}(0) = \Phi_{\mathcal{A}}(0)$ and $\mathcal{K}\,\Phi_{\mathcal{B}}(0) = \Phi_{\mathcal{B}}(0)$. By making such choices we obtain vectors $\Phi_{\mathcal{A}}(X)$ and $\Phi_{\mathcal{B}}(X)$ that satisfy $\mathcal{K}\,\Phi_{\mathcal{A}}(X) = \Phi_{\mathcal{A}}(X)$ and $\mathcal{K}\,\Phi_{\mathcal{B}}(X) = \Phi_{\mathcal{B}}(X)$.

Let $h^{\perp}(X)$ denote the restriction of $h(X)$ to the subspace orthogonal to the range of $P(X)$. By using $\Phi_{\mathcal{A}}(X)$ and $\Phi_{\mathcal{B}}(X)$ as a basis for the range of $P(X)$ and identifying $\mathcal{H} \cong \mathbb{C} \oplus \mathbb{C} \oplus \mathrm{Ran}\,(1 - P(X))$, we can locally represent $h(X)$ by the matrix

$$\tilde{h}(X) = \begin{pmatrix} E_{\mathcal{A}}(X) & 0 & 0 \\ 0 & E_{\mathcal{B}}(X) & 0 \\ 0 & 0 & h^{\perp}(X) \end{pmatrix}.$$

Throughout our discussion, no restrictions have been imposed on the functions $E_{\mathcal{A}}(X)$ and $E_{\mathcal{B}}(X)$, except that they take the same value at the origin. Thus, they could be any two C^2 functions whose values coincide at the origin. Generically the values of two such functions coincide on a submanifold Γ of codimension 1.

STRUCTURE OF CROSSINGS OF TYPES F AND G. Suppose two eigenvalues $E_{\mathcal{A}}(X)$ and $E_{\mathcal{B}}(X)$ of a C^2 electron Hamiltonian function $h(X)$ have a crossing of Type F or Type G at $X = 0$. We may assume the eigenvalues are labeled so that the corepresentation associated with $E_{\mathcal{A}}(X)$ if of type *I* and the corepresentation assiciated with $E_{\mathcal{B}}(X)$ is of type *II* or *III*. Let U_1 and U_2 denote the irreducible corepresentations of G associated with $E_{\mathcal{A}}(X)$ and $E_{\mathcal{B}}(X)$, respectively, and note that the dimension of the U_2 is 2. As in the case of Type A or C crossings, $h(X)$ commutes with the orthogonal projections P_1

and P_2 onto the mutually orthogonal carrier subspaces $\mathcal{H}_1$ and $\mathcal{H}_2$ associated with U_1 and U_2, respectively.

For X in a neighborhood of the origin, one can write the spectral projection $P(X)$ for $h(X)$ associated with the eigenvalues $E_{\mathcal{A}}(X)$ and $E_{\mathcal{B}}(X)$ as an integral of the resolvent of $h(X)$. From this it follows that $P(X)$ is a C^2, rank 3 operator valued function of X near $X = 0$ that commutes with P_1 and P_2. Since U_1 and U_2 are inequivalent, it follows that $P_{\mathcal{A}}(X) = P_1\, P(X)$ and $P_{\mathcal{B}}(X) = P_2\, P(X)$ are C^2, rank one and (respectively) rank two orthogonal projections that project onto mutually orthogonal subspaces.

We construct a C^2 unit-vector valued function $\Phi_{\mathcal{A}}(\cdot)$ exactly as in the case of a Type C crossing, so that $\mathcal{K}\,\Phi_{\mathcal{A}}(X) = \Phi_{\mathcal{A}}(X)$. For a Type F crossing we choose $\Phi_{\mathcal{B},1}(0)$ to be an arbitrary unit vector in the range of $P_{\mathcal{B}}(0)$. We then let

$$\Phi_{\mathcal{B},1}(X) \;=\; \frac{P_{\mathcal{B}}(X)\Phi_{\mathcal{B},1}(0)}{\sqrt{\langle\Phi_{\mathcal{B},1}(0),\, P_{\mathcal{B}}(X)\Phi_{\mathcal{B},1}(0)\rangle}}.$$

and

$$\Phi_{\mathcal{B},2}(X) \;=\; \mathcal{K}\,\Phi_{\mathcal{B},1}(X).$$

Because $\mathcal{K}$ is antiunitary and $D(\mathcal{K}^2) = -1$, it follows that $\Phi_{\mathcal{B},1}(X)$ and $\Phi_{\mathcal{B},2}(X)$ comprise an orthonormal basis for the range of $P_{\mathcal{B}}(X)$.

For Type G crossings, we let P_C and P_D denote the orthogonal projections onto the carrier subspaces for the two representations C and D of the subgroup H that are involved. These projections commute with $P_{\mathcal{B}}(X)$ and project onto mutually orthogonal subspaces. Furthermore, $P_C P_{\mathcal{B}}(X)$ and $P_D P_{\mathcal{B}}(X)$ are rank one projections. We choose $\Phi_{\mathcal{B},1}(0)$ to be a unit vector in the range of $P_D P_{\mathcal{B}}(0)$. We then let

$$\Phi_{\mathcal{B},1}(X) \;=\; \frac{P_{\mathcal{B}}(X)\Phi_{\mathcal{B},1}(0)}{\sqrt{\langle\Phi_{\mathcal{B},1}(0),\, P_{\mathcal{B}}(X)\Phi_{\mathcal{B},1}(0)\rangle}}.$$

and

$$\Phi_{\mathcal{B},2}(X) \;=\; \mathcal{K}\,\Phi_{\mathcal{B},1}(X).$$

From the structure theory of type *III* corepresentations, we see that $\Phi_{\mathcal{B},2}(X)$ belongs to the range of $P_C P_{\mathcal{B}}(X)$, and that $\Phi_{\mathcal{B},1}(X)$ and $\Phi_{\mathcal{B},2}(X)$ comprise a C^2 orthonormal basis for the range of $P_{\mathcal{B}}(X)$.

Let $h^\perp(X)$ denote the restriction of $h(X)$ to the subspace orthogonal to the range of $P(X)$. By using $\Phi_{\mathcal{A}}(X)$, $\Phi_{\mathcal{B},1}(X)$ and $\Phi_{\mathcal{B},2}(X)$ as a basis for the range of $P(X)$ and identifying $\mathcal{H} \cong \mathbb{C} \oplus \mathbb{C}^2 \oplus \mathrm{Ran}\,(1 - P(X))$, we can locally represent $h(X)$ by the matrix

$$\tilde{h}(X) \;=\; \begin{pmatrix} E_{\mathcal{A}}(X) & 0 & 0 & 0 \\ 0 & E_{\mathcal{B}}(X) & 0 & 0 \\ 0 & 0 & E_{\mathcal{B}}(X) & 0 \\ 0 & 0 & 0 & h^\perp(X) \end{pmatrix}.$$

As in the case of Type A and C crossings, no restrictions are imposed on $E_{\mathcal{A}}(X)$ and $E_{\mathcal{B}}(X)$. Thus, they generically cross on a codimension 1 submanifold Γ.

Structure of Crossings of Types D, E, and H. Suppose two eigenvalues $E_{\mathcal{A}}(X)$ and $E_{\mathcal{B}}(X)$ of an electron Hamiltonian function $h(X)$ have a crossing of type D, E, or H at $X = 0$. By mimicking the constructions used for Type F and G crossings, we see that we can choose four smooth, mutually orthogonal unit–vector valued functions $\Phi_{\mathcal{A},1}(X)$, $\Phi_{\mathcal{A},2}(X) = \mathcal{K}\,\Phi_{\mathcal{A},1}(X)$, $\Phi_{\mathcal{B},1}(X)$, and $\Phi_{\mathcal{B},2}(X) = \mathcal{K}\,\Phi_{\mathcal{B},1}(X)$, such that $\Phi_{\mathcal{A},1}(X)$, and $\Phi_{\mathcal{A},2}(X)$ are eigenvectors of $h(X)$ with eigenvalue $E_{\mathcal{A}}(X)$, and $\Phi_{\mathcal{B},1}(X)$, and $\Phi_{\mathcal{B},2}(X)$ are eigenvectors of $h(X)$ with eigenvalue $E_{\mathcal{B}}(X)$. Furthermore, whenever a type III corepresentation is involved, the eigenvector with second subscript 1 belongs to one representation of the subgroup H and the eigenvector with the second subscript 2 belongs to the other representation of the subgroup.

As in the earlier constructions, by using these vectors as part of a basis, and identifying $\mathcal{H} \cong \mathbb{C}^2 \oplus \mathbb{C}^2 \oplus \mathrm{Ran}\,(1 - P(X))$, we can locally represent $h(X)$ by the matrix

$$\tilde{h}(X) \;=\; \begin{pmatrix} E_{\mathcal{A}}(X) & 0 & 0 & 0 & 0 \\ 0 & E_{\mathcal{A}}(X) & 0 & 0 & 0 \\ 0 & 0 & E_{\mathcal{B}}(X) & 0 & 0 \\ 0 & 0 & 0 & E_{\mathcal{B}}(X) & 0 \\ 0 & 0 & 0 & 0 & h^\perp(X) \end{pmatrix}.$$

As in the earlier cases, $E_{\mathcal{A}}(X)$ and $E_{\mathcal{B}}(X)$ generically cross on a submanifold Γ of codimension 1.

STRUCTURE OF TYPE I CROSSINGS Suppose a C^2 electron Hamiltonian function $h(X)$ has a type I crossing of two simple eigenvalues $E_{\mathcal{A}}(X)$ and $E_{\mathcal{B}}(X)$ at $X = 0$. As in the earlier cases, the projection $P(X)$ for $h(X)$ associated with the eigenvalues $E_{\mathcal{A}}(X)$ and $E_{\mathcal{B}}(X)$ is a C^2, rank 2 operator valued function of X near $X = 0$. It follows that $E_{\mathcal{A}}(X) + E_{\mathcal{B}}(X) = \mathrm{trace}\,(h(X)P(X))$ is also C^2. Thus,

$$h_1(X) \;=\; h(X) \,-\, \tfrac{1}{2}\,(\,E_{\mathcal{A}}(X) \,+\, E_{\mathcal{B}}(X)\,)$$

is a C^2 operator–valued function whose restriction to the range of $P(X)$ is traceless.

Let $\{\,\psi_1,\,\psi_2\,\}$ be a basis for the range of $P(0)$. By altering the phases of these two vectors, we may assume that $\mathcal{K}\,\psi_1 \,=\, \psi_1$ and $\mathcal{K}\,\psi_2 \,=\, \psi_2$, where $\mathcal{K}$ is the antiunitary operator chosen for the decomposition $G = H \cup \mathcal{K}H$. Define $\psi_1(X)$ for X by

$$\psi_1(X) \;=\; \frac{P(X)\,\psi_1}{\sqrt{\langle\,\psi_1,\,P(X)\,\psi_1\,\rangle}}.$$

Since $P(X)$ is C^2 and commutes with the action of G, $\psi_1(X)$ is well defined and C^2 in some neighborhood of the origin and satisfies $\mathcal{K}\,\psi_1(X) \,=\, \psi_1(X)$. Let $P_1(X)$ denote the projection onto the subspace spanned by $\psi_1(X)$. It is a C^2 operator–valued function in a neighborhood of X that commutes with $P(X)$ and the action of G. We define

$$\psi_2(X) \;=\; \frac{P(X)\,(1 - P_1(X))\psi_2}{\sqrt{\langle\,\psi_2,\,P(X)\,(1 - P_1(X))\,\psi_2\,\rangle}}.$$

This vector valued function is also C^2 in a neighborhood of the origin; $\mathcal{K}\,\psi_2(X) \,=\, \psi_2(X)$; and $\{\,\psi_1(X),\,\psi_2(X)\,\}$ is an orthonormal basis for the range of $P(X)$, for X in a neighborhood of the origin.

In the basis $\{\,\psi_1(X),\,\psi_2(X)\,\}$, the restriction of $h_1(X)$ to the range of $P(X)$ is represented by a real symmetric, traceless 2×2 matrix valued function $M(X)$ whose entries are C^2 functions that all vanish when $X = 0$. That is,

$$M(X) \;=\; \begin{pmatrix} \alpha(X) & \beta(X) \\ \beta(X) & -\alpha(X) \end{pmatrix},$$

where α and β are real valued C^2 functions. The eigenvalues $E_{\mathcal{A}}(X)$ and $E_{\mathcal{B}}(X)$ cross precisely at those points X where $\alpha(X) \,=\, \beta(X) \,=\, 0$. Generically this defines a codimension 2 submanifold Γ. Furthermore, the difference between $E_{\mathcal{A}}(X)$ and $E_{\mathcal{B}}(X)$ is the same as the difference between the eigenvalues of $M(X)$. By direct computation, the eigenvalues of $M(X)$ are

$$\pm\sqrt{\alpha(X)^2 + \beta(X)^2}.$$

Generically this function is continuous, but not differentiable near Γ. One can easily show that the eigenvectors are not even continuous near Γ.

By standard Taylor series results, $M(X)$ has the form $M(X) = N(X) + O(\|X\|^2)$, where

$$N(X) = \begin{pmatrix} a\cdot X & b\cdot X \\ b\cdot X & -a\cdot X \end{pmatrix},$$

for some vectors a and b. Generically a and b are linearly independent. By a rotation of the coordinate system we may assume that only the first two components of a and b are non-zero.

If η_0 is a vector not tangent to Γ at $X = 0$, then we can rotate the first two coordinate axes so that the projection of η_0 into the two dimensional subspace spanned by a and b lies along the positive X_1 axis.

At this point, the X_j coordinates for $j > 2$ no longer play a role in the structure of $N(X)$. Furthermore, the form of $N(X)$ is not altered if we do X-independent orthogonal transformations of the two dimensional space spanned by the basic electronic wave functions $\psi_1(X)$ and $\psi_2(X)$. We replace $\psi_1(X)$ by $\cos(\theta)\psi_1(X) + \sin(\theta)\psi_2(X)$ and $\psi_2(X)$ by $-\sin(\theta)\psi_1(X) + \cos(\theta)\psi_1(X)$. A simple calculation shows that we can choose θ so that the X_1-component of b is zero. Finally, by possibly interchanging the order of $\psi_1(X)$ and $\psi_2(X)$ or multiplying one of them by -1, we can assume that the X_1-component of a and the X_2-component of b are both positive.

Thus, $N(X)$ has the form

$$N(X) = \begin{pmatrix} a_1X_1 + a_2X_2 & b_2X_2 \\ b_2X_2 & -a_1X_1 - a_2X_2 \end{pmatrix},$$

where a_1 and b_2 have the same sign. So, by identifying $\mathcal{H} \cong \mathbb{C} \oplus \mathbb{C} \oplus \operatorname{Ran}(1 - P(X))$, we can locally approximate $h_1(X)$ by the matrix

$$\tilde{h}_1(X) = \begin{pmatrix} a_1X_1 + a_2X_2 & b_2X_2 & 0 \\ b_2X_2 & -a_1X_1 - a_2X_2 & 0 \\ 0 & 0 & h_1^{\perp}(X) \end{pmatrix}.$$

STRUCTURE OF TYPE B CROSSINGS Suppose a C^2 electron Hamiltonian function $h(X)$ has a type B crossing of two simple eigenvalues $E_{\mathcal{A}}(X)$ and $E_{\mathcal{B}}(X)$ at $X = 0$. In this situation we mimic the construction of the vectors $\psi_1(X)$ and $\psi_2(X)$ in the case of a Type I crossing. Since there is no anitunitary operator $\mathcal{K} \in G$, we choose arbitrary orthogonal unit vectors $\psi_1(0)$ and $\psi_2(0)$ from the range of $P(X)$, and then proceed with the construction. This yields an orthonormal basis $\{\, \psi_1(X),\, \psi_2(X)\,\}$ for the range of $P(X)$.

In this basis, the restriction of

$$h_1(X) \;=\; h(X) \,-\, \tfrac{1}{2}\,(E_{\mathcal{A}}(X) \,+\, E_{\mathcal{B}}(X)\,)$$

to the range of $P(X)$ is represented by a self-adjoint traceless 2×2 matrix valued function $M(X)$ whose entries are C^2 functions that all vanish when $X = 0$. That is,

$$M(X) \;=\; \begin{pmatrix} \alpha(X) & \beta(X) + i\gamma(X) \\ \beta(X) - i\gamma(X) & -\alpha(X) \end{pmatrix},$$

where α, β, and γ are C^2 real valued functions. The difference between $E_{\mathcal{A}}(X)$ and $E_{\mathcal{B}}(X)$ is the same as the difference between the eigenvalues of $M(X)$. By direct computation, the eigenvalues of $M(X)$ are

$$\pm\,\sqrt{\alpha(X)^2 \,+\, \beta(X)^2 \,+\, \gamma(X)^2}.$$

Thus, the eigenvalues $E_{\mathcal{A}}(X)$ and $E_{\mathcal{B}}(X)$ cross precisely at those points X where $\alpha(X) \,=\, \beta(X) \,=\, \gamma(X) \,=\, 0$. Generically this defines a codimension 3 submanifold Γ. Furthermore, it is clear that the eigenvalues $E_{\mathcal{A}}(X)$ and $E_{\mathcal{B}}(X)$ are continuous, but generically not differentiable near Γ.

By standard Taylor series results, $M(X)$ has the form $M(X) = N(X) + O(\|X\|^2)$, where

$$N(X) \;=\; \begin{pmatrix} a \cdot X & b \cdot X + ic \cdot X \\ b \cdot X - ic \cdot X & -a \cdot X \end{pmatrix},$$

for some vectors a, b, and c. Generically a, b, and c are linearly independent. By a rotation of the coordinate system we may assume that only the first three components of a, b, and c are non-zero.

If η_0 is a vector not tangent to Γ at $X=0$, then we can rotate the first three coordinate axes so that the projection of η_0 into the three dimensional subspace spanned by a, b, and c lies along the positive X_1 axis.

At this point, the X_j coordinates for $j>3$ no longer play a role in the structure of $N(X)$. Furthermore, without altering the basic structure obtained so far, we still have the freedom to rotate the X_2 and X_3 coordinate directions, and we can perform X–independent unitary transformations of the two dimensional space spanned by $\psi_1(X)$ and $\psi_2(X)$. By doing both of these in a special way, we claim that we may assume the following:

1. The first component of a is non-zero.
2. The first and third components of b are zero, but its second component is positive.
3. The first and second components of c are zero, but its third component is positive.

Thus, we may assume that $N(X)$ has the form

$$N(X) \;=\; \begin{pmatrix} a_1X_1+a_2X_2+a_3X_3 & b_2X_2+ic_3X_3 \\ b_2X_2-ic_3X_3 & -a_1X_1-a_2X_2-a_3X_3 \end{pmatrix}.$$

To prove these claims we first do a unitary transformation of the span of $\psi_1(X)$ and $\psi_2(X)$ so that when $X_2=X_3=\cdots=X_N=0$, the matrix $M(X)$ is diagonal. Standard one variable perturbation theory shows that this can always be done. Thus, we may assume that $b_1=c_1=0$.

Next, we show that we can do another unitary transformation of the span of $\psi_1(X)$ and $\psi_2(X)$ so that b_1 and c_1 are unchanged, but b and c are transformed into perpendicular vectors. The unitary transformation we use simply multiplies $\psi_2(X)$ by a phase factor $e^{i\theta}$. This diagonal transformation leaves $M(X)$ diagonal when $X_2=X_3=\cdots=X_N=0$, so b_1 and c_1 are not altered. However, the similarity transformation replaces

$$\begin{pmatrix} b_2 & c_2 \\ b_3 & c_3 \end{pmatrix}$$

by

$$\begin{pmatrix} \tilde b_2 & \tilde c_2 \\ \tilde b_3 & \tilde c_3 \end{pmatrix} \;=\; \begin{pmatrix} b_2 & c_2 \\ b_3 & c_3 \end{pmatrix} \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}$$

We need only show that by a proper choice of θ, the columns of $\begin{pmatrix} \tilde{b}_2 & \tilde{c}_2 \\ \tilde{b}_3 & \tilde{c}_3 \end{pmatrix}$ can be forced to be orthogonal. We choose θ so that $\begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix}$ and $\begin{pmatrix} -\sin\theta \\ \cos\theta \end{pmatrix}$ are an orthonormal basis of eigenvectors for the real symmetric matrix $A^t A$, where $A = \begin{pmatrix} b_2 & c_2 \\ b_3 & c_3 \end{pmatrix}$. A simple computation then shows that $\begin{pmatrix} \tilde{b}_2 \\ \tilde{b}_3 \end{pmatrix}$ and $\begin{pmatrix} \tilde{c}_2 \\ \tilde{c}_3 \end{pmatrix}$ are orthogonal to one another.

We can now rotate the X_2 and X_3 coordinate directions so that $\tilde{b}$ and $\tilde{c}$ point along the positive X_2 and X_3 directions, respectively. By adding π to our choice of θ, we can change the signs of both $\tilde{b}$ and $\tilde{c}$. By interchanging $\psi_1(X)$ and $\psi_2(X)$ we can change the sign of $\tilde{c}$ without altering $\tilde{b}$.

Thus, we can arrange for $b_1 = 0$, $b_2 > 0$, $b_3 = 0$, $c_1 = 0$, $c_2 = 0$, and $c_3 > 0$. This proves our claims.

STRUCTURE OF CROSSINGS OF TYPE K Suppose a C^2 electron Hamiltonian function $h(X)$ has a Type K crossing of two multiplicity 2 eigenvalues $E_{\mathcal{A}}(X)$ and $E_{\mathcal{B}}(X)$ at $X = 0$. As in the earlier constructions, we let $P(X)$ be the spectral projection for $h(X)$ corresponding to both the eigenvalues $E_{\mathcal{A}}(X)$ and $E_{\mathcal{B}}(X)$. This projection has rank 4, and its range is the direct sum of a two dimensional subspace that lies in the carrier subspace for the D representation of the subgroup $H \in G$, and a two dimensional subspace that lies in the carrier subspace for the C representation. We arbitrarily pick two orthonormal vectors $\psi_1(0)$ and $\psi_2(0)$ that lie in the range of $P(0)$ and in the carrier subspace for the D representation. We let

$$\psi_1(X) = \frac{P(X)\,\psi_1(0)}{\sqrt{\langle\, \psi_1(0),\, P(X)\,\psi_1(0)\,\rangle}}.$$

We let $P_1(X)$ denote the orthogonal projection onto the span of $\psi_1(X)$ and define

$$\psi_2(X) = \frac{(1 - P_1(X))P(X)\,\psi_2(0)}{\sqrt{\langle\, \psi_2(0),\, (1 - P_1(X))P(X)\,\psi_2(0)\,\rangle}}.$$

In a neighborhood of the origin, these two vectors form an orthonormal basis for the intersection of the range of $P(X)$ and the carrier subspace for the D

representation. We let $\psi_3(X) = \mathcal{K}\,\psi_1(X)$ and $\psi_4(X) = \mathcal{K}\,\psi_2(X)$. Then $\psi_3(X)$ and $\psi_4(X)$ form an orthonormal basis for the intersection of the range of $P(X)$ and the carrier subspace for the C representation. The set of all four vectors is an orthonormal basis for the range of $P(X)$.

In this basis, the restriction of

$$h_1(X) \;=\; h(X) \;-\; \tfrac{1}{4}\,(\,E_{\mathcal{A}}(X) \,+\, E_{\mathcal{B}}(X)\,)$$

to the range of $P(X)$ is represented by a self-adjoint traceless 4×4 matrix valued function $M(X)$ whose entries are C^2 functions that all vanish when $X = 0$. Because $h(X)$ commutes with the two projections onto the carrier subspaces of the C and D representations and with the action of $\mathcal{K}$, $M(X)$ commutes with

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

and

$$\begin{pmatrix} 0 & 0 & e^{i\omega} & 0 \\ 0 & 0 & 0 & e^{i\omega} \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \cdot (\,\text{Conjugation}\,),$$

where $D(\mathcal{K}^2)$ is multiplication by $e^{i\omega}$. It follows that $M(X)$ must have the form

$$\begin{pmatrix} \alpha(X) & \beta(X)+i\gamma(X) & 0 & 0 \\ \beta(X)-i\gamma(X) & -\alpha(X) & 0 & 0 \\ 0 & 0 & \alpha(X) & \beta(X)-i\gamma(X) \\ 0 & 0 & \beta(X)+i\gamma(X) & -\alpha(X) \end{pmatrix}.$$

where α, β, and γ are C^2 real valued functions. By direct computation, the eigenvalues of $M(X)$ are

$$\pm\sqrt{\alpha(X)^2 \,+\, \beta(X)^2 \,+\, \gamma(X)^2}.$$

Thus, the eigenvalues $E_{\mathcal{A}}(X)$ and $E_{\mathcal{B}}(X)$ cross precisely at those points X where $\alpha(X) = \beta(X) = \gamma(X) = 0$, which generically defines a codimension 3 submanifold Γ.

By standard Taylor series results, $M(X)$ has the form $M(X) = N(X) + O(\|X\|^2)$, where

$$N(X) \; = \; \begin{pmatrix} a\cdot X & b\cdot X + ic\cdot X & 0 & 0 \\ b\cdot X - ic\cdot X & -a\cdot X & 0 & 0 \\ 0 & 0 & a\cdot X & b\cdot X - ic\cdot X \\ 0 & 0 & b\cdot X + ic\cdot X & -a\cdot X \end{pmatrix},$$

for some vectors a, b, and c. Generically a, b, and c are linearly independent. By a rotation of the coordinate system we may assume that only the first three components of a, b, and c are non-zero.

If η_0 is any vector not tangent to Γ at $X = 0$, then we can rotate the first three coordinate axes so that the projection of η_0 into the three dimensional subspace spanned by a, b, and c lies along the positive X_1 axis.

At this point, the X_j coordinates for $j > 3$ no longer play a role in the structure of $N(X)$. Furthermore, without altering the basic structure obtained so far, we still have the freedom to rotate the X_2 and X_3 coordinate directions, and we can perform X–independent unitary transformations of the two dimensional space spanned by the basic electronic wave functions $\psi_1(X)$ and $\psi_2(X)$. If we do such unitary transformations, we also redefine $\psi_3(X)$ and $\psi_4(X)$ to preserve the relations $\psi_3(X) = \mathcal{K}\,\psi_1(X)$ and $\psi_4(X) = \mathcal{K}\,\psi_2(X)$. We do these operations, mimicking the procedure used in our discussion of Type B crossings, to see that the following three conditions can be satisfied:

1. The first component of a is non-zero.
2. The first and third components of b are zero, but its second component is positive.
3. The first and second components of c are zero, but its third component is positive.

Thus, we may assume that $N(X)$ has the form

$$\begin{pmatrix} \sum_{j=1}^{3} a_j X_j & b_2 X_2 + i c_3 X_3 & 0 & 0 \\ b_2 X_2 - i c_3 X_3 & -\sum_{j=1}^{3} a_j X_j & 0 & 0 \\ 0 & 0 & \sum_{j=1}^{3} a_j X_j & b_2 X_2 - i c_3 X_3 \\ 0 & 0 & b_2 X_2 + i c_3 X_3 & -\sum_{j=1}^{3} a_j X_j \end{pmatrix}.$$

STRUCTURE OF TYPE J CROSSINGS Suppose a C^2 electron Hamiltonian function $h(X)$ has a Type J crossing of two multiplicity 2 eigenvalues $E_{\mathcal{A}}(X)$ and $E_{\mathcal{B}}(X)$ at $X = 0$. As in the earlier constructions, we let $P(X)$ be the rank 4 spectral projection for $h(X)$ corresponding to both the eigenvalues $E_{\mathcal{A}}(X)$ and $E_{\mathcal{B}}(X)$. We arbitrarily pick a unit vector $\psi_1(0)$ that lies in the range of $P(0)$, and we define $\psi_2(0) = \mathcal{K}\,\psi_1(0)$. We then choose another unit vector $\psi_3(0)$ that is in the range of $P(0)$, but is orthogonal to both $\psi_1(0)$ and $\psi_2(0)$. We then let $\psi_4(0) = \mathcal{K}\,\psi_3(0)$. For Type *II* corepresentations of minimal multiplicity, $D(\mathcal{K}^2) = -1$, and it follows that the four vectors form an orthonormal basis for the range of $P(0)$. We define

$$\psi_1(X) \;=\; \frac{P(X)\,\psi_1(0)}{\sqrt{\langle\,\psi_1(0),\,P(X)\,\psi_1(0)\,\rangle}}.$$

We then define $\psi_2(X) = \mathcal{K}\,\psi_1(X)$. We let $P_{1,2}(X)$ denote the orthogonal projection onto the span of $\psi_1(X)$ and $\psi_2(X)$, and define

$$\psi_3(X) \;=\; \frac{(1 - P_{1,2}(X))P(X)\,\psi_3(0)}{\sqrt{\langle\,\psi_3(0),\,(1 - P_{1,2}(X))P(X)\,\psi_3(0)\,\rangle}}.$$

We then define $\psi_4(X) = \mathcal{K}\,\psi_3(X)$. For each X in a neighborhood of the origin, these four vectors form an orthonormal basis for the range of $P(X)$.

In this basis, the restriction of

$$h_1(X) \;=\; h(X) \,-\, \tfrac{1}{4}\,(\,E_{\mathcal{A}}(X) \,+\, E_{\mathcal{B}}(X)\,)$$

to the range of $P(X)$ is represented by a self-adjoint traceless 4×4 matrix valued function $M(X)$ whose entries are C^2 functions that all vanish when

$X = 0$. Because $h(X)$ commutes with the action of $\mathcal{K}$, $M(X)$ commutes with

$$\begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \cdot (\,\text{Conjugation}\,)\,.$$

It follows that $M(X)$ must have the form

$$\begin{pmatrix} \alpha(X) & 0 & \beta(X)+i\gamma(X) & \delta(X)+i\epsilon(X) \\ 0 & \alpha(X) & -\delta(X)+i\epsilon(X) & \beta(X)-i\gamma(X) \\ \beta(X)-i\gamma(X) & -\delta(X)-i\epsilon(X) & -\alpha(X) & 0 \\ \delta(X)-i\epsilon(X) & \beta(X)+i\gamma(X) & 0 & -\alpha(X) \end{pmatrix}.$$

where α, β, γ, δ, and ϵ are C^2 real valued functions. The difference between $E_{\mathcal{A}}(X)$ and $E_{\mathcal{B}}(X)$ is the same as the difference between the eigenvalues of $M(X)$. By direct computation, the eigenvalues of $M(X)$ are

$$\pm\sqrt{\alpha(X)^2 + \beta(X)^2 + \gamma(X)^2 + \delta(X)^2 + \epsilon(X)^2}.$$

Thus, the eigenvalues $E_{\mathcal{A}}(X)$ and $E_{\mathcal{B}}(X)$ cross precisely at those points X where $\alpha(X) = \beta(X) = \gamma(X) = \delta(X) = \epsilon(X) = 0$, which generically defines a codimension 5 submanifold Γ.

By standard Taylor series results, $M(X)$ has the form $M(X) = N(X) + O(\|X\|^2)$, where

$$\begin{pmatrix} a\cdot X & 0 & b\cdot X+ic\cdot X & d\cdot X+ie\cdot X \\ 0 & a\cdot X & -d\cdot X+ie\cdot X & b\cdot X-ic\cdot X \\ b\cdot X-ic\cdot X & -d\cdot X-ie\cdot X & -a\cdot X & 0 \\ d\cdot X-ie\cdot X & b\cdot X+ic\cdot X & 0 & -a\cdot X \end{pmatrix},$$

for some vectors a, b, c, d, and e. Generically a, b, c, d, and e are linearly independent. By a rotation of the coordinate system we may assume that only the first five components of a, b, c, d, and e are non-zero.

If η_0 is any vector not tangent to Γ at $X = 0$, then we can rotate the first five coordinate axes so that the projection of η_0 into the five dimensional subspace spanned by a, b, c, d, and e lies along the positive X_1 axis.

At this point, the X_j coordinates for $j > 5$ no longer play a role in the structure of $N(X)$. Furthermore, without altering the basic structure obtained so far, we still have the freedom to rotate the X_2, X_3, X_4, and X_5 coordinate directions, and we can perform those X–independent unitary transformations of the four dimensional space spanned by the basic electronic wave functions $\psi_1(X)$, $\psi_2(X)$, $\psi_3(X)$, and $\psi_4(X)$ that preserve the relations $\psi_2(X) = \mathcal{K}\,\psi_1(X)$ and $\psi_4(X) = \mathcal{K}\,\psi_3(X)$. We claim that by doing such operations in generic situations, we can arrange for the following five conditions to be satisfied:

1. The first component of a is non-zero.
2. $b_1 = b_3 = b_4 = b_5 = 0$, but $b_2 \neq 0$.
3. $c_1 = c_2 = c_4 = c_5 = 0$, but $c_3 \neq 0$.
4. $d_1 = d_2 = d_3 = d_5 = 0$, but $d_4 \neq 0$.
5. $e_1 = e_2 = e_3 = e_4 = 0$, but $e_5 \neq 0$.

Thus, we may assume that $N(X)$ has the form

$$\begin{pmatrix} \sum_{j=1}^{5} a_j X_j & 0 & b_2 X_2 + i c_3 X_3 & d_4 X_4 + i e_5 X_5 \\ 0 & \sum_{j=1}^{5} a_j X_j & -d_4 X_4 + i e_5 X_5 & b_2 X_2 - i c_3 X_3 \\ b_2 X_2 - i c_3 X_3 & -d_4 X_4 - i e_5 X_5 & -\sum_{j=1}^{5} a_j X_j & 0 \\ d_4 X_4 - i e_5 X_5 & b_2 X_2 + i c_3 X_3 & 0 & -\sum_{j=1}^{5} a_j X_j \end{pmatrix}.$$

To prove these claims we first note that if we replace $\psi_j(X)$ by $\tilde{\psi}_j(X)$, where

$$\begin{aligned} \tilde{\psi}_1(X) &= z_1\,\psi_1(X) + z_2\,\psi_2(X), && \text{with } |z_1|^2 + |z_2|^2 = 1, \\ \tilde{\psi}_2(X) &= \mathcal{K}\,\tilde{\psi}_1(X), \\ \tilde{\psi}_3(X) &= z_3\,\psi_3(X) + z_4\,\psi_4(X), && \text{with } |z_3|^2 + |z_4|^2 = 1, \qquad \text{and} \\ \tilde{\psi}_4(X) &= \mathcal{K}\,\tilde{\psi}_3(X), \end{aligned}$$

then $N(X)$ is transformed into

$$\begin{pmatrix} \tilde{a}\cdot X & 0 & \tilde{b}\cdot X + i\tilde{c}\cdot X & \tilde{d}\cdot X + i\tilde{e}\cdot X \\ 0 & \tilde{a}\cdot X & -\tilde{d}\cdot X + i\tilde{e}\cdot X & \tilde{b}\cdot X - i\tilde{c}\cdot X \\ \tilde{b}\cdot X - i\tilde{c}\cdot X & -\tilde{d}\cdot X - i\tilde{e}\cdot X & -\tilde{a}\cdot X & 0 \\ \tilde{d}\cdot X - i\tilde{e}\cdot X & \tilde{b}\cdot X + i\tilde{c}\cdot X & 0 & -\tilde{a}\cdot X \end{pmatrix}.$$

We show below that by making an appropriate choice of the z_j, we can force $\tilde{b}$, $\tilde{c}$, $\tilde{d}$, and $\tilde{e}$ to be mutually orthogonal (and all non-zero in generic situations).

Once this is done, we rotate the X_2, X_3, X_4, and X_5 coordinate axes, so that $\tilde{b}$, $\tilde{c}$, $\tilde{d}$, and $\tilde{e}$ point along the X_2, X_3, X_4, and X_5, respectively. This proves the claims.

Arbitrarily choosing the z_j's is equivalent to arbitrarily choosing two matrices $U_1 \in SU(2)$ and $U_2 \in SU(2)$, so that

$$\begin{pmatrix} \tilde{\psi}_1(X) \\ \tilde{\psi}_2(X) \end{pmatrix} = U_1 \begin{pmatrix} \psi_1(X) \\ \psi_2(X) \end{pmatrix}$$

and

$$\begin{pmatrix} \tilde{\psi}_3(X) \\ \tilde{\psi}_4(X) \end{pmatrix} = U_2 \begin{pmatrix} \psi_3(X) \\ \psi_4(X) \end{pmatrix}.$$

In this notation,

$$\begin{pmatrix} \tilde{b} \cdot X - i\tilde{c} \cdot X & -\tilde{d} \cdot X - i\tilde{e} \cdot X \\ \tilde{d} \cdot X - i\tilde{e} \cdot X & \tilde{b} \cdot X + i\tilde{c} \cdot X \end{pmatrix}$$

$$= U_2 \begin{pmatrix} b \cdot X - ic \cdot X & -d \cdot X - ie \cdot X \\ d \cdot X - ie \cdot X & b \cdot X + ic \cdot X \end{pmatrix} U_1^{-1}.$$

The mapping

$$(w_1, w_2, w_3, w_4) \longmapsto W = \begin{pmatrix} w_1 - iw_2 & -w_3 - iw_4 \\ w_3 - iw_4 & w_1 + iw_2 \end{pmatrix}$$

is an isometric isomorphism of standard Euclidean $\mathbb{R}^4$ into a subspace $\mathcal{W}$ of the 4×4 complex matrices endowed with the inner product $\langle W_1, W_2 \rangle = \frac{1}{2}\,\mathrm{trace}\,(W_1^* W_2)$. Furthermore, the action of $SU(2) \times SU(2)$ on $\mathcal{W}$ given by $W \longmapsto \tilde{W} = U_2\, W\, U_1^{-1}$ is isometric on this space. Since $SU(2) \times SU(2)$ is connected, it follows that the corresponding action on Euclidean $\mathbb{R}^4$ is given by

$$(w_1, w_2, w_3, w_4) \longmapsto (\tilde{w}_1, \tilde{w}_2, \tilde{w}_3, \tilde{w}_4) = (w_1, w_2, w_3, w_4)\, \mathcal{O}_{U_1, U_2},$$

where $\mathcal{O}_{U_1, U_2} \in SO(4)$. The mapping $(U_1, U_2) \longmapsto \mathcal{O}_{U_1, U_2}$ is a group homomorphism. By explicit calculation, the differential of this map takes the generators of the Lie algebra $su(2) \times su(2)$ onto the generators of the Lie algebra $so(4)$. Thus, the map is a local isomorphism of the Lie groups. $SU(2) \times SU(2)$ is connected and simply connected, and $SO(4)$ is connected. It follows that the mapping is a covering map, and therefore is surjective (In fact, it is two-to-one with kernel $\{\, (I, I), (-I, -I) \,\}$.). If $(\, b\ c\ d\ e \,)$ denotes the 4×4 matrix whose columns are the vectors b, c, d, and e, then we have

$$\begin{pmatrix} \tilde{b} & \tilde{c} & \tilde{d} & \tilde{e} \end{pmatrix} = \begin{pmatrix} b & c & d & e \end{pmatrix} \mathcal{O}_{U_1, U_2},$$

where $\mathcal{O}_{U_1, U_2}$ can be taken to be any element of $SO(4)$ if U_1 and U_2 are chosen properly. Our claims are thus proved if we can show that any invertible matrix $A = (b\ c\ d\ e)$ has the property that it maps some orthonormal basis (the columns of $\mathcal{O}_{U_1, U_2}$) into non-zero, mutually orthogonal vectors $\{\tilde{b}, \tilde{c}, \tilde{d}, \tilde{e}\}$. To show that this is the case, we choose the orthonormal basis $\{v_1, v_2, v_3, v_4\}$ to be an orthonormal basis in which the real symmetric matrix $A^* A$ is diagonal. Such bases always exist, and one can always arrange for $\mathcal{O}_{U_1, U_2} = (v_1\ v_2\ v_3\ v_4)$ to be in SO(4). Then for $i \neq j$, $\langle Av_i, Av_j \rangle = \langle v_i, A^* Av_j \rangle = \mu_j \langle v_i, v_j \rangle = 0$. This proves the claim.

References

1. Hagedorn, G.A.: High Order Corrections to the Time–Dependent Born–Oppenheimer Approximation I: Smooth Potentials. *Ann. Math.* **124**, 571–590 (1986). Erratum **126**, 219 (1987).
2. Hagedorn, G.A.: High Order Corrections to the Time–Dependent Born–Oppenheimer Approximation II: Coulomb Systems. *Comm. Math. Phys.* **117**, 387–403 (1988).
3. Hagedorn, G.A.: Electron Energy Level Crossings in the Time–Dependent Born–Oppenheimer Approximation. *Theor. Chimica Acta.* **77**, 163–190 (1990).
4. Hagedorn, G.A.: Analysis of Energy Level Crossings in the Time–Dependent Born–Oppenheimer Approximation. (in preparation).
5. Lever, J., and Shaw, R.: Irreducible Multiplier Corepresentations and Generalized Inducing. *Comm. Math. Phys.* **38**, 257–277 (1974).
6. Wigner, E.P.: *Group Theory and its Application to the Quantum Mechanics of Atomic Spectra.* New York: Academic Press, 1959.

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Semiclassical expansions of the thermodynamic limit for a Schrödinger equation

I. The one well case

by B.Helffer and J.Sjöstrand

§1 Presentation of the problem :

One of the motivations of the study presented here is a statistical model introduced by M.Kac $[Ka]_2$ and called the exponential bidimensional model. This model was supposed to present phase transition. Let us just recall here (see $[Ka]_2$ or [Br-He] for details) that after some reductions M.Kac arrive to the question of studying the spectral properties of the following operator:

(1.1) $K_m(h):=$

$$=\exp[-V^{(m)}(x)/2].\exp[h^2\Sigma_{k=1}^{m}\partial^2/\partial x_k^2].\exp[-V^{(m)}(x)/2]$$

with[1] :

(1.2) $V^{(m)}(x) = (1/4)\,\Sigma_{k=1}^{m} x_k^{\,2} - \Sigma_{k=1}^{m}\log \mathrm{ch}(\sqrt{\nu/2}\ (x_k+x_{k+1}))$.

[1] In fact, the operator which appears in Kac is $\exp(-mh/2)K_m(h)$. It is easier w.l.o.g. in this article to work with this modified Kac operator.

The parameter ν is here the inverse of the temperature and h is a semi-classical parameter. The two questions of interest are in this context:

(1.3) If $\mu_1(m;h,\nu)$ is the largest eigenvalue of the Kac's operator, what is the behavior as a function of ν and h of the thermodynamic quantity :

$\mathrm{Lim}_{m\to\infty}(-\mathrm{Log}\ \mu_1(m;h,\nu)/m)$.

(1.4) If $\mu_2(m;h,\nu)$ is the second eigenvalue (which is $< \mu_1(m;h,\nu)$ by standard results), can we study the quantity :

$\mathrm{Lim}_{m\to\infty}(\mu_2(m;h,\nu)/\mu_1(m;h,\nu))$.

From discussions with specialists in statistical mechanics (with T.Spencer for example), we get the impression that this problem is probably well understood and that according to the value of ν with respect to a critical value ν_c the answer to (1.4) will be that the limit will be <1 for $\nu<\nu_c$ and will be 1 for $\nu>\nu_c$. This is a sign of a transition of phase. However, we do not have a precise reference for that and at least the problem of analyzing in detail the behavior of the different thermodynamic quantities near the critical value ν_c seems to remain open.

In his interesting course in Brandeis $[\mathrm{Ka}]_2$, M. Kac explains, at least heuristically, how to compare (in the semi-classical context) the operator $K_m(h)$ to the exponential of (minus) a Schrödinger operator. The validity of this approximation (for m fixed) has been studied more carefully in [He-Br] and [He] using some results of $[\mathrm{He}\text{-}\mathrm{Sj}]_{1,4}$.

If we admit this approximation, we shall find the following problems for the Schrödinger equation :

(1.5) $P_m(h) = -\Sigma_{k=1}^{m} h^2\partial^2/\partial x_k^2 + V^{(m)}(x)$.

(1.6) If $\lambda_1^{(m)}(h,\nu)$ is the smallest eigenvalue of the Schrödinger's operator, study as a function of ν and h the thermodynamic quantity :

$\mathrm{Lim}_{m\to\infty} (\lambda_1(m;h,\nu)/m)$.

(1.7) If $\lambda_2(m;h,\nu)$ is the second eigenvalue (which is $>\lambda_1(m;h,\nu)$ by standard results), study the quantity :

$\mathrm{Lim}_{m\to\infty} (\lambda_2(m;h,\nu) - \lambda_1(m;h,\nu))$.

Forgetting the initial Kac's problem, we shall start to study in this article these two questions (1.6) and (1.7). Because it is a high dimension problem, we shall use (at least in the semi-classical context) the techniques introduced by one of us (J.S). Most of the results which are given here :

(1) existence of the thermodynamic limit $\mathrm{Lim}_{m\to\infty} (\lambda_1(m;h,\nu)/m)$

(2) asymptotic expansion of the limit as a formal series in h

(3) rapidity of the convergence as $m \to \infty$

are given in a relatively general framework but we shall see how it can be applied in our motivating example, in the particular case where $\nu < \nu_c$.

This is of course just the starting point (and the easiest) of a study which has to consider after the case where $\nu > \nu_c$, and then the transition around $\nu = \nu_c$. There is some hope to return later to the initial Kac's problem. This ν_c can be guessed by looking carefully to the properties of $V^{(m)}$. As observed by V.Kac, for $\nu < 1/4$, the potential $V^{(m)}$ has a unique minimum at 0 and appears to be convex. For $\nu > 1/4$, we shall observe a double well problem which is certainly more difficult to analyze.

The principal result of this paper will be :

Theorem 1.1

If $\nu < 1/4$, *the limit* $\Lambda(h,\nu) = \mathrm{Lim}_{m\to\infty} (\lambda_1(m;h,\nu)/m)$ *exists and admit a complete asymptotic expansion :*

$\Lambda(h,\nu) \sim h\Sigma_{j\geq 0}\Lambda_j(\nu).h^j$ *as h tends to 0.*

Moreover, if we denote the corresponding semiclassical expansions for $\lambda_1(m;h,\nu)/m$ *by :*

$(\lambda_1(m;h,\nu)/m) \sim h\Sigma_{j\geq 0}\Lambda_j(m,\nu).h^j$,

there exists k_0 *s.t. for each j, there exists a constant* $C_j(\nu)$, *s.t.*

$|\Lambda_j(\nu) - \Lambda_j(m,\nu)| \leq C_j(\nu).\exp(-k_0 m)$.

$C_j(\nu)$ *can be chosen independently of* ν *in a compact of* $[0,1/4[$.

The problems, we consider here, are also connected to quantum field theory problems and a lot of results have been obtained by other techniques (see for example the new edition of [Gl-Ja] for a updated presentation).

The paper is organized in three parts.

The first part (§ 2 and §3) is essentially devoted to the proof of the existence of the thermodynamic limit. This is a non-semiclassical proof but we shall see that a control of the convergence with respect to parameters can be useful. In §3 we give additional remarks (to $[Sj]_2$) on universal estimates of the splitting of the two first eigenvalues .

The second part (§4 and §5) is the semi-classical part and the natural continuation of two papers by one of us (J.S) $[Sj]_{1,2}$.

In the last part (§6), we shall first recall some preliminary computations by Kac [Ka] and then deduce the Theorem 1.1 as a particular case of the more general results obtained in the preceding sections.

The first author (B.H) thanks V.Tchoulaevski and T.Spencer for useful remarks and stimulating discussions.

§2 On the existence of the thermodynamic limit $\lambda_1(m)/m$

This section is inspired by the reading of the book of Ruelle [Ru] which gives probably the necessary ideas to extend the results we present here to more general interactions.

Let us just consider the following model :

(2.1) $P_m = -h^2\Delta_m + \Sigma_{k=1}^{m} W(x_k x_{k+1})$

(with the convention that $m+1=1$)

operating on $L^2(\mathbb{R}^m)$.

Here :

(2.2) $\Delta_m = \Sigma_{k=1}^{m} (\partial_{x_k})^2$

We forget the semi-classical problem (we take $h=1$) (but if needed the proof will be sufficiently explicit to have a control with respect to h), we assume that W is C^∞ and satisfies :

(2.3) $W \geqslant 0$

There exists a constant $C_0 > 0$ s.t.:

(2.4) $W(t,s) \leqslant C_0 (W(t,r) + W(u,s)+1)$ for all $t,s,r,u \in \mathbb{R}$

which will be called the decoupling inequality.

Moreover, we assume

(2.5) $W (t,s) \to \infty$ as $|t|+|s| \to \infty$.

This last property (which is not necessary at all) permits us to work in the simpler context where the Schrödinger equation has compact resolvent.

Remark 2.1 :

(2.4) and (2.5) follow from the stronger assumptions, that there exists constants $C_1, C_2 > 0$, and C_3 s.t. :

(2.6) $W(t,s) \geqslant (1/C_2) (t^2 + s^2) - C_1$ for all $s,t \in \mathbb{R}$

(2.7) $W(t,s) \leqslant C_2 (t^2 + s^2) + C_3$ for all $s,t \in \mathbb{R}$

We shall denote in this section by $\lambda(m) = \lambda_1(m)$ the first eigenvalue of P_m. This first eigenvalue always exists (the resolvent is compact) and we shall denote by u_m the corresponding eigenfunction uniquely determined if we suppose that the L^2 norm is one and that u_m is positive. Recall that by standard results u_m is strictly positive.

The main result of this section is the following :

Theorem 2.2

Under the assumptions (2.3) - (2.5), the sequence $\lambda(m)/m$ is convergent as m tends to infinity.

Majoration, minoration :

We get from (2.3) that :

(2.8) $\lambda(m) \geqslant 0$

and (2.4) (with $r = u = 0$) and (2.5) imply :

(2.9) $\lambda(m) \leqslant C\, m$

We then have :

(2.10) $\quad 0 \leqslant \text{Lim inf}_{m\to\infty} \lambda(m)/m \leqslant \text{Lim sup}_{m\to\infty} \lambda(m)/m < \infty$

The following simple lemma will play a crucial role

Lemma 2.3

There exists a constant C_4 *such that, for all* $m \geqslant 1$*, we have, for* $j = 1$ *to* m*:*

(2.11) $\|W(x_j x_{j+1})^{1/2} u_m\|^2 \leqslant \lambda(m)/m \leqslant C_4$

Proof :

From (2.3), we get :

$\Sigma_j \|W(x_j x_{j+1})^{1/2} u_m\|^2 \leqslant \lambda(m)$

We observe now that the potential is invariant by circular permutation. By usual arguments, we get that u_m (which is strictly positive and corresponds to an eigenvalue of multiplicity 1) has the same property.

In particular $\|W(x_j x_{j+1})^{1/2} u_m\|^2$ is independent of j. The lemma follows immediately with $C_4 = \text{Sup}_m (\lambda(m)/m)$.

Comparison between $\lambda(m)$, $\lambda(p)$ and $\lambda(m+p)$

In a second step we shall prove the

Lemma 2.4

There exists a constant $C_5 > 0$ *such that, for all integers* m, p *s.t.* $1 \leqslant p$, $1 \leqslant m$ *, we have :*

(2.12) $-C_5+\lambda(m)+\lambda(p) \leqslant \lambda(m+p) \leqslant C_5+\lambda(m)+\lambda(p)$

<u>Proof</u>

We start from the following decomposition of P_{m+p}

(2.13) $P_{m+p} = P_m + \hat{P}_p^{(m+1)} - W(x_m x_1) + W(x_m x_{m+1}) -$

$$-W(x_{m+p} x_{m+1}) + W(x_{m+p} x_1)$$

with : $\hat{P}_p^{(m+1)} = -\hat{\Delta}_p^{(m+1)} + \Sigma_{k=m+1}^{m+p-1} W(x_k x_{k+1}) + W(x_{m+p} x_{m+1})$

and $\hat{\Delta}_p^{(m+1)} = \Sigma_{k=m+1}^{m+p} (\partial_{x_k})^2$

It is then clear that the infimum of the spectrum of $\hat{P}_p^{(m+1)}$ is the same as the infimum of P_p. Sometimes we shall use the notation $P_m \tilde{\oplus} P_p$ instead as $P_m + \hat{P}_p^{(m+1)}$.

For the minoration of $\lambda(m+p)$, one writes :

$\lambda(m+p) = (P_{m+p} u_{m+p} | u_{m+p}) \geqslant (P_m u_{m+p} | u_{m+p}) + (\hat{P}_p^{(m+1)} u_{m+p} | u_{m+p})$
$- \|W^{1/2}(x_m x_1) u_{m+p}\|^2 - \|W^{1/2}(x_{m+p} x_{m+1}) u_{m+p}\|^2$

and we use (2.4) and Lemma 2.3.

By the definition of $\lambda(m)$ (and identifying P_m on $L^2(\mathbb{R}^m)$ and $P_m \otimes I$ on $L^2(\mathbb{R}^m) \otimes L^2(\mathbb{R}^p)$ who have the same spectrum (as a set)) we get the first estimate :

$\lambda(m+p) \geqslant \lambda(m) + \lambda(p) - C_5$ (with $C_5 = 2C_4$).

For the majoration of $\lambda(m+p)$, we proceed similarly using the fonction:

$\hat{u}_{p,m}(x) = u_m(x_1, \ldots\ldots, x_m) . u_p(x_{m+1}, \ldots\ldots, x_{m+p})$

We have :

$\lambda(m+p) \leqslant (P_{m+p} \hat{u}_{m,p} | \hat{u}_{m,p}) \leqslant (P_m \hat{u}_{m,p} | \hat{u}_{m,p}) + (\hat{P}_p^{(m+1)} \hat{u}_{m,p} | \hat{u}_{m,p})$.
$+ \| W^{1/2}(x_m x_{m+1}) \hat{u}_{m,p} \|^2 + \|W^{1/2}(x_{m+p} x_1) \hat{u}_{m,p}\|$

$\leqslant \lambda(m) + \lambda(p) + C_5$

(using the same type of arguments)

The last lemma to prove the proposition is the following :

Lemma 2.5 :

Let C *some fixed constant* $(C \geqslant 0)$. *Let* $\lambda(m)$ $(m \in \mathbb{N}^*)$ *be a sequence of real numbers such that*

(2.14) $|\lambda(m+p) - \lambda(m) - \lambda(p)| \leqslant C$, *for each m,p ,*

then the limit of the sequence $\lambda(m)/m$ *exists and :*

(2.15) $|(\lambda(m)/m) - \mathrm{Lim}_{m \to \infty}(\lambda(m)/m)| \leqslant C/m$.

Proof

Let $\mu(m) = \lambda(m)/m$. Let us rewrite (2.14) on the form :

(2.16) $|\mu(m+p) - ((m/(m+p))\mu(m)) - ((p/(m+p))\mu(p))| \leqslant C/(m+p)$

In particular, for p = m, we get :

$|\mu(2m) - \mu(m)| \leqslant C/2m$

and by iteration :

$|\mu(2^{k+1}m) - \mu(2^k m)| \leqslant C/(2^k m)$.

In particular $\overline{\mu}(m) := \mathrm{Lim}_{k \to \infty} \mu(2^k m)$ exists and

(2.17) $|\overline{\mu}(m) - \mu(m)| \leqslant C/m$.

Replacing m and p in (2.16) by $2^k m$ and $2^k p$ and taking the limit in k, we get :

(2.18) $\overline{\mu}(m+p) = ((m/(m+p))\overline{\mu}(m)) + ((p/(m+p))\overline{\mu}(p))$.

We now define $\overline{\lambda}(m)$ by : $\overline{\lambda}(m) = m\,\overline{\mu}(m)$, and rewrite (2.17) as :

(2.19) $\overline{\lambda}(m+p) = \overline{\lambda}(m) + \overline{\lambda}(p)$.

This implies in particular that $\overline{\lambda}(m) = m\overline{\lambda}(1)$ and then :

(2.20) $\overline{\mu}(m) = \overline{\mu}(1)$.

(2.17) and (2.20) give the lemma.

Examples

Example 2.6 ([Ka])

Let us consider

$$V_m(x_1, \ldots\ldots, x_m) = (1/4)\,\Sigma_{k=1}^{m} x_k^{2} - \Sigma_{k=1}^{m} \log \mathrm{ch}(\sqrt{\nu}\ (\sqrt{\xi}\, x_k + \sqrt{1-\xi}\ \ x_{k+1})),$$

where $\xi \in]0,1[$, $\nu > 0$.

Then this potential can be written on the form (2.1) by taking :

$$W(s,t)) = (1/8)\,(s^2+t^2) - \log \mathrm{ch}(\sqrt{\nu}\ (\sqrt{\xi}\, t + \sqrt{1-\xi}\ \ s))$$

In the introduction we took and in the future we shall take $\xi = 1/2$.

Example 2.7

One gets another example by taking the quadratic approximation at a minimum of the preceding model. Then we arrive to:

$$W(s,t) = (1/16)\,(s-t)^2 + \mu\,(s+t)^2$$

where μ depends on ν but remains > 0.

In this case, very explicit computation can be made (see [Ka] or § 6).

Example 2.8

More generally, T.Spencer indicates to one of us (B.H) that the following more general model is interesting :

$$W(s,t) = g(s^2+t^2) + h\,(s-t)^2 + \lambda\,(f(\mu s)+f(\mu t))$$

where $|f(v)| \leqslant C(|v|+1)$ and $g>0$ and $h>0$ are parameters.

Remark 2.9

It is important to remark that for the application to semi-classical analysis there exists at each step of the proofs in this section a very good control with respect to the different constants.

Remark 2.10

It will be interesting in the case of the Examples (2.6) or (2.7) to have a control of the regularity of the limit with respect to the parameter ν. It is clear that the convergence is uniform with respect to ν, on each compact of $]0,\infty[$, so it is clear that the limit is continuous. Moreover we observe that $(\partial\lambda(m;\nu)/\partial\nu)/m$ is a bounded set (by the Hellman's formula) which implies that the limit as m tends to ∞ of $\lambda(m;\nu)/m$ is Lipschitzian in $]0,\infty[$. But a more interesting result would be to study the properties of analyticity with respect to ν. One suspects of course that the limit is analytic with respect to ν, for $\nu<\nu_c$, in the model presented in the introduction ($\xi=1/2$, in Example (2.6)).

Remark 2.11 (stability by perturbation)

The limit is relatively stable by perturbation. For example, if we consider the following operator

$$P_m = -\Delta_m + \Sigma_{k=1}^{m-1} W(x_k x_{k+1})$$

and if we denote by $\lambda'(m)$ the first eigenvalue of P'_m,

then it is possible to prove, under the additional assumption that there exists a constant C s.t., for all $1 \geq \varepsilon > 0$, we have:

(2.21) $W(s,t) \leqslant (1+\varepsilon)(W(s,r) + W(p,t)) + (C/\varepsilon)$

for all s,t,r,p, that :

(2.22) $\mathrm{Lim}_{m\to\infty} \lambda'(m)/m = \mathrm{Lim}_{m\to\infty} \lambda(m)/m$

§3 Additional remarks on the splitting of the two first eigenvalues

Let us recall the problem mentioned in (1.7). It is also interesting to have theorems on $\underline{\mathrm{Lim}}_{m\to\infty}(\lambda_2(m)-\lambda_1(m))$ and $\overline{\mathrm{Lim}}_{m\to\infty}(\lambda_2(m)-\lambda_1(m))$. If the potential depends on a parameter ν (typically the inverse of the temperature in Example (2.6)), one is interested in knowing for which values of ν we have :

$\underline{\mathrm{Lim}}_{m\to\infty}(\lambda_2(m;\nu)-\lambda_1(m;\nu)) > 0$

or

$\mathrm{Lim}_{m\to\infty}(\lambda_2(m;\nu)-\lambda_1(m;\nu)) = 0.$

We shall not give an answer to the most interesting questions in this paper but we shall recall and improve some results obtained in this context. Let us first recall the :

Proposition 3.1 (cf [SWYY])

If V is a C^∞ positive potential tending to ∞ as $|x|$ tends to ∞, then we have :

(3.2) $(\lambda_2(m)-\lambda_1(m)) \leqslant 4\,\lambda_1(m)/m$

We shall now show how to give a result which is more sensible to the property of the Hessian of the potential V. The proposition is the following:

Proposition 3.2

Under the additional assumption that $x \to (\text{Hess } V)(x)$ is bounded, we have:

(3.3) $\lambda_2 - \lambda_1 \leq \sqrt{2}\ \mathrm{Inf}_{X \in \mathbb{R}^m, \|X\|=1} (\mathrm{Sup}_x\ (\mathrm{Hess} V)_x (X,X))^{1/2}$

Proof

The proof is as in [SWWY] reminiscent of the proof of the Payne-Polya-Weinberger inequality [P-P-W]. Similar ideas are used in the paper by B.Simon $[\mathrm{Si}]_3$ who refers to [Ka-Th], §3.

Let u^1_m the first normalized, strictly positive eigenfunction attached to $\lambda_1(m)$. We forget now the reference to m. Then we have :

(3.4) $(-\Delta + V)\, u^1 = \lambda_1\, u^1$

Let :

$\rho_\ell = \int x_\ell (u^1)^2 dx$

and let us consider :

$u^{1,\ell} = (x_\ell - \rho_\ell)\, u^1$

$u^{1,\ell}$ is orthogonal to u^1 and by the minimax principle we have :

(3.5) $\lambda_2 \leq\ < (-\Delta + V)\, u^{1,\ell} | u^{1,\ell} > / < u^{1,\ell} | u^{1,\ell} >$ for $\ell \in \{1, \ldots, m\}$

Let us observe now that, as a consequence of :

$(-\Delta + V)\, u^{1,\ell} = \lambda_1\, u^{1,\ell} - 2\partial_{x_\ell} u^1,$

we get :

$<(-\Delta+V)\, u^{1,\ell}|u^{1,\ell}> \leq \lambda_1 \; < u^{1,\ell}|u^{1,\ell}> + 1.$

Now the incertainty principle gives :

(3.6) $(1/2) \leq \|\partial_{x_\ell} u^1\| \; \|u^{1,\ell}\|,$

and then finally :

(3.7) $0 < \lambda_2 - \lambda_1 \; \leq 1/ < u^{1,\ell}|u^{1,\ell}>$

and

(3.8) $\lambda_2 - \lambda_1 \leq \; 4 \; \|\partial_{x_\ell} u^1\|^2.$

Summing over ℓ and using the equation we obtain first Proposition 3.1.

We now observe that (because u^1 is real) for all $\ell \in \{1,....,m\}$, we have:

(3.9) $u^1_\ell := \partial_{x_\ell} u^1$ is orthogonal to u^1

Similarly to the proof of (3.5), we deduce :

(3.10) $\lambda_2 \leq \; <(-\Delta+V)\, u^1_\ell|u^1_\ell>/ \; < u^1_\ell|u^1_\ell>$ for $\ell \in \{1,....,m\}$

Let us observe now that :

$(-\Delta+V)\, u^1_\ell = \lambda_1 \; u^1_\ell - (\partial_{x_\ell} V) u^1$

and that :

$<(-\Delta+V)\, u^1_\ell|u^1_\ell> \leq \lambda_1 \; < u^1_\ell|u^1_\ell> \; + (1/2) < (\partial^2_{x_\ell} V) u^1 \, |u^1 >.$

Finally we get

(3.11) $\lambda_2 - \lambda_1 \leq \; (1/(2 < \; u^1_\ell|u^1_\ell>))\, \mathrm{Sup}_x \partial^2_{x_\ell} V$

Then we take the product of (3.8) and (3.11) to get :

(3.12) $\lambda_2 - \lambda_1 \leq \sqrt{2}\, (\mathrm{Sup}_x \; \partial^2_{x_\ell} V)^{1/2}.$

This gives the proposition by observing that all the assumptions are invariant by rotation in $\mathbb{R}^m$.

Example 3.3 (cf Example 2.6):

If $V_v = \Sigma_j W_v(x_j x_{j+1})$, with :

$W_v(s,t) = (1/8)(s^2+t^2) - \log ch(\sqrt{(v/2)}\,(t+s))$

then we get :

$\lambda_2 - \lambda_1 \leqslant 1$

If we introduce the semi-classical parameter h, we shall obtain :

$\lambda_2 - \lambda_1 \leqslant h.$

To finish this section let us give shortly (in the case of $\mathbb{R}^m$) some universal minoration for the splitting. This result was already proved in $[Sj]_2$ in the case of an open bounded convex set Ω and it is not difficult to extend the result to the case of $\mathbb{R}^m$ by taking the limit of Dirichlet problems in balls Ω_R of increasing radius R and using the fact that the two first eigenvalues of the Dirichlet problem $\lambda_1^D(\Omega_R)$ (resp. $\lambda_2^D(\Omega_R)$) converge as R tends to ∞ to the corresponding eigenvalues of the global problem in $\mathbb{R}^m$ $\lambda_1(m)$ (resp. $\lambda_2(m)$).

Proposition 3.4 ($[Sj]_2$) :

Let V be a strictly convex C^∞ positive potential tending to ∞ as $|x|$ tends to ∞. Then we have :

(3.13) $\lambda_2 - \lambda_1 \geqslant \sqrt{2}.\mathrm{Inf}_x \lambda_{\min}((\mathrm{Hess}\,V)^{1/2}(x))$

where $\lambda_{\min}((\mathrm{Hess}\,V)^{1/2}(x))$ *is the smallest eigenvalue of* $(\mathrm{Hess}\,V)^{1/2}(x)$.

To see the interest of such a result let us observe the following :

<u>**Lemma 3.5** (Example 2.6)</u>

If $V_\nu = \Sigma_{j=1}^{m} W_\nu(x_j x_{j+1})$, *with :*

$W_\nu(s,t) = (1/8)(s^2+t^2) - \log \mathrm{ch}(\sqrt{(\nu/2)}\,(t+s))$,

then the potential is convex iff $\nu \leqslant 1/4$.

1/4 is consequently the good candidate to be the critical ν_c.

<u>**Remark 3.6**</u>

The existence of a minoration in the convex case was apparently known to some specialists (as T.Spencer indicated to one of us (B.H.)) at least in the framework of the field theory but surprisingly we do not know a reference before $[Sj]_2$. Recall also that a semiclassical version appears in $[Sj]_1$.

Let us now sketch here a variant (in the case of $\mathbb{R}^m$) of the proof given in $[Sj]_2$. The first step is the following formula for the splitting (cf for example [Ki-Si])

$$(3.14)\ \lambda_2-\lambda_1 = \mathrm{Inf}_\phi\{ [(\int|\nabla\phi|^2 (u^1)^2(x)\,dx)/\int|\phi|^2 (u^1)^2(x)\,dx)],\quad \phi\in C_0^\infty, \int\phi\,(u^1)^2(x)\,dx = 0\}$$

This is just a variant of the minimax principle.

The second step is the

<u>**Proposition 3.7** (cf [BL]) :</u>

Let us assume that $V(x) = (1/2)\omega^2 x^2 + U(x)$ *with* $\omega \geqslant 0$ *and* U *convex.*

Then

$g(x) := -\mathrm{Log}\,(u^1)(x) = (\omega x^2/\sqrt{2}) + v(x)$

with v convex .

This step was also basic in the proof in $[\mathrm{Sj}]_2$ (cf also [SWYY] for a proof based on the maximum principle).

For the last step let us introduce some notations. If ϕ is for example a continuous bounded function we can introduce :

$<\phi> = \int \phi\, (u^1)^2(x)\, dx, \ \mathrm{var}(\phi) = <(\phi - <\phi>)^2>.$

Then Brascamp and Lieb give in [Bra-Li] the following inequality :

(3.15) $\mathrm{var}\ (\phi) \leqslant <(\nabla\phi |\, {g''_{xx}}^{-1} | \nabla\phi)>.$

The proof is then easy by combining the results of the three steps.

__Application 3.8__ __(Example (2.6)__

As seen in Lemma 3.5, Example (2.6) satisfies all the assumptions. In particular we get for all m, and all $\nu < 1/4$:

(3.16) $\lambda_2(m;\nu) - \lambda_1(m;\nu) \geqslant \sqrt{(1-4\nu)}$

This gives us an interesting control with respect to the temperature. Of course, this result is not astonishing for the specialists in statistical physics.

If the semi-classical parameter h is introduced we get :

(3.17) $\lambda_2(m;h,\nu) - \lambda_1(m;h,\nu) \geqslant \sqrt{(1-4\nu)}\ h.$

The most interesting result would be to prove that, for $\nu > 1/4$, the splitting $(\lambda_2(m;h,\nu) - \lambda_1(m;,h,\nu))$ tends to 0 as m tends to infinity. On the other hand we do not know if, for $\nu < 1/4$, the limit $(\lambda_2(m;h,\nu) - \lambda_1(m;,h,\nu))$ exists .

§ 4. Exponentially weighted estimates in the construction of the phase

In this section, we shall develop some complements to the results in $[Sj]_{1,2}$.

To come back to the notations used in these papers, we shall now work with the operator $-(h^2/2)\Delta_m+V$. Let us introduce a set $\mathscr{A}$ as the disjoint union over $\mathbb{N}$ of sets $\mathscr{A}_m$:

$\mathscr{A} = \cup_{m\in\mathbb{N}} \mathscr{A}_m$

where $\mathscr{A}_m \subseteq \mathscr{V}_m \times \mathscr{R}_m$, $\mathscr{V}_m$ is the set of C^∞ potentials on $\mathbb{R}^m$ and $\mathscr{R}_m$ is the set of applications from $\{1,....,m\}$ in $\mathbb{R}^+$.

Let us make on $\mathscr{A}$ the following assumptions :

For all (V,ρ) in $\mathscr{A}$

(4.1) V is holomorphic in $B(0,1)$ with $|\nabla V(x)|_\infty = O(1)$ uniformly in $\mathscr{A}$ and $B(0,1)$, (Here $B(0,1)$ is the open unit ball in $\mathbb{C}^m$ with respect to the norm $|x|_\infty = \sup|x_j|$)

(4.2) $V(0)=0, V'(0)=0$,

$V''(0)=D+A$, where D is diagonal (positive definite) and

(4.3) There exists r_1 and r_0 (independent of (V,ρ) in $\mathscr{A}$) such that :

$\|A\|_{\mathscr{L}(\ell^p_\rho,\ell^p_\rho)} \leq r_1 < r_0 \leq \lambda_{min}(D)$

for all p s.t. $1 \leq p \leq \infty$.

We also assume :

(4.4) $\|\nabla^2 V\|_{\mathscr{L}(\ell^p_\rho,\ell^p_\rho)} = O(1)$

uniformly in $\mathscr{A}$ and p.

Here we write :

$|x|_{p,\rho} = |\rho x|_p = (\Sigma|\rho(j)x_j|^p)^{1/p}$ for $1 \leq p < \infty$

and

$|x|_{\infty,\rho} = |\rho x|_{\infty} = \mathrm{Sup}_j\, |\rho(j)x_j|.$

Because A and $\nabla^2 V$ are symmetric, we deduce from (4.3) and (4.4) that we have the same estimates with ρ replaced by $(1/\rho)$, so we may assume that :

(4.5) $(V,\rho) \in \mathcal{A} \Rightarrow (V,1/\rho) \in \mathcal{A}$.

From this, we get by interpolation that we may assume without loss of generality :

(4.6) If (V,ρ) is in $\mathcal{A}_m$, $(V,1)$ is in $\mathcal{A}_m$ where " 1 " is the constant weight defined by $\rho(j) = 1$ for $1 \leqslant j \leqslant m$.

As in $[Sj]_2$ (Lemma 1.1), we see that :

$(4.7)_1$ $(V''(0))^{1/2} = \tilde{D} + \tilde{A}$

with $\tilde{D}$ diagonal and

$(4.7)_2$ $\|\tilde{A}\|_{\mathcal{L}(\ell^p_\rho,\ell^p_\rho)} \leqslant \tilde{r}_1 < \tilde{r}_0 \leqslant \lambda_{\min}(\tilde{D})$

for all p s.t. $1 \leqslant p \leqslant \infty$ and uniformly in $\mathcal{A}$.

The property (4.6) permits to apply the results of $[Sj]_2$. In particular, let ϕ_0 be the solution of the eikonal equation :

(4.8) $(1/2)\, |\nabla\phi_0|_2^2 = V$

constructed in $[Sj]_2$, §2 for $|x|_\infty < r$. Then we have the following :

<u>**Lemma 4.1**</u>

If r is sufficiently small, then we have :

(4.9) $\|\phi_0''(x)\|_{\mathcal{L}(\ell^p_\rho,\ell^p_\rho)} = O(1)$

uniformly for (V,ρ) in $\mathcal{A}$ and for $|x|_\infty < r$.

Proof.

We recall first that $\phi_0''(0) = V''(0)^{1/2}$ and that $|\nabla\phi_0''(x)|_\infty = O(1)$. Contrary to the situation in $[Sj]_{1,2}$, it seems that we will have to work with ϕ_0'' directly (and not just with the Cauchy inequalities to estimate the Hessian from the gradient as in $[Sj]_1$ §1). Let $q = \xi^2/2 - V$. If we differentiate the H_q flow, we get[2] :

(4.10) $\partial_t(\delta x) = \delta\xi$, $\partial_t(\delta\xi) = V''(x).\ \delta x$

Consider an integral curve $]-\infty,0] \ni t \to (x(t),\xi(t))$ of H_q with : $(x(t),\xi(t)) \to (0,0)$ when $t \to -\infty$, $x(0) = x$, $\xi(0) = \nabla\phi_0(x)$, $|x| < r$ with r small. Recall from $[Sj]_2$ (§2, 2.16) that [3]

(4.11) $|x(t)|_\infty \leqslant \exp(-|t|/C)\ |x|_\infty$

Let $A(t) = \phi_0''(x(t))$. Let Λ_{ϕ_0} be the lagrangian manifold defined by $\{(x,\xi),\ \xi = \nabla\phi_0(x)\}$. Then the tangent space $T_{(x(t),\xi(t))}(\Lambda_{\phi_0})$ is given by :

(4.12) $\delta\xi = A(t).\delta x$

and if we use that the tangent bundle $T(\Lambda_{\phi_0})$ is invariant under the differentiated H_q - flow we get by taking the t-derivative of (4.12) and using (4.10) :

$\partial_t\delta\xi = \partial_t A(t).\delta x + A(t)\ \partial_t\delta x = \partial_t A(t).\delta x + A(t)^2\ \delta x = V''(x)\ \delta x$, and consequently:

[2] If we denote by $x(t,y,\eta)$, $\xi(t,y,\eta)$ the solution starting of the point (y,η) at $t = 0$, the equation means :

$\partial^2 x_\ell/\partial t\partial y_j = \partial\xi_\ell/\partial y_j$, $\partial^2\xi_\ell/\partial t\partial y_j = \Sigma_m \partial^2 V/\partial x_\ell\partial x_m .\ \partial x_m/\partial y_j$

$\partial^2 x_\ell/\partial t\partial\eta_j = \partial\xi_\ell/\partial\eta_j$, $\partial^2\xi_\ell/\partial t\partial\eta_j = \Sigma_m \partial^2 V/\partial x_\ell\partial x_m .\ \partial x_m/\partial\eta_j$

[3] we recall that $x(t)$ is an integral curve of $\nabla\phi_0$.

(4.13) $\partial_t A(t) + A(t)^2 = V''(x(t))$.

Put $A(t) = V''(0)^{1/2} + B(t)$. Then (4.13) becomes :

(4.16) $\partial_t B(t) + \mathcal{V}(B(t)) = V''(x(t)) - V''(0) - B(t)^2$

where

(4.17) $\mathcal{V}(B) = V''(0)^{1/2}B + B.V''(0)^{1/2}$

Here we notice that by the Cauchy inequalities :

(4.18) $\| V''(x(t)) - V''(x(0))\|_{\mathcal{L}(\ell^p_\rho,\ell^p_\rho)} = O(|x(t)|_\infty) = O(1)\exp(-|t|/C)$.

Moreover

(4.19) $\exp(t\mathcal{V})(B) = \exp(tV''(0)^{1/2}).B.\exp(tV''(0)^{1/2})$

and as in $[Sj]_2$ (Proposition 1.2) we see that :

(4.20) $\|\exp(tV''(0)^{1/2})\|_{\mathcal{L}(\ell^p_\rho,\ell^p_\rho)} \leqslant \exp(-|t|/C)$, for $t \leqslant 0$.

Hence :

(4.21) $\|\exp(t\mathcal{V})(B)\|_{\mathcal{L}(\ell^p_\rho,\ell^p_\rho)} \leqslant \exp(-2|t|/C)\,\|B\|_{\mathcal{L}(\ell^p_\rho,\ell^p_\rho)}$, for $t \leqslant 0$.

From (4.16) we get :

(4.22) $B(t) = \int_{-\infty}^{t} \exp(-(t-s)\mathcal{V})\,(V''(x(s)) - V''(0) - B(s)^2)\,ds$

If $M(t) = \mathrm{Sup}_{-\infty<s\leqslant t}\|B(s)\|_{\mathcal{L}(\ell^p_\rho,\ell^p_\rho)}$, then

(4.23) $M(t) \leqslant C\,(M(t)^2 + \exp(-|t|/C)|x|_\infty)$

and it follows that $M(0) \leqslant 1/2$ if $|x|_\infty$ is small enough.

######

Using Lemma 4.1 and the Cauchy inequalities, we see that

(4.24) $\|\phi_0''(x) - \phi_0''(0)\|_{\mathcal{L}(\ell^p_\rho,\ell^p_\rho)} = O(|x|_\infty)$

Noticing that $v(t) = d_x\exp(t\nabla\phi_0(x).\partial_x)(x)(v(0))$ satisfies :

(4.25) $\partial_t v(t) = \phi_0''(x(t))v(t)$, where $x(t) = \exp(t\nabla\phi_0(x).\partial_x)(x)$, using the arguments around the proof of (4.21)-(4.23), it is then easy to prove that

(4.26) $\|d_x \exp(t\nabla\phi_0(x).\partial_x)(x)\|_{\mathcal{L}(\ell^p_\rho,\ell^p_\rho)} = O(1)\exp(-|t|/C),\ t \leqslant 0$

Let $\phi \sim \phi_0 + \phi_1 h + \phi_2 h^2 + \ldots,$

be the (asymptotic) solution of the (complete) eiconal equation with

$E \sim E_0 + E_1 h + E_2 h^2 + \ldots$:

(4.27) $V(x) - (1/2)\,|\nabla\phi(x)|_2^2 + h(\,(\Delta\phi(x)/2) - E) = 0,$

i.e. :

(E) $V(x) - (1/2)\,|\nabla\phi_0|_2^2 = 0\ ,$

$(T_1)\ \nabla\phi_0(x).\partial_x\phi_1(x) = (\Delta\phi_0(x)/2) - E_0\ ,$

.

.

$(T_k)\ \nabla\phi_0(x).\partial_x\phi_k(x) =$

$$= (\Delta\phi_{k-1}(x)/2) - (1/2)\,\Sigma_{j=1}^{k-1}\ \nabla\phi_j(x).\nabla\phi_{k-j}(x) - E_{k-1}\ .$$

Here recall that $E_0, \ldots\ldots, E_{k-1}, \ldots$ are defined by the condition that the r.h.s. of $(T_1), \ldots\ldots, (T_k)$, vanish for $x = 0$.

Let us recall that $u = \exp(-\phi/h)$ is the approximate solution of :

$(-(h^2\Delta/2) + V - hE)(u) = 0$

Proposition 4.2 :

There exists $r > 0$ independent of $\mathcal{A}$ and of j such that

(4.28) $\|\nabla^2\phi_j(x)\|_{\mathcal{L}(\ell^p_\rho,\ell^p_\rho)} = O_j(1)$

for $|x|_\infty < r,\ 1 \leqslant p \leqslant \infty.$

Proof :

We recall from $[Sj]_1$ that we already know that $|\nabla\phi_j|_\infty = O_j(1)$ and combining this with the Cauchy inequalities we obtain (4.28) in the special case when $\rho \equiv 1$. In the general case we have apparently to work with the Hessian directly, and we shall therefore take the Hessians of the r.h.s. of $(T_1),(T_2),\dots$.

Knowing (by Lemma (4.1)) that

$|<\phi_0''(x),t\otimes s>| = O(1)\,|t|_{p,\rho}\,.|s|_{q,1/\rho}$, with $(1/p)+(1/q)=1$,

we get by the Cauchy inequalities :

$|<\nabla^2<\phi_0''(x),t\otimes s>,\nu\otimes\mu>| = O(1)\,|t|_{p,\rho}\,.|s|_{q,1/\rho}.\,|\nu|_\infty.|\mu|_\infty$

and Lemma 1.2 of $[Sj]_1$ [4] implies that

$\Delta<\phi_0''(x),t\otimes s> = O(1)\,|t|_{p,\rho}\,.|s|_{q,1/\rho}$.

Hence

(4.29) $\|\Delta\,\phi_0''(x)\|_{\mathcal{L}(\ell^p_\rho,\ell^p_\rho)} = O(1)$.

We now differentiate (T_1) twice and get :

(4.30) $\nabla\phi_0(x).\partial_x(\nabla^2\phi_1) + \phi_0''.\,\phi_1'' + \phi_1''.\phi_0''$

$$= (1/2)\Delta\phi_0'' - \nabla^3\phi_0(x)\;\mathrm{L}\;\nabla\phi_1(x)$$

where "L" means contraction of tensors :

$<\nabla^3\phi_0(x)\;\mathrm{L}\;\nabla\phi_1(x),\,t\otimes s> \;=\; <\nabla^3\phi_0(x)\,,\nabla\phi_1(x)\otimes t\otimes s>$.

By the Cauchy inequalities, Lemma (4.1) and the fact that $|\nabla\phi_1|_\infty = O(1)$, we get that this expression is $O(1)\,|t|_{p,\rho}\,.|s|_{q,1/\rho}$ and so we have :

(4.31) The norm in $\mathcal{L}(\ell^p_\rho)$ of $\nabla^3\phi_0(x)\;\mathrm{L}\;\nabla\phi_1(x)$ is $O(1)$.

Consider (4.30) along an integral curve $x = x(t) = \exp(t\nabla\phi_0.\partial_x)\,(x)$.

Let $\Phi(t,s)$ be the fundamental matrix for the corresponding problem:

$\partial_t\nu(t) = -\,\phi_0''(x(t))\,\nu(t)$,

[4] If A is a complex $N\times N$ matrix, then $|\mathrm{Tr}A| \leqslant \|A\|_{\mathcal{L}(\ell^\infty,\ell^1)}$

that is the solution of :

(4.32) $\partial_t \Phi(t,s)) = -\phi_0''(x(t))\Phi(t,s)$; $\Phi(s,s)=1$

Then (see the proof of (4.26))

(4.33) $\|\Phi(t,s)\|_{\mathcal{L}(\ell^p_\rho)} = O(1)\exp(-(t-s)/C)$, $\quad -\infty < s \leq t \leq 0$

$\quad = O(1)\exp(C|t-s|)$, $\quad -\infty < t \leq s \leq 0$

If B is a matrix, put :

$\tilde{\Phi}(t,s)\,(B) = \Phi(t,s).B.\,{}^t\Phi(t,s)$.

Then $\tilde{\Phi}(s,s)\,B = B$ and $\tilde{\Phi}(t,s)$ is a solution of :

$\partial_t\tilde{\Phi}(t,s)(B) + \phi_0''(x(t))\,\tilde{\Phi}(t,s)\,(B) + \tilde{\Phi}(t,s)\,(B)\,\phi_0''(x(t)) = 0$

(using that $\phi_0''(x(t))$ is symmetric). Notice that all non-trivial solutions of this equation explode as $t \to -\infty$. The non-exploding solution to (4.30) is then :

(4.34)) $\phi_1''(x(t)) = \int_{-\infty}^{t} \tilde{\Phi}(t,s)\,((1/2)\Delta\phi_0'' - \nabla^3\phi_0(x)\ L\,\nabla\phi_1)(x(s))ds$

which is (using (4.29), (4.31) and (4.33)) $O(1)$ in $\mathcal{L}(\ell^p_\rho)$.

Assume by induction that we have established (4.28) for $1 \leq j \leq k-1$.

Taking the Hessian of (T_k) we get :

(4.35) $\nabla\phi_0(x).\partial_x(\phi_k'') + \phi_0''.\,\phi_k'' + \phi_k''.\,\phi_0'' =$

$= -\nabla^3\phi_0(x)\ L\,\nabla\phi_k(x) + f_k''$

where f_k is the r.h.s. of (T_k).

Here $\|\phi_0''\,L\,\phi_k'\|_{\mathcal{L}(\ell^p_\rho)} = O(1)$ by the same argument as before. Observe now that f_k'' contains terms of the form :

$(1/2)\,\Delta\phi_{k-1}''$, $\phi_j''.\,\phi_{k-j}''$, $\phi_j'''\,L\,\phi_{k-j}'$

which are all $O(1)$ in $\mathcal{L}(\ell^p_\rho)$. The solution of (4.35) is given by a formula analogous to (4.34) and it follows that (4.28) holds for $j = k$.

We shall next analyze the influence of a perturbation $\mathcal{W}$ on V. Let us attach to the set $\mathcal{A}$ the set $\mathcal{B}$ defined again as a disjoint union over $\mathbb{N}$:

$\mathcal{B} = \cup_m \mathcal{B}_m$ where $\mathcal{B}_m \subseteq \mathcal{V}_m \times \mathcal{A}_m$

and let us assume that for all ($\mathcal{W}, \mathcal{V}, \rho$) in $\mathcal{B}$, we have :

$(4.36)_1$ $|\nabla \mathcal{W}(x)|_{\rho,\infty} = O(1)$, uniformly in x and $\mathcal{B}$

and :

$(4.36)_2$ (V_t,ρ) (with $V_t = V + t\,\mathcal{W}$) belongs to $\mathcal{A}$ for all $t \in [0,1]$

(in particular we must have $\mathcal{W}(0) = 0, \mathcal{W}'(0) = 0$, $\|\mathcal{W}''(x)\|_{\mathcal{L}(\ell^p_\rho)} = O(1)$ uniformly).

Let

$\phi = \phi_t \sim \phi_{t,0} + \phi_{t,1}h + \ldots\ldots$

be the phase associated to $V = V_t$.

Differentiating the eiconal equation with respect to t we get

(4.37) $(\nabla_x\phi_0.\partial_x)\ (\partial_t\phi_0) = \mathcal{W}$

(here we take the notation $\phi_0(t,x) = \phi_{t,0}(x)$)

and hence :

(4.38) $(\partial_t\phi_0)(t,x) = \int_{-\infty}^{0} \mathcal{W}(\exp\,(s\nabla_x\phi_0(t,x).\partial_x)(x))ds$.

We now observe that :

$d(\mathcal{W}(\exp\,(s\nabla_x\phi_0(t,x).\partial_x)(x))) = d\,\mathcal{W} \circ d(\exp\,(s\nabla_x\phi_0(t,x).\partial_x)(x))$.

Using (4.5), (4.26) (with $p = 1$ and ρ replaced by $1/\rho$) and (4.36), we see that :

(4.39) $|\nabla_x\partial_t\phi_0|_{\infty,\rho} = O(1)$.

Assume by induction that we have proved that :

$|\nabla_x\partial_t\phi_j|_{\infty,\rho} = O(1)$ for $0 \leqslant j \leqslant k-1$.

Differentiating T_k with respect to t, we get :

(4.40) $\nabla_x\phi_0(t,x).\partial_x\partial_t\phi_k(t,x) = -\nabla\partial_t\phi_0(t,x).\nabla_x\phi_k + (\Delta\partial_t\phi_{k-1}(t,x)/2) - $

$$-\Sigma_{j=1}^{k-1}\ \nabla_x\partial_t\phi_j(t,x).\nabla_x\phi_{k-j}(t,x)\ -\partial_t E_{k-1}(t)\ .$$

The x-gradient of the l.h.s. is

$\nabla_x\phi_0(t,x).\partial_x(\nabla_x\partial_t\phi_k(t,x)) + \phi_0''(t,x).\nabla_x\partial_t\phi_k(t,x)$

and the x-gradient of the r.h.s. is a sum of terms of the form :

$\alpha = \nabla_x^2(f)\ (\nabla_x g),\ \beta = \nabla_x^2(g)\ (\nabla_x f),\ \gamma = \Delta_x\nabla_x f$

for various functions f and g satisfying

(4.41) $|\nabla_x f|_{\infty,\rho}$, $|\nabla_x g|_{\infty}$, $\|\nabla_x^2 g\|_{\mathcal{L}(\ell^\infty_\rho)} = O(1)$.

(a) $f = \partial_t\phi_0(t,x)$, $g = \phi_k$ (the verification of (4.41) is obtained through (4.39), Proposition 3.1 in $[Sj]_1$, and Proposition (4.2)).

(b) $f = \partial_t\phi_{k-1}$ ((4.41) is satisfied by the induction assumption)

(c) $f = \partial_t\phi_j$, $g = \phi_{k-j}$ with $1 \leq j \leq k-1$.

We have by Cauchy (and (4.40)) :

$<\nabla_x^2 f,\ \nu\otimes\mu> \ = \ O(1)\ |\nu|_\infty|\mu|_{1,1/\rho}$

so

$\|\nabla_x^2 f\|_{\mathcal{L}(\ell^\infty,\ell^\infty_\rho)} = \ O(1)$

and hence $|\alpha|_{\infty,\rho} = \ O(1)$.

That $|\beta|_{\infty,\rho} = O(1)$ is immediate.

Finally we get $|\gamma|_{\infty,\rho} \ = \ O(1)$, by starting from $<\nabla_x f,\nu> = \ O(1)|\nu|_{1,1/\rho}$, taking the Hessian , using the Cauchy inequalities :

$<\nabla_x^2<\nabla_x f,\nu>,t\otimes s> \ = \ O(1)|\nu|_{1,1/\rho}|t|_\infty.|s|_\infty$

and finally Lemma 1.2 of $[Sj]_1$ to get :

$<\nabla_x\Delta_x f,\nu> = \ O(1)|\nu|_{1,1/\rho}$.

Then using the analog of (4.38) for $\nabla_x \partial_t \phi_k$ with $\mathcal{W}$ replaced by the r.h.s. of (4.40) we get the control of $|\nabla_x \partial_t \phi_k|_{\infty,\rho}$. Then we have proved:

Proposition 4.3:

Under the assumptions (4.36), let ϕ_t be the phase associated to the perturbation $V_t = V + t\,\mathcal{W}$. Writing

$\phi_t \sim \phi_{t,0} + \phi_{t,1} h + \ldots\ldots,$

we have for every j, and uniformly for $(\mathcal{W}, V, \rho, t)$ in $\mathcal{B} \times [0,1]$:

(4.42) $|\nabla_x \partial_t \phi_{t,j}|_{\infty,\rho} = O(1)$ *for* $|x|_\infty \leq r$.

We shall apply the above estimates to show the exponential convergence of the WKB ground state energy divided by the dimension, for a certain sequence of potentials : $V^{(m)}(x_1, \ldots, x_m)$, $m = 1,2,\ldots\ldots$

Let us describe $\mathcal{A}$ and $\mathcal{B}$ in this case.

We start with this family $V^{(m)}$ defined for each m. For a given m, $\mathcal{A}_m$ will be parametrized by n (with $1 \leq n \leq m-1$) : $\mathcal{A}_m = \cup_{1 \leq n \leq m-1} \mathcal{A}_m^n$.

For given n this is the set of pairs (V,ρ) where (using a notation introduced in the proof of Lemma 2.4)

(4.43) $V = (1-t)\,(V^{(n)} \tilde{\oplus} V^{(m-n)}) + t\,V^{(m)}$ for some $0 \leq t \leq 1$

and

(4.44) ρ belongs to $\mathcal{R}_m^n(\mathcal{k})$ defined as a set of applications on $\{1, \ldots, m\}$ and satisfying[5] :

$\exp(-\mathcal{k}) \leq \rho(j+1)/\rho(j) \leq \exp(\mathcal{k})$

[5] We can (if necessary) reduce ourselves to a smaller class with the additional assumption that $\rho(j) = 1$ for $j \geq n$.

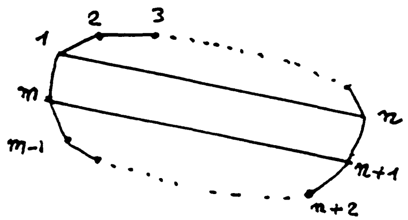
(with the convention that if ρ is defined on $\{1,\dots,m\}$, $\rho(m+1)=\rho(1)$)

$\exp(-\mathscr{k}) \leqslant \rho(n)/\rho(1) \leqslant \exp(\mathscr{k})$

$\exp(-\mathscr{k}) \leqslant \rho(m)/\rho(n+1) \leqslant \exp(\mathscr{k})$

Notice that (4.44) gives bounds for $\rho(j)/\rho(k)$ when (j,k) is a pair of nearest neighbors in the graph :

GRAPH :



Similarly the set $\mathscr{B}$ is defined by describing $\mathscr{B}_m$ as $\cup_n \mathscr{B}_m^n$ where :

(4.45) $\mathscr{B}_m^n$ is the set $\{\mathscr{W}_n^m\} \times \mathscr{A}_m^n$, with $\mathscr{W}_n^m = (V^{(m)} - V^{(n)} \tilde{\oplus} V^{(m-n)})$

Let us assume that, for a suitable $\mathscr{k}$, the assumptions of Proposition (4.3) are satisfied for the set $\mathscr{B}$ associated to the sequence $V^{(m)}$ (we shall give in §6 examples where this is true). Then if $\phi^{(m)}$ denotes the phase associated to $V^{(m)}$ we obtain by integrating

(4.42) with respect to t :

(4.46) $|\nabla(\phi_k^{(m+p)} - \phi_k^{(m)} \tilde{\oplus} \phi_k^{(p)})|_{\infty,\rho} = O(1)$, $|x| < r$.

We choose $\rho(s) = \exp(\mathscr{k}\ \min(s, m+1-s))$ (for $1 \leqslant s \leqslant m+1$) and $=1$ for $s \geqslant m+1$ .We add one more assumption :

(4.47) For every m, $V^{(m)}$ is invariant under cyclic permutations of the coordinates : $V^{(m)}(x_m x_1, \ldots, x_{m-1}) = V^{(m)}(x_1, \ldots, x_m)$.

Then $\phi^{(m)}$ will have the same property. Let

$hE(m) \sim h(E_0(m) + E_1(m)h + \ldots)$

be the WKB ground state of $-(h^2/2)\Delta + V^{(m)}$.

We recall that we have seen just before the Proposition (4.2) the following equality :

(4.48) $E_k(m) = (\Delta\phi_k^{(m)}(0)/2) - (1/2)\Sigma_{j=1}^{k} \nabla\phi_j^{(m)}(0).\nabla\phi_{k+1-j}^{(m)}(0)$

and using the cyclic invariance of $\phi^{(m)}$ we get for any $s \in \{1, \ldots, m\}$:

(4.49) $(E_k(m)/m) = \partial_{x_s}^2\phi_k^{(m)}(0) - (1/2)\Sigma_{j=1}^{k} \partial_{x_s}\phi_j^{(m)}(0).\partial_{x_s}\phi_{k+1-j}^{(m)}(0)$.

Choosing s with $|s-(m/2)| \leqslant 1$, we obtain from (4.46) that :

$\partial_{x_s}\phi_k^{(m+p)}(x_1, \ldots, x_{m+p}) - \partial_{x_s}\phi_k^{(m)}(x_1, \ldots, x_m) = O(\exp(-\Bbbk m/2))$

By Cauchy's inequality, we can replace ∂_{x_s} by $\partial_{x_s}^2$. Using these estimates with (4.49), we get :

(4.50) $(E_k(m+p)/(m+p)) - (E_k(m)/m) = O_k(\exp(-\Bbbk m/2))$.

which gives for each k the exponential convergence of the $E_k(m)/m$ as m tends to ∞.

To summarize, we have proved the

Theorem 4.4

If the sequence of potentials $V^{(m)}$ satisfies uniformly (4.1),(4.2),(4.3),(4.4) and (4.36) for the family of $\rho \in \mathcal{R}_m^n(\Bbbk)$ introduced in (4.44)[6]*, then the first eigenvalue of the Schrödinger operator* : $-(h^2/2)\Delta_m + V^{(m)}$

[6] More precisely, we have associated to the sequence $V^{(m)}$ and to a set of weights $\mathcal{R}_m^n(\Bbbk)$ a set $\mathcal{A}$ and a set $\mathcal{B}$. The exact assumption is that we can find $\Bbbk$ s.t. all the assumptions concerning $\mathcal{A}$ and $\mathcal{B}$ are satisfied.

admits an asymptotic expansion of the form : $h\Sigma_{k\geq 0} E_k(m).h^k$.
The sequence $E_k(m)/m$ is convergent to a limit E_k^∞ and we have the following inequality :
For all k, there exists C_k s.t.
(4.51) $|E_k^\infty - (E_k(m)/m)| \leq C_k \exp(-\not{k}m/2)$.

§5 Comparison between the Dirichlet problem in a box and the global problem

§5.1 Introduction :

In $[Sj]_1$, the semi-classical study of the fundamental level of the Dirichlet realization in a sufficiently small box was achieved. The validity of the results was subsequently extended in $[Sj]_2$. We are here in the apparently very simple case of a one well problem, and it is natural to think (but difficult to control with respect to m) that the first eigenvalue of the Dirichlet problem in a box containing the unique minimum of the potential will be in the semi-classical limit quite near of the first eigenvalue of the global problem in $\mathbb{R}^m$. We shall prove, following essentially the ideas of $[Sj]_1$ § 5-6, that it is effectively the case under the restrictive condition on the dimension that :
(5.1.1) $m = O(h^{-N_0})$ for some fixed N_0.
This is naturally not completely satisfactory for our purpose but we shall see how to circumvent this problem in §6. In the two next sections, we shall construct as a preliminary step for a procedure of localization of

estimates a suitable family of boxes covering $\mathbb{R}^m$. The idea behind this construction is to compare (more precisely to minorize) by a suitable translation the potential in any box of the family and the potential in a box centered at the minimum of the potential.

§5.2 Case of a quadratic potential :

Let us consider

$V(x) = (1/2) < V''(0)x,x >$

with (see the stronger assumptions we make in §4)

(5.2.1) $V''(0) = D+A$, with D diagonal,

$\|A\|_{\mathcal{L}(\ell^\infty)} \leq r_1 < r_0 \leq \lambda_{min}(D) \leq \lambda_{sup}(D) \leq C_0$

r_1, r_0, C_0 are fixed and independent of the dimension m.

These assumptions were introduced in $[Sj]_2$.

Then we know from $[Sj]_2$ (and we have already used in $(4.7)_1$) that

(5.2.2) $V''(0)^{1/2} = \tilde{D}+\tilde{A}$, with $\tilde{D}$ diagonal,

$\|\tilde{A}\|_{\mathcal{L}(\ell^\infty)} \leq \tilde{r}_1 < \tilde{r}_0 \leq \lambda_{min}(\tilde{D}) \leq \lambda_{sup}(\tilde{D}) \leq \tilde{C}_0$

$\tilde{r}_1, \tilde{r}_0, \tilde{C}_0$ are fixed and independent of the dimension m.

It will be easier to work in the Morse coordinates :

(5.2.3) $y = V''(0)^{1/2}x$

since we get in the new coordinates :

(5.2.4) $V(x) = y^2/2$.

As in $[Sj]_1$ §5,6, we consider then the following family of boxes, which depends on 2 parameters C and ε. The center of the box Ω_ρ is $\rho = (\rho_1, \dots, \rho_m)$ and $\Omega_\rho = I_{\rho_1} \times \dots\dots \times I_{\rho_m}$ in the new coordinates. Here for each j, we have

$\rho_j = 0$ or $\rho_j \geqslant C\varepsilon$, and in the first case $I_{\rho_j} = [-C\varepsilon, C\varepsilon]$ while in the second case $I_{\rho_j} = [\rho_j - \varepsilon, \rho_j + \varepsilon]$. Here $C \geqslant 1$, $\varepsilon > 0$.

Using (5.2.4) it is easy to see that :

(5.2.5) $V(x) - V(x-\rho) \geqslant (1-\eta(C))\, V(\rho)$, $x \in \Omega_\rho$,

where $\eta(C)$ is independent of ε and tends to 0 when C tends to ∞.

The Ω_ρ are somewhat distorted boxes, but since

(5.2.7) $|y|_p \sim |x|_p$, $1 \leqslant p \leqslant \infty$,

the ℓ^∞-diameter of Ω_ρ is $O(\varepsilon)$ when C is fixed.

§5.3 The general case.

Let $V : \mathbb{R}^m \to \mathbb{R}$ be smooth with :

(5.3.1) $V(0) = 0$, $V'(0) = 0$ and $V''(0)$ satisfying (5.2.1).

(5.3.2) $\langle V''(x), t_1 \otimes t_2 \rangle = O(1)\, |t_1|_{p_1} |t_2|_{p_2}$

uniformly in x, t_1, t_2 and for all p_1, p_2 s.t. $1 = 1/p_1 + 1/p_2$.

(5.3.3) $\langle V'''(x), t_1 \otimes t_2 \otimes t_3 \rangle = O(1)\, |t_1|_{p_1} |t_2|_{p_2} |t_3|_{p_3}$

uniformly in x, t_1, t_2, t_3 and for all p_1, p_2, p_3 s.t. $1 = 1/p_1 + 1/p_2 + 1/p_3$.

We write

(5.3.4) $V(x) = V_0(x) + \mathcal{W}(x)$ with $V_0(x) = (1/2) \langle V''(0)x, x \rangle$.

So we have the property (5.2.6) for V_0 :

(5.3.5) $V_0(x) - V_0(x-\rho) \geqslant (1-\eta(C))\, V_0(\rho)$, $x \in \Omega_\rho$,

and $\mathcal{W}$ vanishes to the third order at 0 and satisfies (5.3.3).

Let $\rho + x \in \Omega_\rho$ (so that $x \in \Omega_0$). Then :

$\mathcal{W}(\rho + x) - \mathcal{W}(x) = \mathcal{W}(\rho) - \mathcal{W}(0) + \langle \nabla \mathcal{W}(\rho) - \nabla \mathcal{W}(0), x \rangle$

$$+\int_0^1 (1-t) < \nabla^2 \mathcal{W}(\rho+tx) - \nabla^2 \mathcal{W}(tx), x\otimes x > dt$$
$$= \mathcal{W}(\rho) + \int_0^1\int_0^1 < \nabla^3 \mathcal{W}(ts\rho), \rho\otimes\rho\otimes x > t\, dt\, ds$$
$$+\int_0^1\int_0^1 (1-t) < \nabla^3 \mathcal{W}(s\rho+tx), \rho\otimes x\otimes x > dt\, ds$$

(5.3.6) $\quad \mathcal{W}(\rho+x) - \mathcal{W}(x) \quad = \mathcal{W}(\rho) + O(1)|x|_\infty |\rho|_2^2 + O(1)|x|_\infty^2|\rho|_1$.

For the particular choices of ρ which are allowed, we see that

(5.3.7) $C\varepsilon|\rho|_1 \leqslant \tilde{C}_0|\rho|_2^2$

where C and ε appear in the choice of Ω_ρ and $\tilde{C}_0$ only depends on the constants appearing in (5.2.1) (see 5.2.7)).

On the other hand

(5.3.8) $|x|_\infty = O(C\varepsilon)$

so, with a new constant (with the same properties as the first one), we get :

(5.3.9) $|x|_\infty|\rho|_1 \leqslant \tilde{C}_0 |\rho|_2^2$

Finally we get from (5.3.6)-(5.3.9) that :

(5.3.10) $\mathcal{W}(\rho+x) - \mathcal{W}(x) = \mathcal{W}(\rho) + O(1)\, C\varepsilon\, |\rho|_2^2$

If we combine with the properties of V_0, we get for each x in Ω_ρ :

(5.3.11) $V(x) - V(x-\rho) \geqslant V(\rho) - \eta(C)\, V_0(\rho) - O(1)\, C\varepsilon\, |\rho|_2^2$.

For every $\delta > 0$, we get by chosing first C sufficiently large and then ε sufficiently small :

(5.3.12) $V(x) - V(x-\rho) \geqslant V(\rho) - \delta\, |\rho|_2^2$, for $x \in \Omega_\rho$.

(Here we have used (5.3.2) for the first time).

If we have the additional property that :

(5.3.13) $V''(x) \geqslant \omega\, I > 0$, there is a choice of ε and C in the construction of the ball s.t., for some $\delta_0 > 0$, we have :

(5.3.14) $V(x)-V(x-\rho) \geqslant \delta_0 |\rho|_2^2$, for $x \in \Omega_\rho$.

(compare this estimate with (6.2) in $[Sj]_1$)

§5.4 Statement of the result and end of the proof :

Theorem 5.4.1

Let V satisfy (5.2.1), (5.3.1)-(5.3.3), (5.3.13) and

(5.4.1) V extends holomorphically to $\{x \in \mathbb{C}^m; |x|_\infty < r_0\}$ *and* $|\nabla V|_\infty = O(1)$ *in this polydisc.*

We assume that the condition $m = O(h^{-N_0})$ *is satisfied. Then the first eigenvalue of the Schrödinger equation in* $\mathbb{R}^m$ $\lambda_1(m,h)$ *is of the form* $hE(m) + O(h^\infty)$ *(where* $hE(m)$ *is the WKB eigenvalue constructed in* $[Sj]_2$ *, see also §4).*

Sketch of the proof

This is essentially the same proof as in $[Sj]_1$ using the improvements in $[Sj]_2$ and the new construction of boxes we give in sections 5.1-5.3. Let us recall some of the steps.

We choose $\varepsilon > 0$ so that $C\varepsilon << r_0$. Let us first consider the Dirichlet realization P_{Ω_0} of $-(h^2\Delta/2)+V$ in the "twisted" box Ω_0. In view of (5.4.1), we can construct as in $[Sj]_2$ (see our section 4) a WKB-candidate $hE(h)$ for the lowest eigenvalue of P_{Ω_0} with :

(5.4.2) $E(h) \sim E_0 + E_1 h + \ldots$, $E_0 \sim m$, $E_j = O_j(m)$

and modifying E(h) by $O(mh^{\infty})$ we also know from the arguments of $[Sj]_2$ that hE(h) is exactly equal to the lowest eigenvalue of P_{Ω_0}, when h is small enough. The only slightly new point here is that Ω_0 is not exactly a ℓ^{∞}-ball in the x-coordinates. However, it is enough to notice according to (5.2.7) that

(5.4.3) $B(0, C\varepsilon/C_1) \subset \Omega_0 \subset B(0, C_1 C\varepsilon)$

with $B(x_0, r) = \{x \in \mathbb{R}^n;\ |x - x_0| < r\}$.

Let us now observe that by monotonicity we have :

(5.4.4) $\lambda_1(m,h) \leqslant hE(h)$.

In order to get a lower bound, we follow the general strategy of $[Sj]_1$ (sections 5, 6) and start by establishing some exponentially weighted estimates in Ω_0. Lemma 5.1 of $[Sj]_1$ remains valid in the present context and we conclude that if $\tilde{V} = V - \Sigma x_j^{2M}$, and if $h\tilde{E}$ is the lowest eigenvalue of the Dirichlet realization of $-(h^2\Delta/2) + \tilde{V}$ in Ω_0, then

(5.4.5) $E - \tilde{E} = O(1)\, m.h^{M-1}$.

As in the end of section 5 of $[Sj]_1$ we then obtain the estimate

(5.4.6) $(hE - O(1)mh^{M-1})\|u\|^2 \leqslant (\exp(\psi/h)(-(h^2\Delta/2)+V)\exp(-\psi/h)u|u)$,

for each $u \in C_0^{\infty}(\Omega_0)$, provided that ψ is a real valued smooth function, defined on Ω_0 with

(5.4.7) $(1/2)\ |\nabla\psi(x)|^2 \leqslant \Sigma_{j=1}^{m} x_j^{2M}$, $x \in \Omega_0$.

Replacing u by $\exp(\psi/h)u$, we can rewrite (5.4.6) as

(5.4.8) $(hE - O(1)mh^{M-1})\|\exp(\psi/h)u\|^2$

$\leqslant (\exp(\psi/h)(-(h^2\Delta/2)+V)\,u|\exp(\psi/h)u)$, for each $u \in C_0^{\infty}(\Omega_0)$.

Using now (5.3.14), we deduce from (5.4.8)

(5.4.9) $(hE-O(1)mh^{M-1})\|\exp(\psi/h)u\|^2$

$\leqslant (\exp(\psi/h)(-(h^2\Delta/2)+V)\,u|\exp(\psi/h)u)$, for each $u\in C_0^\infty(\Omega_\rho)$, provided that ψ is a real valued smooth function, defined on Ω_ρ with

(5.4.10) $(1/2)\,|\nabla\psi(x)|^2 \leqslant \Sigma_{j=1}^{m}(x_j-\rho_j)^{2M}$, $x\in\Omega_\rho$.

Then we have just to control the patching procedure which appears in the estimate (6.18) in $[Sj]_1$. The patching procedure is based on a resolution of the identity. We just take the same one but in the y variables. The only new problem occurs in the control of the commutators.

For that, we only need to observe that (with the notations of § 5.2), if we introduce cutoff functions of the form

(5.4.11) $\chi\;(x) \;=\; \Pi_1^m\chi_j(y_j)$,

where :

(5.4.12) $|\chi_j(t)|\leqslant 1$

and

(5.4.13) $|\chi_j'(t)| + |\chi_j''(t)| \leqslant D$

(where D is independent of j),

then :

(5.4.14) $|\nabla_x\chi(x)|_\infty\leqslant C(D)$

(5.4.15) $|\Delta_x\chi(x)| \leqslant C\,(D)\,m^3$.[7]

Let us prove for instance (5.4.14) :

$\partial_{x_\nu}\chi \;=\; \Sigma_1^m\chi_1(y_1).....\chi_{k-1}(y_{k-1})\;(\partial_{x_\nu}(\chi_k(y_k)).\chi_{k+1}(y_{k+1}).......\chi_m(y_m))$

with $\underline{(\partial_{x_\nu}(\chi_k(y_k)) = \chi_k'}(y_k)(\partial_{x_\nu}(y_k)) = (V''(0)^{1/2})_{k\nu}\chi_k'(y_k)$.

[7] In fact using lemma 1.2 in $[Sj]_1$ we can get O(m) but this improvement is of no use here.

This gives us :

$$\partial_{x_\nu}\chi = \Sigma_{k=1}^{m} (V''(0)^{1/2})_{k\nu}\chi_1(y_1).....\chi_{k-1}(y_{k-1})\, \chi_k'.\chi_{k+1}(y_{k+1}).......\chi_m(y_m)$$
$$= \Sigma_{k=1}^{m} (V''(0)^{1/2})_{k\nu} t_k(y)$$

with $t_k(y) = \chi_1(y_1).....\chi_{k-1}(y_{k-1})\, \chi_k'.\chi_{k+1}(y_{k+1}).......\chi_m(y_m)$.

According to (5.4.12) and (5.4.13), $(t_k(y))_k$ is in a bounded ball of ℓ^∞ and using (5.2.2), we get (5.4.14).

The control of cut off terms occurs in the proof in §6 of $[Sj]_1$ only in passing from (6.18) to (6.19). These terms are multiplied by an exponentially small (w.r.to h) term and as in $[Sj]_1$ we get

(5.4.15) $(hE - O(1)mh^{M-1})(1 + O(\exp(-1/Ch)))\|u\|^2$

$\leqslant \int(1 + O(\exp(-1/Ch)))(-(h^2\Delta/2)+V)\, u)udx$

$\qquad + \int(O(\exp(-1/Ch))\, |u|.|\nabla u|_2 dx.$

Since $V \geqslant 0$, we have

$(h^2/2)\int|\nabla u|_2^2 dx \leqslant \int(-(h^2\Delta/2)+V)\, u)udx$,

so we end up with

(5.4.16) $(hE - O(1)mh^{M-1})\|u\|^2$

$\leqslant \int(1 + O(\exp(-1/Ch))(-(h^2\Delta/2)+V)\, u)udx.$

Taking for u a sequence of truncations of the first eigenfunction, we get in the limit : $hE - O(1)mh^{M-1} \leqslant (1+O(\exp(-1/\tilde{C}h))\lambda_1(m,h)$

and combining with (5.4.4) :

(5.4.17) $hE - O(1)mh^{M-1} \leqslant \lambda_1(m,h) \leqslant hE.$

§6. Complete study of the model for $\nu < 1/4$, proof of Theorem 1.1 .

We return in this section to the initial conventions to work with

$-h^2\Delta + V$.

(Note that it is easy to go from one convention to the other by a change of h : $\tilde{h} = h/\sqrt{2}$).

§6.1 Summary of the different steps :

As we have seen in Theorem 5.4.1 :

(6.1.1) $\lambda_1(m; h) \sim h\Sigma_{j\geq 0}\, \Lambda_j(m)\, h^j$ if $m = O(h^{-N_0})$

(with $\Lambda_j(m) = E_j(m).2^{-(j+1)/2}$).

But we have seen in §2, that :

(6.1.2) $|\, (\lambda_1(m;h)/m) - \mathrm{Lim}_{m\to\infty}\, (\lambda_1(m;h)/m)\, | \leq Ch/m$

Taking $m = h^{-M}$, we get (using Theorem 4.4) the existence of a sequence Λ_j s.t. :

(6.1.3) $|\, h(\Sigma_{M\geq j\geq 0}\, \Lambda_j \,.\, h^j) - \mathrm{Lim}_{m\to\infty}\, (\lambda_1(m;h)/m)\, | \leq C_M . h^M$

as h tends to 0, where :

(6.1.4) $\Lambda_j = \mathrm{Lim}_{m\to\infty}\, (\Lambda_j(m)/m)$

Of course we have to verify that all the conditions of the different theorems we use are satisfied for Example 2.6.

But before let us give a weaker result which can be obtained easier and some explicit computations on the harmonic approximation permitting to determine Λ_0.

Lemma 6.1.1

There exists a constant C such that, for all $h \in]0,h_0]$ and all $m \geq 1$, we have :

(6.1.5) $0 \leq \lambda_1(m;h,\nu) - (h/2)\Sigma_{k=0}^{m-1}(\sqrt{\omega_k(m;\nu)}) \leq Cm.h^2$

where the $\omega_k(m;\nu)$ are given by :

(6.1.6) $\omega_k(m;\nu) = 1 - 4\nu\cos^2(\pi k/m)$; $k = 0,1,\ldots\ldots,m-1$

Proof

The $(\omega_k(m;\nu)/2)$ are just the eigenvalues of the Hessian of the potential $V^{(m)}$ at 0. An easy computation (cf $[Ka]_2$) gives (6.1.5) (see § 6.2).

The minoration is just that in this case the potential $V^{(m)}$ dominates everywhere its quadratic approximation in view of

(6.1.7) $-\log \mathrm{ch}\, s \geq -s^2/2$

so we get immediately the lower bound in (6.1.5).

For the upper bound, it is sufficient to use the eigenfunction corresponding to the harmonic approximation and to estimate carefully the error using the inequality :

(6.1.8) $|-\log \mathrm{ch}\, s + s^2/2| \leq C s^4$

The details are for example computed in $[Ka]_2$ (p.293-294).

We just give now for completeness some of the computations relative to the harmonic oscillator.

The harmonic approximation at 0 is given in the case of Example (2.6) by the potential :

(6.1.9) $Q_m(x) = (1/4)\Sigma_{k=1}^{m} x_k^2 - (\nu/4)(\Sigma_{k=1}^{m}(x_k + x_{k+1})^2)$

Let us now remark that :

(6.1.10) $\mathrm{Lim}_{m\to\infty}\ [(1/2m)\ \Sigma_{k=0}^{m-1}\ (\sqrt{\omega_k}\ )] =$

$$= (1/2\pi)\ \int_0^\pi \sqrt{1-4\nu.\cos^2\theta}\ d\theta$$

Using directly the Mac-Laurin formula (cf for example [Di], p.302) or Fourier series and Parseval, we get :

(6.1.11) $|[\mathrm{Lim}_{m\to\infty}\ [(1/2m)\ \Sigma_{k=0}^{m-1}\ \sqrt{\omega_k}\ ]] -$

$$-[(1/2\pi)\ \int_0^\pi \sqrt{1-4\nu.\cos^2\theta}\ d\theta\ ] \leqslant [(Cr/m)^{2(r/m)}]^m$$

for all r. By chosing correctly r ($=\alpha m$) we get the exponential convergence which was proved in the general case in §4. We have used here the π-periodicity and the analyticity of the function $\theta \to \sqrt{1-4\nu.\cos^2\theta}$.

§6.2 Verification of the conditions for the Example 2.6

We shall verify the following properties for the potential $V = V^{(m)}$ which is given by

(6.2.1) $V^{(m)}(x) = (1/4)\ \Sigma_{k=1}^{m} x_k^{\ 2}\ -\ \Sigma_{k=1}^{m} \log \mathrm{ch}(\sqrt{\nu/2}\ \ (x_k + x_{k+1}))$.

(6.2.2) V is holomorphic in $B_\infty(0,1)$ with $|\nabla V(x)|_\infty = O(1)$,

(6.2.3) $V(0) = 0, V'(0) = 0$,

(6.2.4) $V''(0) = D + A$, where D is diagonal (positive definite) and

$\|A\|_{\mathcal{L}(\ell^p_\rho,\ell^p_\rho)} \leqslant r_1 < r_0 \leqslant \lambda_{min}(D)$ for all p s.t. $1 \leqslant p \leqslant \infty$ and for all ρ with :

(*) $\exp(-\mathscr{k}) \leqslant \rho(j+1)/\rho(j) \leqslant \exp(\mathscr{k})$.

(6.2.5) $\|\nabla^2 V\|_{\mathcal{L}(\ell^p_\rho,\ell^p_\rho)} = O(1)$

uniformly in $B_\infty(0,1)$ for ρ satisfying (*).

(6.2.6) $V^{(m)\,''}(x) \geqslant ((1-4\nu)/2\ ).\ I_m$

and in particular V is convex for $\nu < 1/4$.

With $\mathcal{W}_n^m = V^{(m)} - (V^{(n)} \tilde{\oplus} V^{(m-n)})$ $(1 \leqslant n \leqslant m-1)$, we must have :

(6.2.7) For all m, for all n $((1 \leqslant n \leqslant m-1))$, for all ρ defined on $\{1,\dots,m\}$ and satisfying (*) and

(**) $\rho(j) = 1$ for $j \geqslant n+1$, and $\rho(1) = 1$,

we have uniformly with respect to ρ, m, n :

$|\nabla \mathcal{W}_n^m|_{\ell_\rho^\infty} = O(1)$ in a complex ball $B(0,1)$.

(6.2.8) $V^{(m)}$ and more generally $(1-t)\ (V^{(n)} \tilde{\oplus} V^{(m-n)}) + t\ V^{(m)}$ for $0 \leqslant t \leqslant 1$ satisfy (6.2.2)-(6.2.4) uniformly for the ρ satisfying (*) and (**) (more generally (*) and

$$\exp(-\mathscr{k}) \leqslant \rho(n)/\rho(1) \leqslant \exp(\mathscr{k})$$
(***)
$$\exp(-\mathscr{k}) \leqslant \rho(m)/\rho(n+1) \leqslant \exp(\mathscr{k}))$$

(6.2.9) $<V''(x), t_1 \otimes t_2> \ = O(1)\, |t_1|_{p_1} |t_2|_{p_2}$

uniformly in x, t_1, t_2 and for all $p_1\, p_2$ s.t. $1 = 1/p_1 + 1/p_2$.

(6.2.10) $< V'''(x), t_1 \otimes t_2 \otimes t_3 > \ = O(1)\, |t_1|_{p_1} |t_2|_{p_2} |t_3|_{p_3}$

uniformly in x, t_1, t_2, t_3 and for all $p_1\, p_2\, p_3$ s.t. $1 = 1/p_1 + 1/p_2 + 1/p_3$.

(6.2.11) For every m, $V^{(m)}$ is invariant under cyclic permutations of the coordinates : $V^{(m)}(x_m x_1, \dots, x_{m-1}) = V^{(m)}(x_1, \dots, x_m)$.

The verification of (6.2.2) is easy. We just observe (always with the convention that $x_{m+1} = x_1$) that :

(6.2.12) $\partial_{x_j} V^{(m)}(x) =$

$= (x_j/2) - \sqrt{\nu/2}\ \mathrm{th}\ (\sqrt{\nu/2}\ (x_j + x_{j+1})) - \sqrt{\nu/2}\ \mathrm{th}\ (\sqrt{\nu/2}\ (x_j + x_{j-1}))$

and that if $|x|_\infty$ is $\leqslant 1$,

$|\sqrt{\nu/2}\,(x_j+x_{j+1})| \leqslant \sqrt{2\nu} \leqslant \sqrt{1/2} < \pi/2$

which implies that $\partial_{x_i} V^{(m)}(x)$ is bounded independently of m.

Let us observe for future use that :

(6.2.13) $(\partial^2_{x_i} V^{(m)})(x) =$

$= ((1/2) - \nu) + (\nu/2)[th^2(\sqrt{\nu/2}\,(x_j+x_{j+1}))+th^2\,(\sqrt{\nu/2}\,(x_j+x_{j-1}))$

(6.2.14) $\partial_{x_i}\partial_{x_{i+1}} V^{(m)}(x) =$

$= -\nu/2\,(1-th^2\,(\sqrt{\nu/2}\,(x_j+x_{j+1}))) = -\nu/(2\,ch^2\,(\sqrt{\nu/2}\,(x_j+x_{j+1})))$

(6.2.15) $\partial_{x_i}\partial_{x_k} V^{(m)}(x) = 0$ if $|j-k| \neq 0,-1,+1$ modulo m.

For (6.2.4) we deduce from (6.2.13) :

(6.2.16) $D = ((1/2) - \nu)\, I_m$

where I_m is the identity in $\mathbb{R}^m$, so we have :

(6.2.17) $r_0 = \lambda_{min}(D) = ((1/2) - \nu)$.

If we denote by τ the operator of translation (by 1) on $\mathbb{R}^m$ defined by: $(\tau x)_i = x_{i-1}$, we can write :

(6.2.18) $A = -(\nu/2)\,(\tau + \tau^{-1})$

The eigenvalues of A are easily computed as $-\nu\,.\,\cos(2\pi k/m)$ for $k = 0,1,\ldots\ldots,m-1$.

It is then easy to verify that for ρ satisfying to (*) :

(6.2.19) $\|A\|_{\mathcal{L}(\ell^p_\rho,\ell^p_\rho)} \leqslant \nu.\exp(\mathcal{k})$

If $\nu < 1/4$, we observe that one can choose $\mathcal{k}$ such that :

(6.2.20) $r_1 = \nu.\exp(\mathcal{k}) < ((1/2) - \nu)$

and we shall make this choice now.

The proof of (6.2.5) is immediate if we observe that all the second derivatives are bounded and that we have (6.2.15). (6.2.6) is a consequence of (6.2.13) - (6.2.15). Let us now verify (6.2.7). We just observe (with the notation of §2) that :

$$\mathcal{W}_n^m = W(x_m x_1) + W(x_n x_{n+1}) - W(x_n x_1) - W(x_m, x_{n+1})$$
$$= \log ch(\sqrt{\nu/2}\ (x_m + x_1)) + \log ch(\sqrt{\nu/2}\ (x_n + x_{n+1}))$$
$$- \log ch(\sqrt{\nu/2}\ (x_n + x_1)) - \log ch(\sqrt{\nu/2}\ (x_m + x_{n+1}))$$

The only j for which $\partial_{x_j} \mathcal{W}_n^m$ are not 0 are $j = 1, n, n+1, m$ and one has for each of these terms :

$$|\partial_{x_j} \mathcal{W}_n^m(x)| \leqslant 4\sqrt{\nu/2}\ \mathrm{Sup}_{\tau \in \mathbb{C}, |\tau| \leqslant 1} (th(\sqrt{2\nu}\,\tau)$$

for $x \in \mathbb{C}^m$, $|x|_\infty \leqslant 1$.

As in the proof of (6.2.12), $\mathrm{Sup}_{\tau \in \mathbb{C}, |\tau| \leqslant 1} (th(\sqrt{2\nu}\,\tau)$ is finite.

According to the (**), the property (6.2.7) is clear.

Let us verify now (6.2.8). We first observe that :

$$D_t^{(m)} = (1-t)\, D^{(n)} \otimes D^{(m-n)} + t\, A^{(m)} \quad \text{and :}$$
$$A_t^{(m)} = (1-t)\, A^{(n)} \otimes A^{(m-n)} + t\, A^{(m)}.$$

All the properties we need are stable by arithmetical means, so it is sufficient to treat the case $(V^{(n)} \tilde{\oplus} V^{(m-n)})$ for ρ satisfying (***) and (*) which can be reduced by separation of variables to the study of $V = V^{(m)}$ for ρ satisfying (*).We now observe that $\lambda_{min}(D) = (1/2) - \nu)$ and that $\|A\| \leqslant \nu.\exp(\kappa)$.

If $\nu < 1/4$, it is easy to choose $\kappa > 0$ s.t :

$\nu.\exp(\kappa) < (1/2) - \nu)$.

(6.2.9) and (6.2.10) are then easy to verify by using (6.2.13) - (6.2.15).

Finally, (6.2.11) is clear from the definition.

<u>Références</u>

[Ag] S.Agmon

Lectures on exponential decay of solutions of second order elliptic equations, Math. Notes, t.29, Princeton University Press.

[Bra-Li] H.J.Brascamp, E.Lieb :

On extensions of the Brunn-Minkovski and Prékopa-Leindler Theorems, including inequalities for Log concave functions, and with an application to diffusion equation

Journal of functional analysis 22 (1976), pp.366-389

[Bru-He] M.Brunaud, B.Helffer :

Un problème de double puits provenant de la théorie statistico-mécanique des changements de phase (ou relecture d'un cours de M.Kac), Preprint de l'ENS (Mars 1991).

[Di] J.Dieudonné :

Calcul infinitésimal, Hermann; collection méthodes

[Gl-Ja] J.Glimm, A.Jaffe

Quantum Physics (second edition), A functional integral point of view. Springer Verlag

[Ha] E.M.Harrell,

On the rate of asymptotic eigenvalue degeneracy

Comm.in Math. Phys., t.75, 1980, p.239-261

[He] B.Helffer :

Décroissance exponentielle des fonctions propres de l'opérateur de Kac : cas de la dimension >1. Manuscrit, Mars 1991

[He-Sj] B.Helffer, J.Sjostrand :

[1] Multiple wells in the semi-classical limit I
Comm. in PDE, 9(4), 337-408 (1984)

[2] Puits multiples en limite semi-classique II
Interaction moléculaire. Symétries. Perturbation
Ann.Inst. Henri Poincaré Vol.42, n°2, 1985, p.127-212

[3] Multiple wells in the semi-classical limit III
Math.Nachrichte 124 (1985) p.263-313

[4]Analyse semi-classique pour l'équation de Harper
Mémoire de la SMF n°34; Tome 116, Fasc.4 (1988)

[Ka] M.Kac

[1] Statistical mechanics of some one-dimensional systems
Studies in mathematical analysis and related topics : essays in honor of Georges Polya (Stanford Univ. Press, Stanford,California 1962), p.165-169

[2] Mathematical mechanisms of phase transitions
Brandeis lectures (1966), Gordon and Breach, New York

[Ka-Th] M.Kac, C.J.Thomson

Phase transition and eigenvalue degeneracy of a one dimensional anharmonic oscillator

Studies in Applied Mathematics 48 (1969) 257-264

[Ki-Si] W.Kirsch, B.Simon :

Comparison theorems for the gap of Schrödinger operators

JFA , Vol.75, n°2, Dec.1987, p.396-410

[PPW] L.E. Payne, G.Polya, H.F.Weinberger :

On the ratio of consecutive eigenvalues,

Journal of Math. and Physics, 35, n°3 (Oct.56), pp.289-298

[Ru] D.Ruelle :

Statistical mechanics

Math. physics monograph series, W.A.Benjamin, Inc. 1969

[Si] B.Simon

[1] Instantons,double wells and large deviations

Bull.AMS.,t.8, 1983 p.323-326

[2] Semi-classical analysis of low lying eigenvalues I

Ann. Inst. Poincaré, t.38, 1983, p.295-307

[3] Semi-classical analysis of low lying eigenvalues

II tunneling, Ann. of Math. 120, p.89-118 (1984)

[SWYY] I.M.Singer, B.Wong, Shing-Tung Yau, Stephen S.-T.Yau :

An estimate of the gap of the first two eigenvalues in the Schrödinger operator.

Ann. d. Scuola Norm. Sup. di Pisa , Série IV Vol. XII,2, p.319-333

[Sj] J.Sjöstrand :

[1] Potential wells in high dimensions I

(to appear in Annales de l'IHP, Section Physique Théorique)

[2] Potential wells in high dimensions II, more about the one well case,

(to appear in Annales de l'IHP, Section Physique Théorique)

[Th] Colin J. Thompson

Mathematical statistical mechanics,

The Macmillan company New York (1972)

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Eigenvalue asymptotics related to impurities in crystals

Astérisque, tome 210 (1992), p. 183-196
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Eigenvalue asymptotics related to impurities in crystals.

Rainer Hempel

1. Introduction.

In the present paper, we continue the analysis of eigenvalues of Schrödinger operators $H - \lambda W$ in a spectral gap of H. As a typical example, one should think of $H = -\Delta + V$ as a periodic Schrödinger operator which, in solid state physics, may be used to describe the energy spectrum of an electron moving in a pure crystal (in the so-called 1-electron model). The perturbation W simulates a localized impurity, and $\lambda \in \mathbf{R}$ is a coupling constant; both V and W are assumed to be real-valued. Here we ask for the existence and number of discrete eigenvalues of $H - \lambda W$ which are moved into or through the gap as λ increases from 0 to ∞. The connection of this question to solid state physics is discussed in more detail in [7,13]; we only mention that "impurity levels" (i. e., energy levels which are introduced into the spectral gap of the pure crystal by impurities) are responsible for the color of crystals in the case of insulators, and strongly influence conductivity in the case of semi-conductors; cf., e. g., [3, 21].

In the mathematical analysis of this problem, it turns out that the case where W doesn't change sign enjoys many simplifying features: fixing E in the gap and assuming $W \geq 0$ for the moment, basic existence and asymptotic results can be read off from the associated (compact and symmetric) *Birman–Schwinger kernel* $W^{1/2}(H - E)^{-1}W^{1/2}$, (cf. Klaus [18] and, most recently, the remarkable work of Birman [4]). This approach is based entirely on functional analysis and avoids PDE–methods.

In the general situation where W changes sign, however, the associated Birman–Schwinger kernel is no longer symmetric and it is hard to extract useful information from its analysis. Here a more direct approach was developed by Deift and Hempel [7] which combines localization techniques and a quasi–classical volume counting in phase space. Led by some simple physical intuition—which says that a localized perturbation should have localized effects— we start from a suitable approximating problem on the ball B_n , and let n tend to ∞. Note, however, that even this approximation step is by no means trivial, since restricting the operator $-\Delta + V$ to B_n and imposing Dirichlet boundary conditions, will in general produce (unwanted!) eigenvalues in the gap. This method was further extended in some work of Hempel [13, 15], Alama, Deift and Hempel [1], where decoupling by an additional Dirichlet boundary condition (DBC) or Neumann boundary condition (NBC) on ∂B_R is used to separate the region where the perturbation λW is active from the remaining portion of B_n. In Section 2, below, a brief outline of this technique is given (for a more detailed description, cf. [1,15]). By now, this approach has been fully developed and it provides various asymptotic results for the eigenvalue counting functions $N_\pm$, where

$$N_\pm(\lambda; H-E, W) = \sum_{0<\mu<\lambda} \dim\ker(H \mp \mu W - E) \tag{1.1}$$

counts the number of crossings of eigenvalue branches, keeping track of multiplicities; here, again, E is a fixed "control point" in the gap. In Section 3, we present upper and lower asymptotic bounds on N_+ in the general case $W = W_+ - W_-$, $W_\pm \geq 0$.

In Section 4, finally, our method will be used in the delicate problem of finding a lower bound for the (finite) quantity

$$N_-(\infty; K) := \sup_{\lambda>0} N_-(\lambda; H-E, \chi_K),$$

where K is a fixed compact subset of $\mathbf{R}^\nu$. $N_-(\infty; K)$ counts the total number of eigenvalue branches which cross E under the influence of a potential "barrier" supported on K, with height going to infinity. While it is known that (in dimension > 2) no eigenvalue branch of $H + \lambda\chi_K$, $\lambda > 0$, will ever cross E if the diameter of K is small enough, we also know that some eigenvalues will cross E if K contains a ball of sufficiently large radius (cf.[13,15]). In the present paper, we'll concentrate on K's which are drastically different from balls. Here it turns out that decoupling by natural DBC plays a crucial role, highlighting once more the fundamental difference between N_+ and N_- in the case where W is non-negative: while N_+ is dominated by the Weyl term, which is related to the volume of the interior of K, the number we are investigating now is more or less independent of the volume of K ; e. g., a set K looking like a swiss cheese with many small holes may be very effective in shifting eigenvalues through the gap although the volume of the cheese might be very small as compared with the volume of the holes.

The approach described above allows us to discover some of the local effects of the perturbation and connects phase space analysis with eigenvalue counting. However, it is neither simple nor short, and there are many results which can be obtained by more direct methods; we conclude this introduction with a brief discussion of some of these alternatives. As mentioned above, a very fruitful idea consists in the recent observation of Birman [4] that one should apply the first resolvent equation to $(H-E)^{-1}$ in the Birman-Schwinger kernel to replace the control point E in the gap by some $E_0 < \inf\sigma(H)$. The transformed kernel can then be analyzed with the aid of the Gokhberg-Krein theory of weak trace ideals. This yields some sharp asymptotic results for N_+ in the case where W is non-negative, and works even for E sitting on the gap edge, if H is periodic. Since this method tests asymptotics on the scale of Weyl's Law, it gives only weak information for N_-, however.

For W changing sign, W of compact support, a very short and elegant proof for the existence of eigenvalues of $H-\lambda W$ in the gap has been given by Gesztesy and Simon [11], while some very detailed and surprising facts concerning the trajectories of eigenvalue branches in the o.d.e.-case ("trapping and cascading") have been discovered by Gesztesy et al. [10]. Of particular interest and difficulty is the question for the number of eigenvalues in a given *interval* in the gap; here we would like to mention some recent 1-dimensional work of Sobolev [28]. For results concerning eigenvalues in gaps under the semi-classical point of view, we refer to Klopp [19] and Outassourt [20]. Finally, Alama and Li [2] have created a non-linear Birman-Schwinger principle which can be successfully applied to non-linear perturbations of periodic Schrödinger operators.

2. Approximation and decoupling.

We are now going to give a condensed description of the approach developed by Deift and Hempel; for details, see [1,15]. Starting from a Schrödinger operator $H=-\Delta+V$, where V is a bounded potential and H is the unique self-adjoint extension of $-\Delta+V$ on $C_c^\infty(\mathbf{R}^\nu)$, we make the *basic assumption* that $\sigma(H)$, the spectrum of H, has a gap. Again, we are mainly interested in the case where the spectral gap occurs above the infimum of $\sigma_{\text{ess}}(H)$, the essential spectrum of H. As a typical example, one may think of H as a periodic Schrödinger operator, but spectral gaps may also occur in Schrödinger operators of disordered matter (Briet, Combes and Duclos [5]). Also, for convenience, we assume that $V\geq 1$. In the sequel, let $a<b$ be such that

$$[a,b]\cap\sigma(H)=\emptyset.$$

We next introduce the perturbation W, a bounded, real-valued function going to 0 at infinity. While $H-\lambda W$ has the same essential spectrum as H, the perturbation λW may produce discrete spectrum in the gap. By Kato-Rellich perturbation theory, the eigenvalues of $H-\lambda W$ depend analytically on the coupling constant λ, as long as they stay inside the gap. In order to count the eigenvalues, we now fix $E\in(a,b)$ and we define $N_\pm(\lambda):=N_\pm(\lambda;H-E,W)$ as in (1.1).

In the case of non-negative W there are some nice quasi-classical heuristics ("volume counting in phase space"; cf. [7,1]) which suggest that one should expect for N_+ an asymptotic behavior with a leading order term as in Weyl's Law,

$$N_+(\lambda)\sim c_\nu\lambda^{\nu/2}\int W^{\nu/2},\quad \lambda\to\infty,$$

if W decays faster than quadratically. In contrast, if W behaves like $c|x|^{-\alpha}$, for x large and some constants c, $\alpha>0$, then N_- is highly dependent on the decay rate α,

$$N_-(\lambda)\sim C\cdot\lambda^{\nu/\alpha},\quad \lambda\to\infty,$$

under certain natural assumptions on W (cf. [1]). Note that the asymptotics of N_+ can be obtained by Birman's method in [4], and this even in the case where E is situated on the edge of a gap. The case where W changes sign is much harder to understand, and there are only a few upper and lower bounds on $N_+(\lambda)$, for λ large; this will be discussed in Section 3 in more detail.

We next describe the sequence of approximating problems which are used to compactify the problem. Let $a' < a$ and $b' > b$ be such that the interval $[a', b']$ doesn't intersect the spectrum of H. As in [13,1,15], we define

$$H_n = -\Delta_n + V|_{B_n},$$

where $-\Delta_n$ denotes the Dirichlet Laplacian on the ball B_n in $\mathbf{R}^\nu$, and we consider the spectral projection $\Pi_n = P_{[a',b']}(H_n)$ associated with the interval $[a', b']$ where $\{P_\lambda\}_{\lambda \in \mathbf{R}}$ denotes the spectral family. Clearly, Π_n is finite dimensional, and for $c' = b' - a'$, we have

$$\sigma\left(H_n + c'\Pi_n\right) \cap (a', b') = \emptyset.$$

In the next step, we apply cut-offs in order to restrict the integral operator Π_n to the region $B_n - B_{n/2}$. Letting ψ_n be defined by $\psi_n(x) = \psi(x/n)$, $x \in \mathbf{R}^\nu$, $n \in \mathbf{N}$, where $\psi \in C^\infty(\mathbf{R}^\nu)$ enjoys the properties $\psi(x) = 1$, for $|x| \geq 3/4$, $\psi(x) = 0$, for $|x| \leq 1/2$, and $0 \leq \psi(x) \leq 1$ else, we define

$$\tilde{H}_n = H_n + c'\psi_n\Pi_n\psi_n.$$

Here the important point is that $\tilde{H}_n$ has a spectral gap containing the interval $[a, b]$, for sufficiently large n, i. e.,

$$\sigma(\tilde{H}_n) \cap [a, b] = \emptyset, \quad n \geq n_0.$$

This basic result is a consequence of Weyl's Law (which yields a bound $\dim \Pi_n \leq cn^\nu$) and the fact that the eigenfunctions of H_n which build up the projection Π_n are exponentially localized near the boundary ∂B_n (cf. [7,1] for details).

The second useful fact is that the Birman-Schwinger kernels associated with $\tilde{H}_n$ and $W|_{B_n}$ converge to the full Birman-Schwinger kernel in norm. This in turn implies the following comparison result for the counting functions ([15; Proposition 2.3]), valid for $W \geq 0$. To keep the notation concise, we'll often write W instead of $W|_{B_n}$, in the sequel.

2.1. PROPOSITION. *Let H and $\tilde{H}_n$, $n \geq n_0$, be as above, and let $E \in (a, b)$. Assume that W is a non-negative, bounded function, tending to 0 at infinity. We then have*

$$N_\pm(\lambda; H - E, W) \geq \limsup_{n\to\infty} N_\pm(\lambda'; \tilde{H}_n - E, W|_{B_n}), \quad 0 < \lambda' < \lambda, \tag{2.1}$$

$$N_\pm(\lambda; H - E, W) \leq \liminf_{n\to\infty} N_\pm(\lambda'; \tilde{H}_n - E, W|_{B_n}), \quad 0 < \lambda < \lambda'. \tag{2.2}$$

By this approximation process, we have gained the following: as the operators $\tilde{H}_n - \mu W$ all have compact resolvent, we can count eigenvalues starting from the bottom of the spectrum. From Kato-Rellich perturbation theory it is then clear that

$$N_+(\lambda; \tilde{H}_n - E, W) = \dim P_{(-\infty,E)}\left(\tilde{H}_n\right) - \dim P_{(-\infty,E)}\left(\tilde{H}_n - \lambda W\right),$$

and similarly for N_-. Therefore, we can obtain information on $N_\pm(\lambda; \tilde{H}_n - E, W)$ by simply counting how many eigenvalues have been moved over the level E by the perturbation λW. Here we use the notation "$\dim P_{(-\infty,E)}(.)$" to denote the number of eigenvalues below E, counting multiplicities.

By a different method, one can prove the following convergence result for the case $W = W_+ - W_-$ (note that we do *not* get an upper bound here).

2.2. PROPOSITION. (cf. [15; Proposition 2.4]) *Let H and $\tilde{H}_n$, $n \geq n_0$, be as above, and let $E \in (a, b)$. Suppose that W is a bounded function tending to zero at infinity. Then, for $0 < \lambda < \lambda'$, we have*

$$N_\pm(\lambda'; H - E, W) \geq \limsup_{n\to\infty} \left|\dim P_{(-\infty,E)}\left(\tilde{H}_n\right) - \dim P_{(-\infty,E)}\left(\tilde{H}_n \mp \lambda W\right)\right|.$$

The above approximation scheme has simplified the problem, but the eigenvalue counting for $\tilde{H}_n$ and $\tilde{H}_n - \lambda W$ is by no means trivial. As a second main step in the proof, we use decoupling inside the ball B_n to separate the region where λW is active from the region where λW may be neglected. As W decays, this will in particular ensure that the interaction between W and the non-local operator $\psi_n \Pi_n \psi_n$ will be negligable. To obtain upper or lower bounds, we decouple by means of a DBC or NBC on ∂B_R, where the radius R is chosen in such a way that W is sufficiently small outside B_R; note that this can be done independently of n, at least for n large. Here our basic lemma reads as follows ($\mathcal{B}_p$ denotes the p-th Schatten ideal or trace ideal, for $1 \leq p < \infty$; cf. Simon [25]):

2.3. LEMMA. (*cf.* [15; Proposition 1.3]) *Let A, B be compact, symmetric operators and suppose that $B \in \mathcal{B}_p$, for some $p \in [1, \infty)$. Also let $\eta > 0$, $\eta \in \rho(A)$. Then*

$$\left|\dim P_{(\eta,\infty)}(A) - \dim P_{(\eta,\infty)}(A + B)\right| \leq \left|\left|(A - \eta)^{-1}\right|\right|^p \cdot ||B||^p_{\mathcal{B}_p},$$

where $\dim P_{(\eta,\infty)}$ counts the eigenvalues in (η, ∞), repeated according to their multiplicities.

In order to apply this perturbation result in our situation, we need some more notation: Letting $-\Delta_{R;N}$ denote the Neumann Laplacian on B_R, and $-\Delta_{R,n;N,D}$ the Laplacian on the spherical shell $B_n - \bar{B}_R$, with NBC on ∂B_R and DBC on ∂B_n, we have the following trace ideal estimate:

2.4. PROPOSITION. *Let $m > 0$ and let $p > \nu/2$, $p = 2^q$, for some $q \in \mathbf{N}$. Then there exist constants $c, C > 0$ such that*

$$\left\|(-\Delta_n + m)^{-1} - (-\Delta_{R;N} \oplus -\Delta_{R,n;N,D} + m)^{-1}\right\|_{\mathcal{B}_p}^p \leq cR^{\nu-1},$$

and

$$\left\|(-\Delta_n + m)^{-1} - (0|_{B_R}) \oplus (-\Delta_{R,n;N,D} + m)^{-1}\right\|_{\mathcal{B}_p}^p \leq CR^{\nu},$$

for $1 \leq R < n$, where $0|_{B_R}$ denotes the zero operator on $L_2(B_R)$.

A proof of this basic decoupling result can be found in [15;Appendix]; of course, there is a corresponding result for DBC on ∂B_R.

While min-max methods and monotonicity imply that adding Neumann (resp., Dirichlet) boundary conditions increases (resp., decreases) the number of eigenvalues below E, we need estimates which go in the other direction. In the following proposition, we let $-\Delta_{R;N}$ denote the Neumann Laplacian on B_R, $-\Delta_{R,n;ND}$ the Laplacian on $B_n - \bar{B}_R$ with NBC on ∂B_R and DBC on ∂B_n. Then $H_{R;N}$ denotes the operator $-\Delta_{R;N} + V|_{B_R}$ while $\tilde{H}_{R,n;N,D} = -\Delta_{R,n;ND} + V|_{B_n - \bar{B}_R} + c'\psi_n\Pi_n\psi_n$, so that the direct sum $H_{R;N} \oplus \tilde{H}_{R,n;N,D}$ is nothing else but $\tilde{H}_n$ with an additional NBC on ∂B_R.

2.5. PROPOSITION. (*cf.* [15; Lemma 3.2]) *Let H and $\tilde{H}_n$, $n \geq n_0$, be as above and let $E' \in (a, b)$. Then, for $n \geq n_0$ and $1 \leq R \leq n/2$, we have*

$$\begin{aligned}\dim P_{(-\infty,E')}(H_{R;N}) + &\dim P_{(-\infty,E')}\left(\tilde{H}_{R,n;N,D}\right) \\ &\leq \dim P_{(-\infty,E')}\left(\tilde{H}_n\right) + CR^{\nu-1},\end{aligned}$$

with a constant C which is independent of n and R.

To prove an estimate of this type, we apply Lemma 2.3 to the resolvents, use the second resolvent equation to get rid of the potential V and the $\psi_n\Pi_n\psi_n$-term and conclude with an application of the trace ideal estimate given in Proposition 2.4. Of course, decoupling by a DBC on ∂B_R leads to a similar estimate; in the subsequent proposition, we let $-\Delta_{R,n;D}$ denote the Dirichlet Laplacian on $B_n - \bar{B}_R$ and $\tilde{H}_{R,n;D} := -\Delta_{R,n;D} + V|_{B_n - B_R} + c'\psi_n\Pi_n\psi_n$.

2.6. PROPOSITION. (*cf.* [15; Lemma 3.2]) *Let H and $\tilde{H}_n$, $n \geq n_0$, be as above and let $E' \in (a,b)$. Then, for $n \geq n_0$ and $1 \leq R \leq n/2$, we have*

$$\dim P_{(-\infty,E')}(H_R) + \dim P_{(-\infty,E')}\left(\tilde{H}_{R,n;D}\right) \geq \dim P_{(-\infty,E')}\left(\tilde{H}_n\right) - CR^{\nu-1},$$

with a constant C which is independent of n and R.

3. Some asymptotic bounds.

As a first illustration of our approach, we prove a simple *lower* bound for N_+ in the general case $W = W_+ - W_-$, with $W_\pm \geq 0$; note that there is now no need to consider N_- separately because this would only mean to switch from W to $-W$.

Here the main difficulty comes from the competition between the attractive part W_+ and the repulsive part W_-. If W_- decays faster than quadratically, then W_+ always wins over W_- (cf. [1, 15]), and we'll concentrate now on a case where W_- decays slowly,

$$W_-(x) \leq c_0(1+|x|)^{-\alpha}, \qquad x \in \mathbf{R}^\nu, \tag{3.1}$$

for some constants $c > 0$ and $0 < \alpha \leq 2$. The following Theorem 3.1 is a refinement of Corollary 3.5 in [15], where some other related results may be found.

3.1. THEOREM. *Let H be as above, $E \in \mathbf{R} - \sigma(H)$ and suppose that W is bounded and tends to 0 at infinity, with W_- satisfying condition (3.1) for some $0 < \alpha \leq 2$. For W_+ we assume that there exist constants $k \geq 2$, $c_1, c_1' > 0$, $0 < \beta < \alpha$ and γ, where γ satisfies*

$$\nu - 1 \geq \gamma > \nu - 1 - \nu(\alpha - \beta)/2, \tag{3.2}$$

with the property that each spherical shell $B_{nk} - B_{(n-1)k}$, $n = 1, 2, \ldots$, contains at least $c_1'[n^\gamma]$ mutually disjoint balls of radius 1 on which W is bounded from below by $c_1 n^{-\beta}$.

Then there exists a positive constant C such that

$$N_+(\lambda; H - E, W) \geq C\lambda^\kappa, \quad \lambda \geq 1,$$

where $\kappa := (\nu(\alpha - \beta) + 2\gamma + 2)/2\alpha$.

PROOF. As in [1, 15], we let $E_1 := (a+E)/2$ and define

$$R = R(\lambda) = (c_0\lambda/(E - E_1))^{1/\alpha}, \quad \lambda \geq 1.$$

Then it is clear from (3.1) that $0 \leq \lambda W_-(x) \leq E - E_1$, for $|x| \geq R(\lambda)$. We now decouple by means of a DBC on ∂B_R to obtain

$$\begin{aligned}\dim P_{(-\infty,E)}(\tilde{H}_n - \lambda W) \\ \geq \dim P_{(-\infty,E)}(H_R - \lambda W) + \dim P_{(-\infty,E_1)}\left(\tilde{H}_{R,n;D}\right).\end{aligned} \tag{3.3}$$

We first consider the second term on the RHS of (3.3) where Proposition 2.2 implies that

$$\begin{aligned}\dim P_{(-\infty,E_1)}\left(\tilde{H}_{R,n;D}\right) &\geq \dim P_{(-\infty,E_1)}\left(\tilde{H}_n\right) - \dim P_{(-\infty,E_1)}(H_R) - c' R^{\nu-1} \\ &= \dim P_{(-\infty,E)}\left(\tilde{H}_n\right) - \dim P_{(-\infty,E_1)}(H_R) - c' R^{\nu-1},\end{aligned}$$

as E and E_1 belong to the same gap of $\tilde{H}_n$. For the second term on the RHS of (3.3), we introduce DBC on the boundaries of the balls where the lower bound for W holds; we discard the remaining portion of B_R. By Weyl's Law, there exist constants $c_2 > 0$ and c_3 such that

$$\dim P_{(-\infty,\mu)}(-\Delta_1) \geq c_2 \mu^{\nu/2} - c_3, \qquad \mu \geq 0,$$

and it follows that

$$\dim P_{(-\infty,E)}\left(-\Delta_1 + \|V\|_\infty - c_1 \lambda n^{-\beta}\right) \geq c_4 \lambda^{\nu/2} n^{-\nu\beta/2} - c_5, \qquad \lambda \geq 0.$$

Summing up the individual contributions coming from the balls of radius 1 where the lower bound for W holds, we now obtain

$$\begin{aligned}\dim P_{(-\infty,E)}(H_R - \lambda W) &\geq c_5 \sum_{n \leq R/k} n^\gamma \lambda^{\nu/2} n^{-\nu\beta/2} - c_6\, Vol(B_R) \\ &\geq c_7 \lambda^{\nu/2} \lambda^{(1+\gamma-\nu\beta/2)/\alpha} - c_8 \lambda^{\nu/\alpha},\end{aligned}$$

as $R \sim \lambda^{1/\alpha}$; also note that our assumptions imply that $\gamma - \nu\beta/2 > -1$.

Using all of the above information in the RHS of (3.3) and also the estimate

$$\dim P_{(-\infty,E_1)}(H_R) \leq c_9 \lambda^{\nu/\alpha}, \qquad \lambda \geq 1,$$

which is immediate by Weyl's Law, we finally see that

$$\begin{aligned}&\dim P_{(-\infty,E)}\left(\tilde{H}_n - \lambda W\right) - \dim P_{(-\infty,E)}\left(\tilde{H}_n\right) \\ &\quad\geq \dim P_{(-\infty,E)}(H_R - \lambda W) - \dim P_{(-\infty,E_1)}(H_R) - c' R^{\nu-1} \\ &\quad\geq C_1 \lambda^\kappa - C_2 \lambda^{\nu/\alpha} - C_3 \lambda^{\nu/\alpha} - C_4 \lambda^{(\nu-1)/\alpha} \\ &\quad\geq C \lambda^\kappa,\end{aligned}$$

for λ large, since $\kappa > \nu/\alpha$ for γ in the interval defined by (3.2). Now the result follows immediately via Proposition 2.2. ∎

To obtain an upper bound for $N_+(\lambda; H-E, W)$, we next try to squeeze some information from the associated (non-symmetric) Birman-Schwinger kernel.

3.2. THEOREM. *Let H be as above, and let $E \in (a,b)$. Suppose that W satisfies the decay condition*

$$|W(x)| \leq c(1+|x|)^{-\alpha}. \qquad x \in \mathbf{R}^\nu,$$

with some positive constants c and α. Then, for any $p > \nu/\min\{\alpha, 2\}$, we have

$$\limsup_{\lambda \to \infty} \lambda^{-p} N_+(\lambda; H-E, W) < \infty.$$

PROOF. (1) Suppose $0 < \lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_j \leq \ldots$, with $\lambda_j \to \infty$, are the positive coupling constants where the kernel of $H - \lambda_j W - E$ is non-trivial, repeated according to the dimension of $\ker(H - \lambda_j W - E)$. By the Birman–Schwinger–principle, the numbers $\kappa_j := \lambda_j^{-1}$ are eigenvalues of the Birman–Schwinger kernel

$$\mathcal{K} := (\operatorname{sgn} W)|W|^{1/2}(H-E)^{-1}|W|^{1/2},$$

and (geometric) multiplicities are preserved. Now the Schur–Lalesco–Weyl theorem (*cf.*, *e. g.*, [24, 25]) implies that

$$\sum_j \kappa_j^p \leq \sum_j \mu_j^p,$$

where the μ_j denote the singular values of $\mathcal{K}$. As a consequence, we obtain the estimate

$$\left(\sum \lambda_j^{-p}\right)^{1/p} \leq \|\mathcal{K}\|_{\mathcal{B}_p}.$$

We next plug in $(-\Delta+1)^{1/2}(-\Delta+1)^{-1/2}$ and write

$$A := (-\Delta+1)^{1/2}(H-E)^{-1}(-\Delta+1)^{1/2},$$

which is a bounded operator, to conclude that

$$\begin{aligned}\|\mathcal{K}\|_{\mathcal{B}_p} &= \left\|W^{1/2}(-\Delta+1)^{-1/2}A(-\Delta+1)^{-1/2}|W|^{1/2}\right\|_{\mathcal{B}_p}\\ &\leq \left\|W^{1/2}(-\Delta+1)^{-1/2}\right\|_{\mathcal{B}_{2p}} \cdot \|A\| \cdot \left\|(-\Delta+1)^{-1/2}|W|^{1/2}\right\|_{\mathcal{B}_{2p}},\end{aligned}$$

by Hölder's inequality for trace ideals ([25]). By the estimates given in [23; Theorem XI.20], it is clear that the trace-ideal norms on the RHS are finite, since, by assumption, $p > \nu/2$ and $p > \nu/\alpha$. We have therefore shown that $\sum_j \lambda_j^{-p}$ is finite, and the result follows. ∎

REMARKS. (a)Our result falls short of proving the more "natural" estimate $N_+(\lambda; H-E, W) \leq c\lambda^{\nu/\min\{2,\alpha\}}$. However, in the case of W changing its sign we can't exclude that eigenvalue branches wiggle around the level E for a while which might increase the counting function considerably.

(b) The bound derived above is not only valid for positive coupling constants, but it gives as well a bound for *all* complex eigenvalues λ in the generalized eigenvalue problem $(H-E)u = \lambda W u$.

4. High barriers with compact support.

In this section, we consider $H + \lambda\chi_K$, for positive λ tending to ∞, where χ_K denotes the characteristic function of the compact set $K \subset \mathbf{R}^\nu$. It is shown in [15] that a potential barrier of the type $\lambda\chi_{B_R}$ sweeps out all the states of H having energy below E and "living" in the ball B_R, provided λ is large enough, up to an error term of order $R^{\nu-1}$. We are now trying to understand the mechanism working for compact K's which are very different from balls. Here, again, we ask for the large coupling constant limit

$$N_-(\infty; K) := \lim_{\lambda\to\infty} N_-(\lambda; H-E, \chi_K), \tag{4.1}$$

that is, the total number of eigenvalues of $H + \lambda\chi_K$ which are shifted over the level E as λ grows from 0 to $+\infty$. Note that the quantity $N_-(\infty; K)$ is always finite if K is bounded.

Here we'll see the following mechanism at work: as λ tends to infinity, the operators $H + \lambda\chi_K$ converge in strong resolvent sense to the operator $-\Delta + V$ in the exterior domain $\mathbf{R}^\nu - K$, with DBC on ∂K. This leads to a decoupling via DBC on ∂K, and, as a consequence, the mere *volume* of the set K doesn't tell much about $N_-(\infty; K)$.

In the sequel, we shall always assume that K is a compact subset of $\mathbf{R}^\nu$ and that $R > 0$ is so large that $K \subset B_R$. Our estimates will involve two auxiliary operators defined on the domain $\Omega(R) = B_R - K$: first, we let $H_{\Omega(R);D}$ denote $-\Delta + V$, acting in $L_2(\Omega(R))$, with DBC on $\partial\Omega(R)$; second, we let $H_{\Omega(R);D,N}$ denote $-\Delta + V$ on $\Omega(R)$, with DBC on ∂K and NBC on ∂B_R. As we shall see below, the quantities relevant for the eigenvalue counting are given by

$$n_{K;N} = \dim P_{(-\infty,E)}(H_{R;N}) - \dim P_{(-\infty,E)}\left(H_{\Omega(R);D,N}\right) \tag{4.2}$$

and

$$n_{K;D} = \dim P_{(-\infty,E)}(H_R) - \dim P_{(-\infty,E)}\left(H_{\Omega(R);D}\right). \tag{4.3}$$

The numbers $n_{K;N}$ and $n_{K;D}$ give lower (respectively, upper) bounds for the quantity $N_-(\infty; K)$, up to an error of order $R^{\nu-1}$. This reduces the problem to the study of an explicit situation on the finite region B_R; in view of the error terms, R should be chosen as small as possible.

4.1. THEOREM. *Suppose K is a compact subset of $\mathbf{R}^\nu$ and $R \geq 1$ is such that $K \subset B_R$. With the above notation, we then have*

$$N_-(\infty; K) \geq n_{K;N} - CR^{\nu-1},$$

where the constant C is independent of K and R.

PROOF. By Proposition 2.1, it is enough to produce a lower bound

$$\sup_{\lambda>0} N_-(\lambda; \tilde{H}_n - E, \chi_K) \geq n_{K;N} - CR^{\nu-1}, \tag{4.4}$$

for n large. Without restriction, we may assume that E is not an eigenvalue of $H_{\Omega(R);D,N}$. Introducing NBCs on ∂B_R, monotonicity of the associated quadratic forms implies that

$$\begin{aligned}
&\dim P_{(-\infty,E)}(\tilde{H}_n + \mu\chi_K) \\
&\qquad \leq \dim P_{(-\infty,E)}\left(\tilde{H}_{R,n;N,D}\right) + \dim P_{(-\infty,E)}\left(H_{R;N} + \mu\chi_K\right) \\
&\qquad \leq \dim P_{(-\infty,E)}\left(\tilde{H}_n\right) - \dim P_{(-\infty,E)}\left(H_{R;N}\right) + CR^{\nu-1} \\
&\qquad\qquad + \dim P_{(-\infty,E)}\left(H_{R;N} + \mu\chi_K\right),
\end{aligned}$$

by Proposition 2.5, whence

$$\begin{aligned}
&\dim P_{(-\infty,E)}\left(\tilde{H}_n\right) - \dim P_{(-\infty,E)}\left(\tilde{H}_n + \mu\chi_K\right) \\
&\quad \geq \dim P_{(-\infty,E)}\left(H_{R;N}\right) - \dim P_{(-\infty,E)}\left(H_{R;N} + \mu\chi_K\right) - CR^{\nu-1}.
\end{aligned} \tag{4.5}$$

By classical convergence results for eigenvalues (cf. Simon [26], Weidmann [27]), the eigenvalues of $H_{R;N} + \mu\chi_K$ increase monotonically to the corresponding eigenvalues of $H_{\Omega(R);D,N}$, as $\mu \to \infty$. Taking into account the definition of $n_{K;N}$, we have therefore shown that the LHS of (4.5) is eventually greater or equal to $n_{K;N} - CR^{\nu-1}$, for $\mu \to \infty$. By Kato–Rellich perturbation theory, this implies (4.4), and we are done. ∎

REMARK. The decoupling effect becomes most visible if K has lots of holes which are so small that the Dirichlet Laplacian on each hole has no eigenvalue below E ("swiss cheese"). In this case, we see that $n_{K;N} = n_{\tilde{K};N}$, where $\tilde{K}$

is obtained from K by taking the union of K with all bounded components of $\mathbf{R}^\nu - K$. For example, it is possible to have $\tilde{K} = B_R$ while the volume of K itself is arbitrarily small.

In $\mathbf{R}^\nu$, $\nu \geq 2$, the opposite situation is also possible. In fact, it is easy to construct examples where K has large volume while *no* eigenvalues cross E (think of K as a union of many small balls which are well separated; cf. [13, 1]).

The corresponding upper bound is somewhat easier.

4.2. THEOREM. *Suppose K is a compact subset of $\mathbf{R}^\nu$ and $R \geq 1$ is such that $K \subset B_R$. With the above notation, we then have*

$$N_-(\infty; K) \leq n_{K;D} + CR^{\nu-1},$$

where the constant C is independent of K and R.

PROOF. Proceeding as in the proof of the lower bound, we now use Dirichlet decoupling on ∂B_R and Proposition 2.6 to obtain

$$\begin{aligned}\dim P_{(-\infty,E)}\left(\tilde{H}_n\right) - \dim P_{(-\infty,E)}\left(\tilde{H}_n + \mu\chi_K\right)&\\ \leq &\dim P_{(-\infty,E)}(H_R) - \dim P_{(-\infty,E)}(H_R + \mu\chi_K) + CR^{\nu-1}\\ \leq &n_{K;D} + CR^{\nu-1}, \qquad \mu > 0, \quad n \geq n_0,\end{aligned}$$

by monotonicity and the definition of $n_{K;D}$. By Kato–Rellich perturbation theory, this implies that $N_-(\mu; \tilde{H}_n - E, \chi_K) \leq n_{K;D} + CR^{\nu-1}$, for n large, and the desired result follows via Proposition 2.1. ∎

REMARK. It is clear that one can use the standard techniques of Dirichlet–Neumann bracketing in order to derive (crude) estimates for $n_{K;D}$ in concrete situations, but sharp information on $n_{K;D}$ may be difficult to obtain (cf. also Kirsch [17]). An even more challenging problem consists in finding bounds for $n_{K;N} - n_{K;D}$.

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References.

[1] S. Alama, P. A. Deift and R. Hempel: Eigenvalue branches of the Schrödinger operator $H - \lambda W$ in a spectral gap of H. Commun. Math. Phys. **121** (1989), 291-321.

[2] S. Alama and Y.Y. Li: Existence of solutions for semilinear elliptic equations with indefinite linear part. Preprint, 1990.

[3] N. W. Ashcroft and N. D. Mermin: *Solid State Physics.* Holt, Rinehart and Winston, New York 1976.

[4] M. Sh. Birman: Discrete spectrum in the gaps of the continuous one in the large coupling constant limit. In: *Operator Theory: Advance and Applications*, Vol. 46. Birkhäuser, Basel 1990.

[5] Ph. Briet, J. M. Combes and P. Duclos: Spectral stability under tunneling. Commun. Math. Phys. **126** (1989), 133-156.

[6] R. Courant and D. Hilbert: *Methods of Mathematical Physics.* Vol. I. Interscience, New York 1953.

[7] P. A. Deift and R. Hempel: On the existence of eigenvalues of the Schrödinger operator $H - \lambda W$ in a gap of $\sigma(H)$. Commun. Math. Phys. **103** (1986), 461-490.

[8] P. A. Deift and B. Simon: On the decoupling of finite singularities from the question of asymptotic completeness in two-body quantum systems. J. Funct. Anal. **23** (1976), 218-238.

[9] M. S. P. Eastham:*The spectral theory of periodic differential equations.* Scottish Academic Press, Edinburgh 1973.

[10] F. Gesztesy, D. Gurarie, H. Holden, M. Klaus, L. Sadun, B. Simon and P. Vogl: Trapping and cascading of eigenvalues in the large coupling limit. Commun. Math. Phys. **116** (1988), 597-634.

[11] F. Gesztesy and B. Simon: On a theorem of Deift and Hempel. Commun. Math. Phys. **116** (1988), 503-505.

[12] I. C. Gohberg and M. G. Krein: *Introduction to the Theory of Linear Nonselfadjoint Operators.* Amer. Math. Soc., Providence (R. I.) 1969.

[13] R. Hempel: *A left-indefinite generalized eigenvalue problem for Schrödinger operators.* Habilitationsschrift, Univ. München 1987.

[14] R. Hempel: On the asymptotic distribution of the eigenvalue branches of the Schrödinger operator $H + \lambda W$ in a spectral gap of H. J. Reine Angew. Math. **399** (1989), 38-59.

[15] R. Hempel: Eigenvalues in gaps and decoupling by Neumann boundary conditions. J. Math. Anal. Appl., to appear.

[16] T. Kato: *Perturbation theory for linear operators.* Springer, New York 1966.

[17] W. Kirsch: Small perturbations and the eigenvalues of the Laplacian on large bounded domains. Proc. Amer. Math. Soc. **101** (1987), 509-512.

[18] M. Klaus: Some applications of the Birman-Schwinger principle. Helv. Phys. Acta **55** (1982), 49-68.

[19] F. Klopp: Impuretés dans une structure périodique. *Journées "Equations aux dérivés partielles"* (Saint Jean des Monts, 1990), Exp. No. XX, Ecole Polytech., Palaiseau, 1990

[20] A. Outassourt: Comportement semi-classique pour l'opérateur de Schrödinger à potentiel périodique. J. Funct. Anal. **72** (1987), 65-93.

[21] S.T. Pantelides: The electronic structure of impurities and other point defects in semiconductors. Rev. Mod. Phys. **50** (1978), 797-858.

[22] M. Reed and B. Simon: *Methods of modern mathematical physics.* Vol. I. *Functional Analysis. Revised and enlarged ed.* Academic Press, New York 1981.

[23] M. Reed and B. Simon: *Methods of modern mathematical physics.* Vol. III. *Scattering theory.* Academic Press, New York 1979.

[24] M. Reed and B. Simon: *Methods of modern mathematical physics.* Vol. IV.*Analysis of operators.* Academic Press, New York 1978.

[25] B. Simon:*Trace Ideals and their applications.* Cambridge Univ. Press, London 1979.

[26] B. Simon: A canonical decomposition for quadratic forms with application to monotone convergence theorems. J. Funct. Anal. **28** (1978), 377-385.

[27] J. Weidmann: Stetige Abhängigkeit der Eigenwerte und Eigenfunktionen elliptischer Differentialoperatoren vom Gebiet. Math. Scand. **54**(1984), 51-69.

[28] A. V. Sobolev: The Weyl asymptotics for discrete spectrum of the perturbed Hill operator. Preprint, 1991

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Singular perturbations of Dirichlet and Neumann domains and resonances for obstacle scattering

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SINGULAR PERTURBATIONS OF DIRICHLET AND NEUMANN DOMAINS AND RESONANCES FOR OBSTACLE SCATTERING

Peter D. Hislop [1]

1. Introduction

Some of the work reported in this article is joint with R.M. Brown, University of Kentucky, and A. Martinez, Université de Paris XIII. We want to describe some recent results concerning the existence and estimation of the poles of the S-matrix for the scattering of waves by a single, compact obstacle. The details of the calculations appear in [6], [12], [11]. We are interested in the scattering poles for a class of obstacles known as Helmholtz resonators. These obstacles are characterized by a large cavity $\mathcal{C}$ which is coupled to the (unbounded) exterior $\mathcal{E}$ by means of a tube $T(\varepsilon)$ of diameter ε. The waves propagate in $\Omega(\varepsilon) \equiv Int(\overline{\mathcal{C} \cup T(\varepsilon) \cup \mathcal{E}})$ and we consider either Dirichlet or Neumann boundary conditions (DBC or NBC) on the boundary of $\Omega(\varepsilon), \partial\Omega(\varepsilon)$. We consider two classes of problems : (1) local in energy : for a fixed compact subset $K \subset \mathbf{C}$, intersecting the real axis $\mathbf{R}$, describe and estimate the position of all scattering poles in K for all ε sufficiently small; (2) global in energy : for a fixed ε (say $\varepsilon = 1$), consider the high energy behavior of the scattering poles and show that there exists a sequence of poles converging to the real axis.

The problem of a local characterization of scattering poles for a Helmholtz resonator has been considered by Beale [4] and Arsen'ev [3]. For the case of DBC, the poles arise from either eigenvalues of the cavity Laplacian $-\Delta_{\mathcal{C}}$ with DBC or resonances of the exterior Laplacian $-\Delta_{\mathcal{E}}$ with DBC. In particular for K as above, they prove that there exists $\varepsilon_K > 0$ such that for all $\varepsilon < \varepsilon_K$, there exists a bijection between the scattering poles in K and the set consisting of the eigenvalues of $-\Delta_{\mathcal{C}}$ in K and the resonances of $-\Delta_{\mathcal{E}}$ in K (including multiplicities).

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When there are NBC and $T(\varepsilon)$ is a straight tube $D_\varepsilon \times [0,1], D_\varepsilon = \varepsilon D_1$ and $D_1 = \{x' \epsilon \mathbf{R}^{n-1} \mid |x'| \leq 1\}$, there is an addition set of poles coming from the longitudinal modes of the tube. We reprove these results and give precise upper bounds on the displacement of the poles from the cavity eigenvalues or exterior resonances as a function of ε. For the case of DBC these are exponentially small in ε. For the NBC case, the upper bound is $\mathcal{O}(\varepsilon^\beta)$ where $\beta = 1/2$ for dimension $n \geq 4$ and $0 < \beta < 1/2$ for $n = 3$.

In order to derive these results, we also study the effect of adding a small tube $T(\varepsilon)$ to the cavity $\mathcal{C}$ on the eigenvalues of $-\Delta_{\mathcal{C}}$. We consider both DBC and NBC. In the DBC case, we find that the shift of the eigenvalues is bounded above by $\mathcal{O}(\varepsilon^\beta)$ where $\beta = 1/2$ for $n \geq 3$ and $0 < \beta < 1/2$ for $n = 2$.

In the NBC case, we must restrict ourselves to a straight tube. We find a similar estimate for the shift of the eigenvalues. We mention that singular perturbations of NBC have been recently discussed by several authors, for example [2], [10], [16].

The second type of problem is related to a conjecture of Lax and Phillips [18] concerning the behavior of scattering poles in the case that the obstacle has trapped rays. They conjectured that if an obstacle, like a Helmholtz resonator, has trapped rays, then there is a sequence of scattering poles converging to the real axis as the energy diverges to infinity. Although this conjecture is false, as shown by Ikawa [13] for the case of two bounded, convex obstacles with a single trapped hyperbolic ray, we show that it holds for a class of symmetric Helmholtz resonators (see section 4). In the case studied by Ikawa and, later, by Gérard [9], there is an infinite number of scattering poles but they are bounded a fixed distance from the real axis. This may be a manifestation of the instability of the trapped ray in this example. Indeed, Ikawa [14] later showed that if the obstacles are sufficiently flat in the neighborhood of the trapped ray, there is a sequence of poles converging to the real axis. A similar situation of stability occurs in an example studied by Ralston [20]. He examined the poles for scattering in spherically symmetric inhomogeneous media for which there is an infinite family of stable, trapped rays. Again in this case, there is a sequence of poles converging exponentially fast to the real axis. This model can also be treated by the methods of section 4.

The outline of this paper is as follows. In sections 2 and 3 we discuss the local in energy problem for the Helmholtz resonator. Section 2 is devoted to the DBC case and section 3 to the NBC case. In section 4 we turn to the global in energy problem and sketch the proof of the Lax-Phillips conjecture on the existence of a sequence of scattering poles converging to the real axis for a family of symmetric Helmholtz resonators.

Finally, we mention that a scattering pole is also a pole of the meromorphic continuation of matrix elements of the resolvent of $-\Delta_{\Omega(\varepsilon)}$ for vectors in a certain dense set. Hence they are resonance of the operator $-\Delta_{\Omega(\varepsilon)}$ on $L^2(\Omega(\varepsilon))$. We will freely use the results of the theory of quantum resonances and spectral deformation below. In particular, we will assume the application of spectral deformation techniques as discussed in [12].

2. Perturbation of Dirichlet Domains and Resonances

The first situation for which we will consider the local resonance structure is the Helmholtz resonator with DBC. This material has already been published so we will be brief and simply review the results. The notation and general ideas, however, will be used in the other sections. To be more specific about the geometry, let $\widetilde{\Omega} \subset \mathbf{R}^n$ be an open set with C^2-boundary admitting a decomposition into two disjoint components $\mathcal{C}$, the cavity, and $\mathcal{E}$, the exterior, such that $\mathcal{C} \subset \mathbf{R}^n \backslash \mathcal{E}$ and $\mathcal{C}$ is bounded. Let $x_o \epsilon \partial\mathcal{C}$ and $x_1 \epsilon \partial\mathcal{E}$. We join these two points by a tube $T(\varepsilon)$ which is an open subset of $\mathbf{R}^n \backslash \widetilde{\Omega}$ diffeomorphic to the standard tube $D_\varepsilon \times [0,1]$ where $D_\varepsilon = \varepsilon D_1$ and $D_1 \equiv \{x' \epsilon \mathbf{R}^{n-1} \mid |x'| \leq 1\}$. As in the introduction, we set $\Omega(\varepsilon) \equiv Int(\overline{\mathcal{C} \cup T(\varepsilon) \cup \mathcal{E}})$ and consider the Laplacian $H_\varepsilon = -\Delta$ on $\Omega(\varepsilon)$ with DBC on $\partial\Omega(\varepsilon)$. Our main result is to characterize the resonances of H_ε in a compact complex set K intersecting $\mathbf{R}$ for all ε sufficiently small.

To this end, we need a preliminary estimate of some interest in itself. Consider the cavity $\mathcal{C}$ and the cavity with the tube $T(\varepsilon)$ attached : $\mathcal{C}(\varepsilon) \equiv Int(\overline{\mathcal{C} \cup T(\varepsilon)})$, both with DBC. We want to know by how much the eigenvalues of the Dirichlet Laplacian $-\Delta_{\mathcal{C}}$ shift when the tube is adjoined to the cavity. By the Poincaré inequality for $-\Delta_{T(\varepsilon)}$, one expects that the effect is small.

PROPOSITION **2.1.** *Let $\lambda_0 \epsilon\ \sigma(-\Delta_{\mathcal{C}})$ with multiplicity N_0. Then there exists $\varepsilon_0 > 0, c > 0$ such that for all $\varepsilon < \varepsilon_0, -\Delta_{\mathcal{C}(\varepsilon)}$ has N_0 eigenvalues (counting multiplicity) $\lambda_1(\varepsilon), \ldots, \lambda_{N_0}(\varepsilon)$, satisfying for all $j = 1, \ldots, N_0$:*

$$|\lambda_0 - \lambda_j(\varepsilon)| \leq c\varepsilon^\beta$$

where $\beta = 1/2$ for $n \geq 3$ and $0 < \beta < 1/2$ for $n = 2$.

The proof of this theorem begins with Green's formula expressing the difference of the two Laplacians, $-\Delta_{\mathcal{C}} \oplus -\Delta_{T(\varepsilon)}$ and $-\Delta_{\mathcal{C}(\varepsilon)}$, in terms of normal derivatives and surface integrals. These integrals are then estimated using Sobolev embedding and trace theorems.

The basis for the existence of resonances in K is the fact that a narrow tube with Dirichlet boundary conditions cannot support states with energy in K if ε is sufficiently small. Consequently, the coupling between the cavity and the exterior is very weak. This weak coupling, however, is sufficient to change the bound states of $-\Delta_{\mathcal{C}}$ to resonances of H_ε and to shift the resonances of $-\Delta_{\mathcal{E}}$ a small amount to become resonances of H_ε. We note that $\sigma(H_\varepsilon) = [0,\infty)$ and is absolutely continuous whereas the spectrum of the operator obtained when $\varepsilon = 0$, a direct sum, has eigenvalues embedded in the continuous spectrum.

As described in the introduction, the poles of the S-matrix are characterized also as the complex eigenvalues of the spectrally deformed Hamiltonian. We denote by $H_\varepsilon(\mu), H_\varepsilon^{ext}(\mu)$ and $H_{ext,\varepsilon}^{D}(\mu)$ the spectrally deformed operators obtained from $H_\varepsilon, -\Delta_{\mathcal{E}(\varepsilon)}$ and $-\Delta_{T(\varepsilon)} \oplus -\Delta_{\mathcal{E}}$, respectively, where $\mathcal{E}(\varepsilon) \equiv Int(\overline{\mathcal{E} \cup T(\varepsilon)})$. There is a result for the shift of the resonances of $-\Delta_{\mathcal{E}}$ by the addition of $T(\varepsilon)$, which is the analog of Proposition 2.1.

PROPOSITION **2.2.** *Let λ_0 be a resonance of $-\Delta_{\mathcal{E}}$ for some $\mu \epsilon\ i]0,1[$ of (algebraic) multiplicity N_0. Then there exists $\varepsilon_0 > 0, c > 0$ such that for all $\varepsilon < \varepsilon_0, H_\varepsilon^{ext}(\mu)$ has N_0 eigenvalues $\lambda_1(\varepsilon),\ldots,\lambda_{N_0}(\varepsilon)$ satisfying for all $j = 1,\ldots,N_0$:*

$$|\lambda_0 - \lambda_j(\varepsilon)| \leq c\varepsilon^\beta$$

where $\beta = 1/2$ for $n \geq 3$ and $0 < \beta < 1/2$ for $n = 2$.

To prove that H_ε has resonances in some fixed $K \subset \mathbf{C}$, for all small ε, and that these resonances are precisely, those coming from the eigenvalues of $-\Delta_{\mathcal{C}}$ in K and the resonances of $-\Delta_{\mathcal{E}}$ in K, we show that for z in a neighborhood of any of these latter points, the difference of the resolvents of $H_{\varepsilon,\mu}$ and of $-\Delta_{\mathcal{C}(\varepsilon)} \oplus H_\varepsilon^{ext}(\mu)$, $\mu \epsilon\ i]0,1[$ vanishes as $\varepsilon \to 0$. Note that $\mathcal{C}(\varepsilon) \cap \mathcal{E}(\varepsilon) = T(\varepsilon)$ and it is in this region where states of energy in K are, in fact, exponentially small (see below). To quantify this idea, we use geometric perturbation theory. Let (J_1, J_2) be a partition of unity covering $\Omega(\varepsilon)$, independent of ε, such that $\text{supp}|\nabla J_i|$ is well inside the tube. Indeed, if $d(x,\Omega) \equiv$ Euclidean distance from x to Ω, then we take

$$J_1 | \{x | d(x,\mathcal{E}) \geq 2\delta\} = 1$$
$$J_2 | \{x | d(x,\mathcal{E}) \geq \delta\} = 1$$

so $\text{supp}|\nabla J_i| \subset \{x | \delta \leq d(x,\mathcal{E}) \leq 2\delta\}$. Set $\mathcal{H}_0 \equiv L^2(\mathcal{C}(\varepsilon)) \oplus L^2(\mathcal{E}(\varepsilon))$ and $\mathcal{H} \equiv L^2(\Omega(\varepsilon))$ and define $J : \mathcal{H} \to \mathcal{H}_0$ by

$$Ju = J_1 u \oplus J_2 u$$

so that $J^\star J = 1_{\mathcal{H}}$. Let $R(z) \equiv (H_{\varepsilon,\mu} - z)^{-1}$ and $R_0(z) = (-\Delta_{\mathcal{C}(\varepsilon)} \oplus H_\varepsilon^{ext}(\mu) - z)^{-1}$. Then for z in the intersection of the resolvent sets, we have the geometric resolvent equation on $\mathcal{H}$:

$$R(z) = J^\star R_0(z) J + R(z) M R_0(z) J$$

where $M : \mathcal{H}_0 \to \mathcal{H}$ is given by

$$M(u_1 \oplus u_2) = [-\Delta, J_1]u_1 + [-\Delta, J_2]u_2,$$

for $u_1 \epsilon H^1(\mathcal{C}(\varepsilon)), u_2 \epsilon H^1(\mathcal{E}(\varepsilon))$. We want to show that $||JMR_0(z)||$ vanishes as $\varepsilon \to 0$.

LEMMA **2.3.** *Let $\lambda_0 \epsilon \sigma(-\Delta_C)$ and let Γ_ε be a simple closed contour about λ_0 of radius $2c\varepsilon^\beta$, where β is defined in Prop.2.1. Let $\chi \epsilon C_0^\infty$ (supp$|\nabla J_i|$). Then for each $\delta > 0 \exists c_\delta > 0$ such that uniformly on Γ_ε,*

$$||\chi(-\Delta_{C(\varepsilon)} - z)^{-1}|| \leq c_\delta \varepsilon^{2-\delta}$$
$$||\nabla\chi(-\Delta_{C(\varepsilon)} - z)^{-1}|| \leq c_\delta \varepsilon^{1-\delta}$$

Similar estimates hold for $H_\varepsilon^{ext}(\mu)$.

Idea of the Proof. The proof is based on the inequality

$$| < \chi u, (-\Delta_{C(\varepsilon)} - z)\chi u > | \geq \ ||\nabla(\chi u)||^2_{L^2(T(\varepsilon))} - |z| \ ||\chi u||^2_{L^2(T(\varepsilon))} \ . \quad (2.1)$$

Now, the Poincaré inequality states that for any $\phi \epsilon H_0^1(T(\varepsilon))$,

$$\int_{T(\varepsilon)} |\phi|^2 \leq c\varepsilon^2 \int_{T(\varepsilon)} |\nabla\phi|^2.$$

Applying this to the right side of (2.1), we obtain

$$| < \chi u, (-\Delta_{C(\varepsilon)} - z)\chi u > | \geq (c\varepsilon^{-2} - |z|) \ ||\chi u||^2_{L^2(T(\varepsilon))} \ .$$

Finally, we take $u = (-\Delta_{C(\varepsilon)} - z)^{-1}v$ and compute the left side of (2.1). $\diamondsuit$

COROLLARY **2.4.** *Let Γ_ε be as in Lemma 2.3. Define $K(z) : \mathcal{H}_0 \to \mathcal{H}_0$ as $JMR_0(z)$. Then for any $\delta > 0 \exists c_\delta > 0, \varepsilon_0 > 0$ such that for $\varepsilon < \varepsilon_0$, and uniformly on Γ_ε*

$$||K(z)|| \leq c_\delta \varepsilon^{2-\delta} \ .$$

We use this result to solve the geometric resolvent equation for $z \epsilon \Gamma_\varepsilon$ and ε sufficiently small. This gives

$$R(z) - J^\star R_0(z)J = J^\star R_0(z)(1 - K(z))^{-1}K(z)J \ . \quad (2.2)$$

We can now state our main theorem on the existence of resonances.

THEOREM **2.5.** (1) *Let $\lambda_0 \epsilon \sigma(-\Delta_C)$ with multiplicity N_0 and let $\lambda_j(\varepsilon)\epsilon\sigma$ $(-\Delta_{C(\varepsilon)}), j = 1, \ldots, N_0$, be such that $|\lambda_0 - \lambda_j(\varepsilon)| \leq c\varepsilon^\beta, \beta \leq 1/2$ according to n.*

Then $\exists c > 0$ *and* $\varepsilon_0 > 0$ *such that for all* $\varepsilon < \varepsilon_0, H_\varepsilon(\mu)$ *has* N_0 *eigenvalues (counting multiplicity)* $\rho_1(\varepsilon), \ldots, \rho_{N_0}(\varepsilon)$ *and* $\forall_j, k = 1, \ldots, N_0$*:*

$$|\lambda_j(\varepsilon) - \rho_k(\varepsilon)| \leq c\varepsilon^\beta \ .$$

(2) *Fix* $\mu\epsilon]0,1[$ *and let* λ_0 *be a resonance of* $-\Delta_{\mathcal{E}}$ *of multiplicity* N_0. *Let* $\lambda_j(\varepsilon)\epsilon\sigma_d(H_\varepsilon^{ext}(\mu))$ *be the eigenvalues satisfying* $|\lambda_0 - \lambda_j(\varepsilon)| \leq c\varepsilon^\beta$. *Then* $\exists c > 0$ *and* $\varepsilon_0 > 0$ *such that* $\forall\varepsilon < \varepsilon_0, H_\varepsilon(\mu)$ *has* N_0 *eigenvalues* $\rho_1(\varepsilon), \ldots, \rho_{N_0}(\varepsilon)$ *such that* $\forall_j, k = 1, \ldots, N_0$,

$$|\lambda_j(\varepsilon) - \rho_k(\varepsilon)| \leq c\varepsilon^\beta \ .$$

As a final part of this description of the DBC case, we want to make precise the location of the resonances of H_ε. That is, we show that the shifts between $\lambda_j(\varepsilon)$ and $\rho_k(\varepsilon)$, as described in Theorem 2.5, are exponentially small in ε. The key to this is the fact that eigenfunctions of $-\Delta_{C(\varepsilon)}$ and of $H_\varepsilon^{ext}(\mu)$ decay exponentially in $T(\varepsilon)$.

PROPOSITION **2.6.** *Let* $\lambda(\varepsilon)\epsilon\sigma(-\Delta_{C(\varepsilon)})$ *be such that* $\lambda(\varepsilon) \to \lambda_0\epsilon\sigma(-\Delta_C)$ *as* $\varepsilon \to 0$ *and let* u_ε *be the corresponding eigenfunction with* $||u_\varepsilon|| = 1$. *Then for all* $\alpha\epsilon\mathbf{N}^n$, *for all* $\delta > 0, \exists\widetilde{c}_{\alpha,\delta} > 0$ *such that for all* ε *small enough:*

$$||e^{(1-\delta)\widetilde{d}_\varepsilon(\cdot,x_0)/\varepsilon}\partial^\alpha u_\varepsilon||_{L^2(T(\varepsilon))} \leq \widetilde{c}_{\alpha,\delta}\varepsilon^{-c_{\alpha,\delta}}$$

and $c_{0,\delta} = 0, c_{1,\delta} = 1$, *and* $\widetilde{d}_\varepsilon(x,y)$ *is the minimum distance from* x *to* y *along paths lying in* $\Omega(\varepsilon)$. *A similar estimate holds for eigenfunctions of* $H_\varepsilon^{ext}(\mu)$ *corresponding to eigenvalues* $\lambda(\varepsilon) \to \lambda_0$, *a resonance of* $-\Delta_{\mathcal{E}}$.

THEOREM **2.7.** *Let* $\lambda_j(\varepsilon)$ *and* $\rho_k(\varepsilon)$ *be as in Theorem 2.5. For each* $j, j = 1, \ldots, N_0, \exists$ *a permutation* k *of* $\{1, \ldots, N_0\}$ *such that*

$$|\rho_{k(j)}(\varepsilon) - \lambda_j(\varepsilon)| \leq c\exp[-2(1-\delta)S(\varepsilon,\delta)/\varepsilon]$$

where $S(\varepsilon,\delta) \equiv \max\{\widetilde{d}_\varepsilon(x,y)|\ x, y\epsilon\overline{T(\varepsilon)}, d(x, \mathcal{E}\cup\mathcal{C}) \geq \delta, d(y, \mathcal{E}\cup\mathcal{C}) \geq \delta\}$ *and* $\widetilde{d}_\varepsilon$ *is defined in Prop.2.6.*

The proof of this theorem follows from the construction of an approximate basis for the invariant subspace of H_ε corresponding to $\{\rho_j(\varepsilon)\}$ using the eigenfunctions of $-\Delta_{C(\varepsilon)}$ or $H_\varepsilon^{ext}(\mu)$. In this basis, H_ε is diagonal up to exponentially small terms.

3. Perturbation of Neumann Domains and Resonances

In this section, we first consider the effect of adding a small tube $T(\varepsilon)$ to the cavity $\mathcal{C}$ when NBC are imposed on the boundary. We then consider the determination and estimation of resonances for Helmholtz resonators in the NBC case. The geometry is as in the DBC case with one additional requirement. The tube $T(\varepsilon)$ must be straight, i.e. $T(\varepsilon) \subset D_\varepsilon \times \mathbf{R}$. We fix coordinates $(x', x_n) \in \mathbf{R}^{n-1} \times \mathbf{R}$ so that $(0,0) \in \partial\mathcal{C} \cap T(\varepsilon)$ and $(0,1) \in \partial\mathcal{E} \cap T(\varepsilon)$. As above, we let $\mathcal{C}(\varepsilon) \equiv \mathcal{C} \cup T(\varepsilon)$ and $\mathcal{E}(\varepsilon) \equiv \mathcal{E} \cup T(\varepsilon)$. We must make an assumption on the smoothness of $\partial\mathcal{C}(\varepsilon)$ and $\partial\mathcal{E}(\varepsilon)$.

Boundary regularity assumption: $\partial\mathcal{C}(\varepsilon)$ and $\partial\mathcal{E}(\varepsilon)$ are in $C^{0,1}(\mathbf{R}^{n-1})$, i.e. they are both locally the graph of a Lipschitz continuous function.

We note that this implies that the tube $T(\varepsilon)$ is bounded by Lipschitz surfaces. Moreover, both $-\Delta_{\mathcal{C}}$ and $-\Delta_{\mathcal{C}(\varepsilon)}$ have compact resolvents. We recall [15] that if $\mathcal{C}$ is a region such that $\partial\mathcal{C} \epsilon C^{0,1}(\mathbf{R}^{n-1})$, then the Neumann resolvent $R_N(z)$ followed by restriction to the boundary maps $L^2(\mathcal{C})$ to $H^1(\partial\mathcal{C})$.

We denote by D_ε^0 and D_ε^1 subsets of $T(\varepsilon)$ given by $\partial\mathcal{C} \cap T(\varepsilon)$ and $\partial\mathcal{E} \cap T(\varepsilon)$, respectively. We will consider the eigenvalues of $\mathcal{C}(\varepsilon)$ as $\varepsilon \to 0$ in two cases : (1) NBC everywhere on $\partial\mathcal{C}(\varepsilon)$, and (2) NBC on $\partial\mathcal{C}(\varepsilon)\backslash D_\varepsilon^1$ and DBC on D_ε^1. Case 2 will be important for the study of resonances given in the next section. As in the DBC case, the eigenvalues of $\mathcal{C}(\varepsilon)$ should be well (locally) approximated by eigenvalues of $\mathcal{C}$ with NBC and of $T(\varepsilon)$, where $T(\varepsilon)$ has NBC on $T(\varepsilon)\backslash(D_\varepsilon^0 \cup D_\varepsilon^1)$, DBC on D_ε^0, and either NBC or DBC on D_ε^1, for case 1 or 2, respectively. We introduce the following operators indexed by $i = 1, 2$ depending on NBC or DBC on D_ε^1.

Cavity $-\Delta_{\mathcal{C}} \geq 0$ Cavity Laplacian with NBC on $\partial\mathcal{C}$
$$R_{\mathcal{C}}(z) \equiv (-\Delta_{\mathcal{C}} - z)^{-1}$$

Tube $-\Delta_T^i \geq 0, i = 1, 2$. Tube Laplacian
$$R_T^i(z) \equiv (-\Delta_T - z)^{-1}$$

Unperturbed $\Delta_0^i \equiv \Delta_{\mathcal{C}} \oplus \Delta_T^i,\ i = 1, 2$
$$R_0^i(z) \equiv (-\Delta_0^i - z)^{-1} = (-\Delta_{\mathcal{C}} - z)^{-1} \oplus (-\Delta_T^i - z)^{-1}$$

Coupled $-\Delta_N^i \geq 0$ Laplacian for $\mathcal{C}(\varepsilon)$ in case 1 (NBC on D_ε^1) or case 2 (DBC on D_ε^1)

$$R_N^i(z) \equiv (-\Delta_N^i - z)^{-1}.$$

We will omit the index i when the results hold in both cases. We note that $\sigma(-\Delta_0^i) = \sigma(-\Delta_C) \cup \sigma(-\Delta_T^i)$ and that $\sigma(-\Delta_C)$ is independent of ε and $\lambda_1 = 0$. Unlike the Dirichlet case, we can write $\sigma(-\Delta_T^i) = \sigma_L^i \cup \sigma_T^i$, where σ_L^i, the longitudinal modes, consists of those eigenvalues which differ by $\mathcal{O}(\varepsilon^{1/2})$ from the eigenvalues of the boundary value problem on $[0,1]$:

$$\begin{cases} -u'' = \lambda u \text{ on } [0,1] \\ u(0) = 0 \\ u(1) = 0 \text{ case 1 or } u'(1) = 0 \text{ case 2 .} \end{cases}$$

In case 1, $\sigma_L^1 = \{(n\pi)^2 | n\epsilon \mathbf{Z}^+\}$ and in case 2, $\sigma_L^2 = \{((2n+1)\pi/2)^2 | n\epsilon\mathbf{Z}\}$ (up to $\mathcal{O}(\varepsilon^{1/2})$), which are both independent of ε and each eigenvalue has multiplicity one. Hence we expect these eigenvalues to contribute to $\sigma(-\Delta_N^i)$. The other set of tube eigenvalues, σ_T^i, consists of transverse mode eigenvalues and satisfy a Poincaré-type inequality reminiscent of the Dirichlet case: $\lambda \geq c_0\varepsilon^{-2}$. Accordingly, these do not contribute to the local spectrum of $-\Delta_N^i$ in any compact subset of $\mathbf{R}^+$ for ε sufficiently small.

The case $n = 2$ requires some special treatment so we omit it here (see [6]).

THEOREM **3.1.** *Let $n \geq 3$ and $\mathcal{C}(\varepsilon) = \mathcal{C} \cup T(\varepsilon)$ as described above.*

1) *Let $\lambda_0 \epsilon \sigma(-\Delta_C)$, $\lambda_0 \notin \sigma_L^i$, and let N_0 be the multiplicity of λ_0. Then $-\Delta_N^i$ has N_0 eigenvalues (counting multiplicity) $\lambda_k(\varepsilon) \to \lambda_0$ as $\varepsilon \to 0$ such that for all ε sufficiently small $\exists c_0 > 0$ s.t.*

$$|\lambda_k(\varepsilon) - \lambda_0| \leq c_0 \varepsilon^\alpha$$

where $\alpha = 1/2$ for $n \geq 4$ and $0 < \alpha < 1/2$ for $n = 3$.

2) *$\lambda_0 \epsilon \sigma_L^i, \lambda_0 \notin \sigma(-\Delta_C)$. Then $-\Delta_N^i$ has exactly one eigenvalue $\lambda_0(\varepsilon) \to \lambda_0$ as $\varepsilon \to 0$ and the bound in (1) is satisfied. If it happens that $\lambda_0 \epsilon \sigma_L^i \cap \sigma(-\Delta_C)$ then $-\Delta_N^i$ has $N_0 + 1$ eigenvalues $\lambda_k(\varepsilon) \to \lambda_0$ as $\varepsilon \to 0$ (where N_0 is the multiplicity of λ_0 in $\sigma(-\Delta_C)$) and satisfying the bound in (1).*

We remark that the convergence of Neumann eigenvalues under singular perturbations of the domain has been considered by several researchers. For $n = 2$, Hempel, Seco and Simon [10] show norm resolvent convergence of $R^i(z)$ to $R_0^i(z)$ (and for unperturbed resolvents corresponding to more than one tube) as $\varepsilon \to 0$ but they do not give any estimate on the rate of convergence. Jimbo [16] considers a similar problem in $\mathbf{R}^n$ and gives pointwise asymptotics on the eigenfunctions as $\varepsilon \to 0$. Arrieta, Hale and Han [2] consider more singular perturbations of Neumann domains for which the attached region is shrinking at different rates in different directions.

Theorem 3.1 follows from the main technical lemma which estimates the convergence of resolvents.

LEMMA **3.2.** *Under the hypotheses of Theorem 3.1, for any* $z \epsilon \rho(-\Delta_N^i) \cup \rho(-\Delta_0^i)$, *we have*

$$||R^i(z) - R_0^i(z)|| \leq c_z \varepsilon^\alpha (1 + ||R^i(z)||)(1 + ||R_0^i(z)||)$$

where $c_z \equiv c_0(1+|z|)^{3/2}, c_0$ *dependents on the smoothness of* $\partial\mathcal{C}$, *and* $\alpha = 1/2,\ n \geq 4$, *and* $\alpha < 1/2,\ n = 3$.

We sketch the proof of this lemma. As in the Dirichlet case, it is based on Green's formula.

Proof of Lemma 3.2.

The basic formula is the following. Let $w = w_{\mathcal{C}} \oplus w_T \epsilon D(-\Delta_0)$ and let $u \epsilon D(-\Delta_N)$ (we drop the index i). Then

$$D \equiv \int_{\mathcal{C}(\varepsilon)} w\Delta_N u - u\Delta_0 w = \sum_{X=\mathcal{C},T} \int_{\partial X} \left(u\frac{\partial w_X}{\partial \nu} - w_X \frac{\partial u}{\partial \nu} \right)$$

where $\partial/\partial\nu$ denotes the outward normal derivative from $X = T$ or $\mathcal{C}$. Applying the various BC, we obtain :

$$D = -\int_{D_\varepsilon^0} w_{\mathcal{C}} \frac{\partial u}{\partial \nu} + \int_{D_\varepsilon^0} u \frac{\partial w_T}{\partial \nu} \tag{3.1}$$

in both cases. If we recall that $w = R_0(z)g, g\epsilon L^2(\mathcal{C}) \oplus L^2(T(\varepsilon))$ and $u = R(z)f, f\epsilon L^2(\mathcal{C}(\varepsilon))$, then estimates on the integrals in D give directly an upper bound on $R(z) - R_0(z)$. To estimate the integral involving w_T we will use the following two facts.

1) $||u||_{L^2(D_\varepsilon^0)} \leq c_0 \varepsilon^\alpha (1 + ||R(z)||)||f||_{L^2(\mathcal{C}(\varepsilon))}$,
   where $u = R(z)f$ and α is as in the lemma.

2) $||\frac{\partial w_T}{\partial \nu}||_{L^2(D_\varepsilon^0)} \leq c_z(1 + ||R_T(z)||)||g||_{L^2(T(\varepsilon))}$,
   where $w_T = R_T(z)g$.

It is then clear that we obtain an estimate of the type on the right side of (3.1) for the w_T term in D. The estimate on the $w_{\mathcal{C}}$ term is more involved. Here we use $(H^{1/2}(\partial\mathcal{C}),\ H^{-1/2}(\partial\mathcal{C}))$ duality. Let η be a smooth cut-off function such that $|\nabla\eta| \leq c_0\varepsilon^{-1}$ and $\chi_{D_\varepsilon^0} \leq \eta \leq \chi_{D_{2\varepsilon}^0}$, where $\chi_{D_\varepsilon^0}$ is the characteristic function on D_ε^0. We show that

3) $\|\eta w_{\mathcal{C}}\|_{H^{1/2}(\partial\mathcal{C})} \leq c_z \varepsilon^\alpha (1 + \|R_{\mathcal{C}}(z)\|)\|g\|_{L^2(\mathcal{C})}$,
where $w_{\mathcal{C}} = R_{\mathcal{C}}(z)g,\ g\epsilon L^2(\mathcal{C})$.

4) $\|\frac{\partial u}{\partial \nu}\|_{H^{-1/2}(\partial\mathcal{C})} \leq c(1 + \|R(z)\|)\|f\|_{L^2(\mathcal{C}(\varepsilon))}$,
where $u = R(z)f,\ f\epsilon L^2(\mathcal{C}(\varepsilon))$.

These two estimates allow us to establish (note that $\partial u/\partial x_n = 0$ on $\partial\mathcal{C}\backslash D^0_\varepsilon$):

$$\left|\int_{D^0_\varepsilon} w_{\mathcal{C}} \frac{\partial u}{\partial \nu}\right| \leq \int_{\partial\mathcal{C}} \left|\eta w_{\mathcal{C}} \frac{\partial u}{\partial \nu}\right| \leq \|\eta w_{\mathcal{C}}\|_{H^{1/2}(\partial\mathcal{C})} \left\|\frac{\partial u}{\partial \nu}\right\|_{H^{-1/2}(\partial\mathcal{C})}$$
$$\leq c_0 \varepsilon^\alpha (1 + \|R_{\mathcal{C}}(z)\|)(1 + \|R(z)\|)\|g\|_{L^2(\mathcal{C})}\|f\|_{L^2(\mathcal{C}(\varepsilon))}$$

This result, plus the similar estimate for the integral involving w_T, proves the lemma. It remains to prove (1)-(4). We sketch their proof below. ◇

The proofs of statements (1), (3) and (4) relay on various, but standard, trace estimates and Sobolev embedding theorems. The Lipschitz condition on $\partial\mathcal{C}$ insures that Sobolev embedding theorems hold in our case. For example, to prove (1), note that $u|\partial\mathcal{C}\epsilon H^1(\partial\mathcal{C})$ and, consequently, $u|\partial\mathcal{C}\epsilon H^{1/2}(\partial\mathcal{C})$ by a natural embedding. A Sobolev embedding theorem states in this case $H^{1/2}(\partial\mathcal{C}) \hookrightarrow L^q(\partial\mathcal{C})$, where $q \equiv 2(n-1)(n-2)^{-1},\ n \geq 3$. By this and the Hölder inequality, we obtain

$$\int_{D^0_\varepsilon} u^2 \leq c\varepsilon \left[\int_{\partial\mathcal{C}} u^q\right]^{2/q} \leq c\varepsilon\|u\|^2_{H^{1/2}(\partial\mathcal{C})}$$
$$\leq c\varepsilon\|u\|^2_{H^{3/2}(\mathcal{C})} \leq c\varepsilon(1 + \|R(z)\|)^2\|f\|^2_{L^2(\mathcal{C}(\varepsilon))}\ .$$

The proof of (3) follows a similar line. We obtain the estimate

$$\|\eta w\|_{H^s(\partial\mathcal{C})} \leq c\varepsilon^{\alpha'-s}\|w\|_{H^1(\partial\mathcal{C})}$$

for any $0 \leq s \leq 1, w\epsilon H^1(\partial\mathcal{C})$ and $\alpha' = 1, n \geq 4, \alpha' = 1/2$ for $n = 3$. Combining this with trace estimates gives (3). The proof of (4) follows from an application of the divergence theorem to the integral

$$\int_{\partial\mathcal{C}} \phi . \frac{\partial u}{\partial \nu}$$

as a sum of integrals over $\mathcal{C}$. Here $\phi\epsilon H^{1/2}(\partial\mathcal{C})$ has an extension $\widetilde{\phi}\epsilon H^1(\mathcal{C})$.

Finally, we consider (2). Let α be a C^1 vector field in a neighborhood of $T(\varepsilon)$ such that $0 < \delta < \alpha.\nu < 1$ on D^0_ε, $\alpha.\nu = 0$ on $\partial T(\varepsilon)\backslash D^0_\varepsilon$ and $\alpha = 0$ on D^0_ε. Here ν is the normal vector field. Such a vector field can be constructed by cutting-off the vector field in the x_n-direction. We easily verify the identity on $\partial T(\varepsilon)$:

$$\left|\frac{\partial w_T}{\partial \nu}\right|^2 (\alpha.\nu) = 2\left(\frac{\partial w_T}{\partial \alpha}\right)\left(\overline{\frac{\partial w_T}{\partial \nu}}\right) - (\alpha.\nu)|\nabla w_T|^2$$

where $\partial/\partial\alpha$ is the directional derivative for α. Finally, we write

$$\begin{aligned}\delta\int_{D_\varepsilon^0}\left|\frac{\partial w_T}{\partial\nu}\right|^2 &\le \int_{D_\varepsilon^0}\left|\frac{\partial w_T}{\partial\nu}\right|^2(\alpha.\nu)\\ &\le Re\int_{\partial T(\varepsilon)}\left[2\left(\frac{\partial w_T}{\partial\nu}\right)\left(\overline{\frac{\partial w_T}{\partial\alpha}}\right)-(\alpha.\nu)|\nabla w_T|^2\right]\\ &= Re\int_{T(\varepsilon)}\nabla.\left[2\nabla w_T\left(\overline{\frac{\partial w_T}{\partial\alpha}}\right)-\alpha|\nabla w_T|^2\right]\\ &\le Re\int_{T(\varepsilon)}\left[-2(g+zw_T)\frac{\partial\overline{w}_T}{\partial\alpha}+c_0|\nabla w_T|^2\right]\quad.\end{aligned}$$

Here $w_T = R_T(z)g, g\epsilon L^2(T(\varepsilon))$. The terms involving ∇w_T can be estimated by $(1+\|R_T(z)\|)\|g\|_{L^2(T)}$. Noting that α and its derivatives are independent of ε, this proves the result. (Actually, the integration by parts requires a certain regularity of ∇w_T. See [6] for the details).$\diamondsuit$

We now turn to the existence of resonances in the case of NBC. This case is different from the Dirichlet case since, as we will show below, none of the eigenfunctions of $-\Delta_0^i$ decay exponentially in $T(\varepsilon)$ and there are the longitudinal modes, σ_L^i, of the tube which should become resonances. Because we do not have eigenfunction decay in $T(\varepsilon)$, we do not expect that the localized resolvents satisfy estimates like those in Lemma 2.3. However, with the use of suitable projection operators, one can prove the existence of resonances for $-\Delta_{\Omega(\varepsilon)}$ with NBC near the eigenvalues of $-\Delta_C$ and near the resonances of the exterior Laplacian $-\Delta_\varepsilon$. The proof of this follows as in section 2.

We wish to consider the cavity eigenvalues and the longitudinal modes of $T(\varepsilon)$, with DBC on D_ε^0 and D_ε^1, on an equal footing. Consequently, we take as an approximate Laplacian $H_{0,\varepsilon} \equiv -\Delta_{\mathcal{C}(\varepsilon)} \oplus -\Delta_{\mathcal{E}}$, where $-\Delta_{\mathcal{C}(\varepsilon)}$ has NBC on $\partial\mathcal{C}(\varepsilon)\backslash D_\varepsilon^1$ and DBC on D_ε^1 and $-\Delta_{\mathcal{E}}$ is the exterior Laplacian with mixed boundary conditions : NBC on $\partial\mathcal{E}\backslash D_\varepsilon^1$ and DBC on D_ε^1. After spectral deformation, we find that $R_0(z) \equiv (H_{0,\varepsilon}(\mu)-z)^{-1}$ and $R(z) \equiv (-\Delta_{\Omega(\varepsilon),\mu} - z)^{-1}$ satisfy an estimate similar to that in Lemma 3.2.

LEMMA **3.3.** *Under the hypotheses describe above and for $\mu\epsilon]0,1[$ fixed we have for any $z\epsilon\rho(H_{0,\varepsilon}(\mu))\cap\rho(-\Delta_{\Omega(\varepsilon),\mu})$,*

$$\|R(z)-R_0(z)\| \le c_z\varepsilon^\alpha(1+\|R(z)\|)(1+\|R_0(z)\|)\ ,$$

where $c_z = c_0(1+|z|)^{3/2}$ and $\alpha = 1/2$ for $n \ge 4, 0 < \alpha < 1/2$ for $n = 3$.

Sketch of the proof. We first note that Green's formula holds for $H_{0,\varepsilon}(\mu)$ and $-\Delta_{\Omega(\varepsilon),\mu}$ provided we choose the vector field for the spectral deformation to be spherically symmetric, which we can always do. For $u = u_{\mathcal{C}(\varepsilon)} \oplus u_{\mathcal{E}} =$

$R_0(z)g, g\epsilon L^2(\Omega(\varepsilon))$, and $v = R(z)f,\ f\epsilon L^2(\Omega(\varepsilon))$, we have

$$\int_{\Omega(\varepsilon)} \left[v(H_{0,\varepsilon}(\mu)u) - (-\Delta_{\Omega(\varepsilon),\mu}v)u\right] = \int_{D_\varepsilon^1} v\left[\frac{\partial u_{C(\varepsilon)}}{\partial\nu} - \frac{\partial u_{\mathcal{E}}}{\partial\nu}\right]$$

Since $-\Delta_{\Omega(\varepsilon),\mu}$ and $H_{0,\varepsilon}(\mu)$ are both analytic families of type A, their resolvents enjoy the same Sobolev space mapping properties as the resolvents of their undeformed counterparts. For the term involving $u_{C(\varepsilon)}$ we utilize L^2-estimates:

1) $\int_{D_\varepsilon^1}\left|\frac{\partial u_{C(\varepsilon)}}{\partial\nu}(x',1)\right|^2 \leq c_z(1+\|R_{C(\varepsilon)}(z)\|)^2\|g\|^2$

2) $\|\nu\|_{L^2(D_\varepsilon^1)} \leq c_0\varepsilon^\alpha(1+\|R(z)\|)\|f\|$

The proof of (2) follows as above due to the mapping properties of the resolvent just commented upon. The proof of (1) follows by the same integration by parts identity used in the eigenvalue case. As for the term involving the exterior function, we again use the $(H^{-1/2}, H^{1/2})$-duality. Again, the same type of proof implies :

3) $\|\frac{\partial u_{\mathcal{E}}}{\partial\nu}\|_{H^{-1/2}(\partial\mathcal{E})} \leq c_0(1+\|R_{\mathcal{E}}(z)\|)\|g\|$

4) For η as described in the proof of Lemma 3.2, $\|\eta\nu\|_{H^{-1/2}(\partial\mathcal{E})} \leq c_0\varepsilon^\alpha(1+\|R(z)\|)\|f\|$ where α is as in the lemma.

These estimates prove the result.$\diamondsuit$

Give Lemma 3.3, it is now easy to prove the existence of resonances for $-\Delta_{\Omega(\varepsilon)}$ near the ε-independent eigenvalues of $-\Delta_{C(\varepsilon)}$ with mixed NBC and DBC and near the resonances of $-\Delta_{\mathcal{E}}$, with mixed BC also. We omit the details. We do mention, however, that we do not expect exponentially small upper bounds on the shift of the resonances in the NBC case as in Theorem 2.7. Instead, we can prove $|\rho_k(\varepsilon) - \lambda_j(\varepsilon)| \leq c_0\varepsilon^{1/2}$ for $n \geq 3$. However, we do not have a lower bound.

As a final topic, we give an estimate on the decay of $u - \bar{u}, T(z)$ where u is an eigenfunction of $-\Delta_{C(\varepsilon)}$ and

$$\bar{u}(x_n) = \frac{1}{|D_\varepsilon|}\int_{D_\varepsilon} u(x', x_n)dx'$$

For this result, we must require that $\partial\mathcal{E}\cap T(\varepsilon) = \{(x',1) \;\mid\; |\, x' \,| \leq \varepsilon\}$, i.e. the surface is flat.

THEOREM 3.4. *Let α be the first non-zero eigenvalue of the Laplacian on D_1 with NBC. Then*

$$\|\exp\left[\frac{\alpha}{\varepsilon}\inf(x_1, 1-x_1)\right](u-\bar{u})\|_{L^2(T(\varepsilon))} = \mathcal{O}(\varepsilon^{1-n/2})\ .$$

We remark that this is proved using the following Agmon-type formula:

$$-\left\langle e^{\phi/\varepsilon}\Delta u, e^{\phi/\varepsilon}u\right\rangle = -\int \nabla(e^{2\phi/\varepsilon}(\overline{\nabla u})u)$$
$$+\int \overline{u}\nabla(e^{2\phi/\varepsilon}).\nabla u + \int e^{2\phi/\varepsilon}|\nabla u|^2$$

and the Poincaré inequality:

$$\|\nabla'(u-\bar{u})\|_{L^2(D_\varepsilon)} \geq (\alpha/\varepsilon)\ \|u-\bar{u}\|_{L^2(D_\varepsilon)}\ .$$

4. The Lax-Phillips Conjecture for Helmholtz Resonators

We now turn to the second class of problems mentioned in the introduction, namely, a description of resonances for a trapping obstacle at all energies. Since we are interested in "global-in-energy" results, we fix the diameter ε of the tube $T(\varepsilon)$ equal to 1 and write $T \equiv T(1), \Omega \equiv \Omega(1)$, etc. In order to obtain results, we must restrict the family of Helmholtz resonators to those in dimension $n \geq 3$ which are symmetric with respect to an axis passing through the tube T, which we call the z-axis. This symmetry allows us to use the eigenvalues $\sigma_\ell > 0$ of the square of the angular momentum operator with respect to the z-axis as a perturbation parameter in the theory. To see this, we introduce generalized cylindrical coordinates $(\rho, \widehat{\Theta}, z)$ where $\rho \equiv \left[\sum_{i=1}^{n-1} x_i^2\right]^{1/2}$ and $\widehat{\Theta}\epsilon S^{n-2}$ are any suitable coordinates on the $(n-2)$-sphere. The Laplacian admits a direct sum decomposition

$$-\Delta_\Omega = \bigoplus_\ell \left(-\frac{\partial^2}{\partial z^2} - \frac{\partial^2}{\partial \rho^2} - \frac{(n-2)}{\rho}\frac{\partial}{\partial \rho} + \frac{\sigma_\ell}{\rho^2}\right)$$

on the Hilbert space

$$L^2(\Omega) = \bigoplus_\ell L^2(\widehat{\Omega}, \rho^{n-2}d\rho dz)$$

where $\widehat{\Omega}$ is defined as follows :

$$\widehat{\Omega} \equiv \left\{(\rho, z)\epsilon\mathbf{R}^+ \times \mathbf{R} | \exists \widehat{\Theta}\epsilon S^{n-2}\ s.t.(\rho, \widehat{\Theta}, z)\epsilon\Omega\right\}\ .$$

In an analogous manner we define $\widehat{\mathcal{C}}, \widehat{T}$ and $\widehat{\mathcal{E}}$. After a unitary transformation, we find that $-\Delta_\Omega$ is equivalent to a direct sum of operators

$$H_\ell = -\frac{\partial^2}{\partial z^2} - \frac{\partial^2}{\partial \rho^2} + \frac{\sigma_\ell}{\rho^2}$$

on the spaces $L^2(\widehat{\Omega}, d\rho dz)$. We will show that for all ℓ sufficiently large, the first eigenvalue of H_ℓ on $\widehat{\Omega}$ with DBC will generate a resonance of $-\Delta_\Omega$.

In this way, we obtain a sequence of resonances $\{z_\ell\}$ of $-\Delta_\Omega$ such that $Rez_\ell \to \infty$ and $\exists c_0 > 0$ and $\alpha > 0$, independent of ℓ, such that $|Imz_\ell| \leq c_0 e^{-\alpha \ell^{-1}}$. The idea of using $\{\sigma_\ell\}$ as a perturbation parameter appears already in [8].

We notice that the classical system has trapped rays running along the interior of the cavity which correspond to the resonances. It appears as if the resonances concentrate more strongly on these trapped rays as the eigenvalue parameter ℓ (and hence the real part of the energy) increases. We mention that R. Lavine [17] has obtained similar results for a resonator formed by a sphere with a small cap removed. We also note that we do not have any results in the 2 dimensional case. The method of proof outlined here also applies to the problem of spherically symmetry media which was considered by Ralston [20].

The family of resonators we consider are constructed as in Section 2 with the tube T centered on the z-axis, which is the axis of symmetry. In particular, T contains the interval $[z_0, z_1]$ where $z_0 \epsilon \overline{\mathcal{C}}$ and $z_1 \epsilon \overline{\mathcal{E}}$. The diameter of the tube is $\rho_0 \equiv \max\{\rho | \exists z \epsilon [z_0, z_1], \widehat{\Theta} \epsilon S^{n-2} \text{ s.t. } (\rho, \widehat{\Theta}, z) \epsilon T\}$. Similarly, we define $\rho_1 \equiv max\{\rho | \exists z, \widehat{\Theta} s.t. (\rho, \widehat{\Theta}, z) \epsilon \mathcal{C}\}$. We require $\rho_1 > \rho_0$, which simply says that the tube is small relative to the cavity. We need a final condition on $\partial\mathcal{E}$ and on T near z_1. Let $D_{ext} \equiv \partial\mathcal{E} \cap \overline{T}$ $(z_1 \epsilon D_{ext})$. Define a neighborhood of T near $\partial\mathcal{E}$ by

$$\mathcal{N}(T, \varepsilon) \equiv \{x \epsilon T | z(x) \epsilon [z_1 - \varepsilon, z_1]\}$$

Exterior non-trapping hypothesis The surface $(\partial\mathcal{E} \backslash D_{ext}) \cup (\partial\mathcal{N}(T, \varepsilon))$ admits an escape function $p(x, \xi)$ for some $\varepsilon > 0$.

The notion of an escape function which we use is given in [MRS]. Whereas some non-trapping condition is necessary on $\partial\mathcal{E} \backslash D_{ext}$ to control the exterior resolvent, the condition on the end of the tube can probably be relaxed. Roughly, the condition states that the boundary of the tube must join smoothly with $\partial\mathcal{E} \backslash D_{ext}$ and that there be no trapped rays in the end of the tube. Given these geometric considerations, we can state the main theorem.

THEOREM **4.1.** *Let $\Omega = Int(\overline{\mathcal{C} \cup T \cup \mathcal{E}})$ be a symmetric resonator in $\mathbf{R}^n, n \geq 3$, defined above, satisfying the exterior non-trapping hypothesis. Let $-\Delta_\Omega$ be the Dirichlet Laplacian on Ω. Then $-\Delta_\Omega$ has a sequence of resonances $\{z_\ell\}$ satisfying (1) $0 < Rez_\ell \to \infty$ as $\ell \to \infty$, and (2) $Imz_\ell < 0$ and $\exists c_0 > 0, \alpha > 0$ such that for all ℓ sufficiently large, $|Imz_\ell| \leq c_0 e^{-\alpha \ell}$.*

Sketch of the proof of Theorem 4.1

As above, we will study $-\Delta_{\Omega,\mu} \equiv -U_\mu \Delta_\Omega U_\mu^{-1} \equiv \bigoplus_\ell H_{\ell,\mu}, \mu \epsilon \mathbf{R}$ and it's analytic continuation. Here U_μ is an appropriate spectral deformation group which vanishes inside a ball of radius R (R large enough so that $\widetilde{\Omega} \subset\subset$

$B_R(0)$) and implements the dilations in $\mathbf{R}^n \backslash B_{2R}(0)$. To define the approximate Hamiltonian, we consider two overlapping subsets of Ω. We define $\widetilde{\mathcal{C}} \equiv Int\,[\mathcal{C} \cup \{x\epsilon T | z(x)\epsilon[z_0, z_1 - \varepsilon/2]\}]^{c\ell}$, where $c\ell$ denotes closure and $\varepsilon > 0$ is fixed by the exterior non-trapping hypothesis. Similarly, we define $\widetilde{\mathcal{E}} \equiv Int\,[\mathcal{E} \cup \{x\epsilon T | z(x)\epsilon[z_1 - \varepsilon, z_1]\}]^{c\ell}$. We denote by $\mathcal{O}$ the overlap region : $\mathcal{O} = \{x\epsilon T | z(x)\epsilon[z_1 - \varepsilon/2, z_1 - \varepsilon]\}\} \subset T$. We associate a Dirichlet Laplacian to each $\widetilde{\mathcal{C}}$ and $\widetilde{\mathcal{E}}, -\Delta_{\widetilde{\mathcal{C}}}$ and $-\Delta_{\widetilde{\mathcal{E}}}$, respectively. Then the approximate Laplacian is $-\Delta^0_\Omega \equiv -\Delta_{\widetilde{\mathcal{C}}} \oplus -\Delta_{\widetilde{\mathcal{E}},\mu}$, after the exterior Laplacian has been dilated. Finally, we construct a partition of unity depending only on ρ and z, $\{J_i\}_{i=1}^2, \sum_{i=1}^2 J_i = 1$, such that $supp|\nabla J_i| \subset \mathcal{O}, J_i$ is a function of z only in a neighborhood of $\mathcal{O}$ and $J_1|\widetilde{\mathcal{C}}\backslash\mathcal{O} = 1, J_2|\widetilde{\mathcal{E}}\backslash\mathcal{O} = 1$.

1. Interior estimates

Let H^{int}_ℓ denote the Dirichlet Laplacian on $\widehat{\mathcal{C}}$ and write its spectrum as $\{\lambda_n(\ell)\}_{n=1}^\infty$. Then we have $\lambda_n(\ell) \geq \sigma_\ell/\rho_1^2$, due to the effective potential. For perturbation theory uniform in ℓ, we need to know that the gap between the first two eigenvalues of $H^{int}_\ell, \delta_\ell \equiv \lambda_2(\ell) - \lambda_1(\ell)$, does not decrease as $\ell \to \infty$.

LEMMA **4.2.** *There exists ℓ_0 sufficiently large and a constant $c > 0$ such that for all $\ell > \ell_0, \delta_\ell \geq c > 0$.*

This lemma is proved with the help of a lower bound on the gap between the first two eigenvalues of a Schrödinger operator on a convex domain with DBC and with a smooth, non-negative convex potential due to Singer, Wong, Yau and Yau [21]. We find a convex region $K \subset \widehat{\mathcal{C}}$ such that $\partial K \cap \partial\widehat{\mathcal{C}} \neq \phi$. For all large ℓ, the part of K nearest $\rho = 0$ will be in the classically forbidden region for the energy $\lambda_1(\ell)$. Consequently, the eigenfunctions will be exponentially small there [1]. We then apply the Variational Principle with appropriate test functions constructed from the eigenfunctions of H^{int}_ℓ localized to K and the eigenfunctions of $H^{int}_\ell|K$ with DBC.

We also need decay estimates on $R^{int}_\ell(z) \equiv (H^{int}_\ell - z)^{-1}$ localized in the region $\mathcal{O}$. These essentially follow from the Poincaré inequality as in the proof of Lemma 2.3.

LEMMA **4.3.** *Let χ be a smooth characteristic function supported on $\mathcal{O}$. Then for any $z\epsilon\rho(H^{int}_\ell)$,*

$$\|\chi R^{int}_\ell(z)\| \leq ((\ell/\rho_0)^2 - |z|)^{-1} d(z)^{-1}(1 + c_z)$$
$$\|\chi\widetilde{\nabla} R^{int}_\ell(z)\| \leq ((\ell/\rho_0)^2 - |z|)^{-1/2} d(z)^{-1}(1 + c_z)$$
$$\|\chi\widetilde{\nabla} R^{int}_\ell(z)\widetilde{\nabla}\chi\| \leq c_z$$

where $\widetilde{\nabla} \equiv (\partial_\rho, \partial_z), d(z) \equiv dist(z, \sigma(H^{int}_\ell))$ and $c_z \equiv c(z, d(z)) \geq 0$.

2. Exterior estimates

We need to estimate $R^{ext}_{\ell,\mu}(z) \equiv (H^{ext}_{\ell,\mu} - z)^{-1}$ for $\mu \in \mathbf{C}$, $Im\mu > 0$, and z in a neighborhood of $\lambda_1(\ell)$, for each ℓ sufficiently large. This estimate must be uniform in ℓ. By the geometric perturbation theory described below in part 3, we will need a priori bounds on $\chi R^{ext}_{\ell,\mu}(z)\chi$, $\chi\tilde{\nabla} R^{ext}_{\ell,\mu}(z)\chi$ and $\chi\tilde{\nabla} R^{ext}_{\ell,\mu}\tilde{\nabla}\chi$, where *supp* $\chi \subset \mathcal{O}$ and $\tilde{\nabla} \equiv (\partial_\rho, \partial_z)$, as above. It is precisely for these estimates that we assume the exterior non-trapping hypothesis. Indeed, [19] show how to obtain such bounds given an escape function for a boundary. We briefly review the main points and refer to [18] and [19] for the details.

PROPOSITION 4.4. *Assume that an exterior domain $\mathcal{D}$ admits an escape function. Then the local energy decays as $t \to \infty$ (at least as $\mathcal{O}(t^{-1})$) for all solutions of the wave equation on the exterior domain $\mathcal{D}$ with initial conditions $B_R(0) \cap \mathcal{D}$ (for R large enough). Let B be the generator of the Lax-Phillips semigroup $Z(t) = P_+ \; U(t) \; P_-$, $t \geq 0$. Then there exists $\alpha > 0$ such that $(\mu - B)^{-1}$ is holomorphic on $Re\; \mu > -\alpha$.*

This proposition and standard spectral deformation results imply that $R^{ext}_{\ell,\mu}(z)$ is holomorphic in the region

$$\mathcal{O}_{\alpha,\mu} \equiv \{z \in \mathbf{C} \mid Im\; z > -\alpha \text{ and } arg\; z > -2\; arg(1+\mu)\}.$$

Next, from the construction of $Z(t)$, if f, g are initial conditions for the wave equation with support in $\tilde{\mathcal{E}} \cap B_R(0)$, it follows that [18]

$$((\mu - B)^{-1} f, g)_E = ((\mu - A)^{-1} f, g)_E$$

where $(.,.)_E$ is the energy inner product and A is the generator of $U(t)$, the unitary evolution group for the wave equation. Consequently, by Proposition 4.4., we get an analytic continuation of $((\mu - A)^{-1} f, g)_E$ into $Re\; \mu > -\alpha$. It follows by a simple calculation and suitable choice of initial conditions that $(\chi R^{ext}_{\ell,\mu}(z)\chi\phi,\; \psi)$ can be bounded for $z \in \mathcal{O}_{\alpha,\mu}$, uniformly in the L^2-norms of ϕ and ψ, by $\|(\mu - B)^{-1}\|_E$ for $Re\; \mu > -\alpha$. This latter norm is bounded as follows. The local energy decay implies $\exists c > 0$, $\alpha > 0$ such that

$$\|Z(t)\| \leq ce^{-\alpha t}, \; t > 0.$$

Hence, the Laplace transform of $Z(t)$ converges for $Re\; \mu > -\alpha$:

$$(\mu - B)^{-1} = \int_0^\infty e^{-\mu t} Z(t) dt$$

and thus, for some $c_0 > 0$:

$$\|(\mu - B)^{-1}\| \leq c_0(\alpha + Re\; \mu)^{-1}$$

provided $Re\; \mu > -\alpha$. Consequently, we derive that

$$\|\chi R^{ext}_{\ell,\mu}(z)\chi\| \le c_0[Im\ z + \alpha]^{-1}$$

for $z \in \mathcal{O}_{\alpha,\mu}$, uniformly in ℓ. Combining this a priori estimate with a Poincaré inequality valid for the region $\mathcal{O}$, we obtain an analog of Lemma 4.3.

Lemma 4.5. *Let χ be a smooth characteristic function with support in $\mathcal{O}$ and let*
$\rho_2 \equiv max\{\rho \mid \rho(x) \in \mathcal{O}\}$. *Then for any $z \in \mathcal{O}_{\alpha,\mu}$*

$$\|\chi R^{ext}_{\ell,\mu}(z)\chi\| \le c_1((\ell/\rho_2)^2 - \mid z \mid)^{-1}$$
$$\|\chi \widetilde{\nabla} R^{ext}_{\ell,\mu}(z)\chi\| \le c_2((\ell/\rho_2)^2 - \mid z \mid)^{-1/2}$$
$$\|\chi \widetilde{\nabla} R^{ext}_{\ell,\mu}(z)\widetilde{\nabla}\chi\| \le c_3$$

where the constants c_i depend only on $\mathcal{O}_{\alpha,\mu}$ and are uniform in ℓ.

We remark that the proof of the third estimate requires some machinery of [5] (see [11] and below).

3. Geometric perturbation theory

We use the methods of [5] (see also [7]) to prove that $H_{\ell,\mu}$ has an eigenvalue near $\lambda_1(\ell) \in \sigma(H^{int}_\ell)$. This more detailed form of pertubation theory is necessary since we only have the localized resolvent estimates of Lemmas 4.3 and 4.5. As in section 2, define $\mathcal{H}_0 \equiv L^2(\widetilde{\mathcal{C}}) \oplus L^2(\widetilde{\mathcal{E}})$, $\mathcal{H} \equiv L^2(\widehat{\Omega})$ and $J : \mathcal{H}_0 \to \mathcal{H}$ by $J(u_1 \oplus u_2) = J_1\, u_1 + J_2\, u_2$, where $\{J_i\}_{i=1}^2$ is the partition of unity introduced above such that $supp \mid \nabla J_i \mid \subset \mathcal{O}$. Let $\{\widetilde{J}_i\}_{i=1}^2$ be another pair of functions such that $\widetilde{J}_i\, J_i = J_i$, $\widetilde{J}_i \mid supp\ J_i = 1$, and define $\widetilde{J} : \mathcal{H}_0 \to \mathcal{H}$ as above. Then $J\, \widetilde{J}^\star = 1_{\mathcal{H}}$. We will supress the indices (ℓ, μ) when the meaning is clear. As in section 2, we obtain a geometric resolvent equation

$$R(z)J = JR_0(z) + R(z)JMR_0(z)$$

where M : $\mathcal{H}_0 \to \mathcal{H}_0$ is given by

$$M(u_1 \oplus u_2) \equiv (\widetilde{\nabla} J_1' + J_1'\widetilde{\nabla})u_1 \oplus (\widetilde{\nabla} J_2' + J_2'\widetilde{\nabla})u_2$$

with a prime denoting the z derivative and $\widetilde{\nabla} \equiv (\partial_\rho,\ \partial_z)$. We factorize M with the aid of two auxiliary operators $M_i : \mathcal{H}_0 \to \mathcal{H}_0 \oplus \mathcal{H}_0$:

$$M_1(u_1 \oplus u_2) \equiv (J_1' u_1 \oplus \chi\widetilde{\nabla} u_1) \oplus (J_2' u_2 \oplus \chi\widetilde{\nabla} u_2)$$
$$M_2(v_1 \oplus v_2) \equiv (\chi\widetilde{\nabla} v_1 \oplus J_1' v_1) \oplus (\chi\widetilde{\nabla} v_2 \oplus J_2' v_2)$$

so that $M = -M_2^\star M_1$. Using this factorization and solving for $R(z)J\ M_2^\star$, we obtain

$$R(z) = JR_0(z)\widetilde{J}^\star - JR_0(z)M_2^\star(1 - K(z))^{-1}M_1\ R_0(z)\widetilde{J}^\star \qquad (4.1)$$

where $K(z)\ :\ \mathcal{H}_0 \oplus \mathcal{H}_0 \to \mathcal{H}_0 \oplus \mathcal{H}_0$ is defined by

$$K(z) \equiv -M_1\ R_0(z)\ M_2^\star$$

For (4.1) to be valid, it is sufficient that $\|K(z)\| < 1$. If we write out the form of $K(z)$, we see that the estimates of Lemmas 4.3 and 4.5 guarantee this for all large ℓ and z on a contour Γ_ℓ about $\lambda_1(\ell)$, for each ℓ large enough. It is a consequence of Lemma 4.2 that we can take $rad(\Gamma_\ell) = \mathcal{O}(1)$ for all ℓ. We now integrate both sides of (4.1) about Γ_ℓ. The estimates of Lemma 4.3 and the holomorphy of $R^{ext}_{\ell,\mu}(z)$ on and inside Γ_ℓ allow us to prove

$$\|(z\pi i)^{-1} \oint_{\Gamma_\ell} R(z)dz - JP_0\widetilde{J}^\star\| \leq c_0\ \ell^{-1/2},$$

where P_0 is the projection onto the eigenspace of $\lambda_1(\ell)$. The estimates discussed in section 4 below insure that for any $\varepsilon > 0$, $\|JP_0\widetilde{J}^\star\| \geq 1 - \varepsilon$ for all large ℓ. Consequently, $H_{\ell,\mu}$ has an eigenvalue near $\lambda_1(\ell)$ with the same algebraic multiplicity as $\lambda_1(\ell)$. This proves the existence of resonances for Δ_Ω near $\lambda_1(\ell)$ for all large ℓ.

4. Exponential decay

Estimates on the resonance width come from exponential decay estimates on the eigenfunctions of H_ℓ^{int} in the tube region and bounds on the interior resolvents as in Lemma 4.3. The procedure is as in [12]. Agmon-type calculations as presented there give the necessary decay estimates with constants uniform in ℓ. These estimates also allow us to establish the uniform bound on $\|JP_0\widetilde{J}^\star\|$ mentioned above. Note that the decay of an eigenfunction of H_ℓ^{int} is due to the fact that the tube T and a neighborhood of $\rho.= 0$ in $\hat{e}$ lie in the classically forbidden region for $\lambda_1(\ell)$ for all large ℓ. ◇

References

[1] S. Agmon, Lectures on Exponential Decay of Solutions of Second Order Elliptic Equations. Princeton, N.J. : Princeton University Press (1982).

[2] J.M. Arrieta, J.K. Hale, Q. Han, Eigenvalue Problems for Nonsmoothly Perturbed Domains. J. Diff. Eqns. **91** (1991) 24-52.

[3] A.A. Arsen'ev, On the singularities of analytic continuations and resonance properties of a solution of the scattering problem for the Helmholtz equation. Zh. Vyohisl. Mat. i Mat. Fiz. **12** (1972) 112-138.

[4] J.T. Beale, Scattering frequencies of resonators. Comm. Pure and Applied Math. **26** (1973) 549-563.

[5] Ph. Briet, J.-M. Combes, P. Duclos, Spectral Stability under Tunnelling. Commun. Math. Phys. **126** (1989) 133-156.

[6] R.M. Brown, P.D. Hislop, A. Martinez, in preparation.

[7] J.-M. Combes, P.D. Hislop, Stark Ladder Resonances for Small Electric Fields. Commun. Math. Phys. **140** (1991) 291-320.

[8] S. De Bièvre, P.D. Hislop, Spectral Resonances for the Laplace-Beltrami Operator. Ann. Inst. H. Poincaré **48** (1988) 103-129.

[9] C. Gérard, Asymptotique des poles de la matrice de scattering pour deux obstacles strictement convexes. Bull. S.M.F. **116** n° 31 (1989).

[10] R. Hempel, L. Seco, B. Simon, The Essential Spectrum of Neumann Laplacians on some Bounded Singular Domains. preprint 1991.

[11] P.D. Hislop, The Lax-Phillips Conjecture for a Class of Helmholtz Resonators, in preparation.

[12] P.D. Hislop, A. Martinez, Scattering Resonances of a Helmholtz Resonator. Indiana U. Math. J. **40** (1991) 767-788.

[13] M. Ikawa, On the poles of the scattering matrix for two strictly convex obstacles. J. Math. Kyoto Univ. **23** (1983) 127-194.

[14] M. Ikawa, Trapping Obstacles with a sequence of poles of the scattering matrix converging to the real axis. Osaka J. Math. **22** (1985) 657-689.

[15] D.S. Jerison, C.E. Kenig, The Neumann Problem on Lipschitz Domains. Bull. Amer. Math. Soc. **4** (1981) 203-207.

[16] S. Jimbo, The Singularly Perturbed Domain and the Characterization for Eigenfunctions with Neumann Boundary Conditions. J. Diff. Eqns. **77** (1989) 322-350.

[17] R. Lavine, private communication.

[18] P. Lax and R. Phillips, Scattering Theory. New York : Academic Press (1967).

[19] C. Morawetz, J.V. Ralston, W.A. Strauss, Decay of Solutions of the Wave Equation outside Nontrapping Obstacles. Commun. Pure and Applied Math. **30** (1977) 447-508.

[20] J.V. Ralston, Trapped Rays in Spherically Symmetric Media and Poles of the Scattering Matrix. Commun. Pure and Applied Math. **24** (1971) 571-582.

[21] I.M. Singer, B. Wong, S.T. Yau, S.S.T. Yau, An Estimate of the Gap of the First two Eigenvalues in the Schrödinger Operator. Ann. Scuola Norm. Sup. Pisa **12** (1985) 319-333.

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Singular perturbation of symbolic flows and the modified Lax-Phillips conjecture

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SINGULAR PERTURBATION OF SYMBOLIC FLOWS AND THE MODIFIED LAX-PHILLIPS CONJECTURE

MITSURU IKAWA

1. Introduction. In the study of scattering by an obstacle consisting of several convex bodies, it is known that the distribution of poles of the scattering matrix has a close relationship to the zeta functions associated with a dynamical system in the exterior of the obstacle. When we want to consider the validity of the modified Lax-Phillips conjecture, we can derive it from the existence of poles of the zeta functions. That is, roughly speaking, if the zeta function has a pole in a certain region, the scattering matrix for the obstacle has an infinite number of poles in a strip $\{z \in \mathbf{C}; 0 < \operatorname{Im} z < \alpha\}$ for some $\alpha > 0$. The modified Lax-Phillips conjectrue will be explained in the next section.

Therefore, in order to consider distributions of poles of scattering matrices for an obstacle consisting of several convex bodies, the zeta functions play a crucial role. But unfortunately, it is not so easy to show the existence of a pole of the zeta functions in general.

In this talk, we shall develop a theory of singular perturbations of symbolic dynamics, with which we shall show the existence of a pole of the zeta function when the obstacle is consisted of several small balls.

In Section 2, we explain the modified Lax-Phillips conjecture and consider the scattering by obstacles consisting of several convex bodies. In Section 3, we shall discuss singular perturbations of symbolic dynamics. In Section 4, we shall show how to apply the theorem on singular perturbations of symbolic dynamics to considerations of the matrices for obstacles consisting of several small balls.

2. Scattering by several convex bodies.

Let $\mathcal{O}$ be a bounded open set in $\mathbf{R}^3$ with smooth boundary Γ. We set

$$\Omega = \mathbf{R}^3 - \overline{\mathcal{O}},$$

and assume that Ω is connected. Consider the following acoustic problem:

$$
(2.1) \qquad \begin{cases} \Box u = \dfrac{\partial^2 u}{\partial t^2} - \Delta u = 0 & \text{in } \Omega \times (-\infty, \infty), \\ u = 0 & \text{on } \Gamma \times (-\infty, \infty), \\ u(x,0) = f_1(x), \dfrac{\partial u}{\partial t}(x,0) = f_2(x). \end{cases}
$$

We denote by $\mathcal{S}(z)$ the scattering matrix for this problem. The scattering matrix $\mathcal{S}(z)$ is an $\mathcal{L}(L^2(S^2))$−valued function analytic in $\{z; \operatorname{Im} z \leq 0\}$ and meromorphic in the whole complex plane $\mathbf{C}$, and that the correspondance from obstacles to scattering matrices

$$
\mathcal{O} \to \mathcal{S}(z)
$$

is one to one(see for example [LP]).

Concerning the above correspondance, we are interested in the problem to know how the distribution of poles of scattering matrices relates to the geometry of obstacles. As to this problem, we would like to present the following conjecture:

Modified Lax-Phillips Conjecture. *When $\mathcal{O}$ is trapping, there is a positive constant α such that the scattering matrix $\mathcal{S}(z)$ has an infinite number of poles in $\{z; 0 < Im\, z \leq \alpha\}$.*

Hereafter, we say that MLPC(abbreviation of the modified Lax-Phillips conjecture) is valid for obstacle $\mathcal{O}$, when there is $\alpha > 0$ such that the scattering matrix $\mathcal{S}(z)$ corresponding to $\mathcal{O}$ has an infinite number of poles in $\{z; \operatorname{Im} z \leq \alpha\}$.

About this conjecture, obstacles consisting of two convex bodies were studied first. By the works [BGR], [G], [Ik1] and [S], the distribution of poles are well studied, and it is shown that MLPC is valid for obstacles consisting of two convex bodies. It is very natural to proceed to obstacles consisting of three strictly convex bodies. But the problem for three bodies exposes an essential difference from that of two bodies. Namely, for an obstacle consisting of three bodies, there exist infinitely many primitive periodic rays in the exterior of the obstacle in general. Thus, we have to consider geometric property of the totality of the periodic rays in the exterior, and it seems that the asymptotic behavior of the periodic rays with very large period plays an essential role.

Here, we present a theorem in [Ik3,4], which allows us to connect the asymptotic behavior of the periodic rays and the distribution of poles of the scattering matrix.

Let $\mathcal{O}_j,\ j=1,2,\cdots,L$, be bounded open sets with smooth boundary Γ_j satisfying

$$\text{(H.1)} \qquad \text{every } \mathcal{O}_j \text{ is strictly convex,}$$

(H.2) for every $\{j_1,j_2,j_3\}\in\{1,2,\cdots,L\}^3$ such that $j_l\neq j_{l'}$ if $l\neq l'$,

$$(\text{convex hull of } \overline{\mathcal{O}_{j_1}} \text{and } \overline{\mathcal{O}_{j_2}})\cap\overline{\mathcal{O}_{j_3}}=\phi.$$

We set

$$\mathcal{O}=\cup_{j=1}^{L}\mathcal{O}_j,\quad \Omega=\mathbf{R}^3-\overline{\mathcal{O}} \text{ and } \Gamma=\partial\Omega. \tag{2.2}$$

Denote by γ an oriented periodic ray in Ω, and we shall use the following notations:

d_γ : the length of γ,
T_γ : the primitive period of γ,
i_γ : the number of the reflecting points of γ,
P_γ : the Poincaré map of γ.

We define a function $F_D(s)$ ($s\in\mathbf{C}$) by

$$F_D(s)=\sum_\gamma(-1)^{i_\gamma}T_\gamma|I-P_\gamma|^{-1/2}e^{-sd_\gamma} \tag{2.3}$$

where the summation is taken over all the oriented periodic rays in Ω and $|I-P_\gamma|$ denotes the determinant of $I-P_\gamma$.

Concerning the periodic rays in Ω we have

$$\#\{\gamma;\text{periodic ray in } \Omega \text{ such that } d_\gamma<r\}<e^{a_0 r} \tag{2.4}$$

and

$$|I-P_\gamma|\geq e^{2a_1 d_\gamma}, \tag{2.5}$$

where a_0 and a_1 are positive constants depending on $\mathcal{O}$. The estimates (2.4) and (2.5) imply that the right hand side of (2.3) converges absolutely in $\{s\in\mathbf{C};\ \mathrm{Re}\,s>a_0-a_1\}$. Thus $F_D(s)$ is well defined in $\{s\in\mathbf{C};\ \mathrm{Re}\,s>a_0-a_1\}$, and holomorphic in this domain.

Now we have

Theorem 2.1. *Let $\mathcal{O}$ be an obstacle given by (2.2) satisfying (H.1) and (H.2). If $F_D(s)$ cannot be prolonged analytically to an entire function, then MLPC is valid for $\mathcal{O}$.*

We cannot give here the proof of the above theorem. We would like to refer that the trace formula due to [BGR] is the starting point of the proof. This trace formula is written as follows:

$$\begin{aligned}(2.6)\qquad &\mathrm{Trace}_{L^2(\mathbf{R}^3)} \int \rho(t) \left(\cos t\sqrt{-A} \oplus 0 - \cos t\sqrt{-A_0}\right) dt \\ &= \frac{1}{2}\sum_{j=1}^{\infty} \hat{\rho}(z_j), \qquad \text{for all } \rho \in C_0^\infty(0,\infty)\end{aligned}$$

where

$$\hat{\rho}(z) = \int e^{izt}\rho(t)dt,$$

$\{z_j\}_{j=1}^{\infty}$ is a numbering of all the poles of $\mathcal{S}(z)$, A is the selfajoint realization in $L^2(\Omega)$ of the Laplacian with the Dirichlet boundary condition and A_0 the one in $L^2(\mathbf{R}^3)$, and $\oplus 0$ indicates the extension into $\mathcal{O}$ by 0. It gives us an relationship between the distribution of poles of the scattering matrix and the singularities of the trace of the evolution operator of (2.1). We shall use (2.6) in the following way: Suppose that $F_D(s)$ has a singularity. This enable us to choose a sequence of ρ of the form

$$\rho_q(t) = \rho(m_q(t - l_q))$$

in such way that

$$l_q \to \infty, \quad m_q \to \infty \quad \text{as } q \to \infty,$$

and that the left hand side does not decay so fast as q tends to the infinity. But if MLPC is not valid, the right hand side of (2.6) for ρ_q decreases very rapidely. The difference in decreasing speeds brings a contradiction. Thus MLPC is valid. The detailed proof is given in [Ik3].

By virtue of Theorem 2.1, the proof of the validity of MLPC is transfered to the consideration of singularities of $F_D(s)$. But it is not easy to show the existence of singularities of $F_D(s)$ in general. At present we can show it only for obstacles consisting of small balls.

Theorem 2.2. *Let $P_j, j = 1, 2, \cdots, L$, be points in $\mathbf{R}^3$, and set for $\varepsilon > 0$*

$$\mathcal{O}_\varepsilon = \cup_{j=1}^{L}\mathcal{O}_{j,\varepsilon}, \quad \mathcal{O}_{j,\varepsilon} = \{x; |x - P_j| < \varepsilon\}.$$

Suppose that

(A) *any triple of P_j's does not lie on a straight line.*

Then, there is a positive constant ε_0 such that the modified Lax-Phillips conjecture holds for $\mathcal{O}_\varepsilon$ for all $0 < \varepsilon \le \varepsilon_0$.

To prove the above theorem we have to show the existence of singularities of $F_D(s)$ associated with $\mathcal{O}_\varepsilon$. To do this, we need a theory of singular perturbation of symbolic dynamics, which will be developed in the next section.

3. Singular perturbations of symbolic dynamics

In this section we consider singular perturbations. First we shall give some notations concerning the symbolic dynamics.

3.1. Notations and statement of a theorem.

Let $L \ge 2$ be an integer, and let $A = (A(i,j))_{i,j=1,2,\cdots,L}$ be a zero-one $L \times L$ matrix. We set

$$\Sigma_A^+ = \{\xi = (\xi_1, \xi_2, \cdots); 1 \le \xi_j \le L \text{ and } A(\xi_j, \xi_{j+1}) = 1 \text{ for } j = 1, 2, \cdots\},$$

and denote by σ_A the shift operator defined by

$$(\sigma_A(\xi))_j = \xi_{j+1} \quad \text{for all } j.$$

We regard Σ_A^+ as a compact metric space by introducing the usual discrete metric. Define $\operatorname{var}_n r$ and $\|r\|_\infty$ for $r \in C(\Sigma_A^+)$ by

$$\operatorname{var}_n r = \sup\{|r(\xi) - r(\psi)|; \xi, \psi \in \Sigma_A^+ \text{ and } \xi_j = \psi_i \text{ for } j \le n\},$$
$$\|r\|_\infty = \sup\{|r(\xi)|; \xi \in \Sigma_A^+\}.$$

We set for $0 < \theta < 1$

$$\|r\|_\theta = \sup_{n \ge 1} \frac{\operatorname{var}_n r}{\theta^n}, \quad |||r|||_\theta, = \max\{\|r\|_\theta, \|r\|_\infty\}$$
$$\mathcal{F}_\theta(\Sigma_A^+) = \{r \in C(\Sigma_A^+); |||r|||_\theta < \infty\}.$$

Assume that A satisfies

(3.1) $$A^N > 0 \qquad \text{for some positive integer } N,$$

that is, all the entries of the matrix A^N are positive. Let $B = [B(i,j)]_{i,j=1,2,\cdots,L}$ be another zero-one $L \times L$ matrix.

Definition. Let $i, j \in \{1, 2, \cdots, L\}$. The notation

$$i \underset{B}{\longrightarrow} j$$

indicates the existence of a sequence $i_1, i_2. \cdots, i_p$ such that $B(i_1, i) = 1$, $B(i_{q+1}, i_q) = 1$ for $q = 1, 2, \cdots, p-1$ and $B(j, i_p) = 1$.

We assume on B the following:
There is $1 < K \leq L$ such that

$$B(i,j) = 0 \quad \text{for all} \quad j \text{ if } \ i \geq K+1, \tag{3.2}$$

$$i \underset{B}{\longrightarrow} i \quad \text{for all } 1 \leq i \leq K, \tag{3.3}$$

$$i \underset{B}{\longrightarrow} j \quad \text{implies} \quad j \underset{B}{\longrightarrow} i \quad \text{if } i, j \leq K \tag{3.4}$$

and

$$B(i,j) = 1 \quad \text{implies} \quad A(i,j) = 1. \tag{3.5}$$

Let $f_\varepsilon,\ h_\varepsilon$ are functions with parameter $\varepsilon \geq 0$ satisfying

$$f_\varepsilon,\ h_\varepsilon \in \mathcal{F}_\theta(\Sigma_A^+) \qquad \text{for all } 0 \leq \varepsilon \leq \varepsilon_1, \tag{3.5}$$

where ε_1 is a positive constant, and let $k \in \mathcal{F}_\theta(\Sigma_A^+)$ satisfy

$$k(\xi) = \begin{cases} k(\xi) = 0 & \text{if } \ B(\xi_1, \xi_2) = 1 \\ k(\xi) > 0 & \text{if } \ B(\xi_1, \xi_2) = 0. \end{cases} \tag{3.6}$$

Suppose that

$$|||f_\varepsilon - f_0|||_\theta,\ |||h_\varepsilon - h_0|||_\theta \longrightarrow \infty \quad \text{as} \quad \varepsilon \longrightarrow 0. \tag{3.7}$$

For $0 < \varepsilon \leq \varepsilon_1$, we define zeta function $Z_\varepsilon(s)$ by

$$Z(s;\varepsilon) = \exp\left(\sum_n^\infty \frac{1}{n} \sum_{\sigma_A^n \xi = \xi} \exp S_n r(\xi, s; \varepsilon)\right) \tag{3.8}$$

where

$$r(\xi, s; \varepsilon) = -s f_\varepsilon(\xi) + h_\varepsilon(\xi) + k(\xi) \log \varepsilon$$

and

$$S_n r(\xi, s; \varepsilon) = \sum_{j=0}^{n-1} r({\sigma_A}^j \xi, s; \varepsilon).$$

The following theorem is on the existence of singularities of $Z(s;\varepsilon)$, which is the main result of [Ik5].

Theorem 3.1. *Suppose that (3.1)$\sim$(3.7) are satisfied, and that*

$$f_0(\xi) > 0 \qquad \textit{for all } \xi \in \Sigma_A^+, \tag{3.9}$$

$$h_0(\xi) \textit{ is real for all } \xi \in \Sigma_A^+ \textit{ such that } \quad B(\xi_1, \xi_2) = 1. \tag{3.10}$$

Then there exist $s_0 \in \mathbf{R}$, D a neighborhood of s_0 in $\mathbf{C}$ and $\varepsilon_0 > 0$ such that, for every $0 < \varepsilon \leq \varepsilon_0$, $Z(s;\varepsilon)$ is meromorphic in D and it has a pole s_ε in D with

$$s_\varepsilon \longrightarrow s_0 \qquad \textit{as} \quad \varepsilon \longrightarrow 0.$$

Here we would like to mention about the reason why we call the above result as singular perturbation.

Let us set

$$C = (B(i,j))_{i,j=1,2,\cdots,K}$$

and

$$\Sigma_C^+ = \{\xi = (\xi_1, \xi_2, \cdots);\ 1 \leq \xi_j \leq K \text{ and } B(\xi_j, \xi_{j+1}) = 1 \text{ for all } j\}.$$

Consider a term in (3.8)

$$\sum_{\sigma_A^n \xi = \xi} \exp\, S_n\, r(\xi, s; \varepsilon).$$

If we make ε tend to zero, because of the effect of $k(\xi)\log\varepsilon$, for all $\xi \in \Sigma_A^+$ such that $k({\sigma_A}^m \xi) > 0$ for at least one m, $\exp\, S_n\, r(\xi, s; \varepsilon)$ tends to zero. Therefore, the above summation tends to

$$\sum_{\sigma_C^n \xi = \xi} \exp\, S_n\, r(\xi, s; \varepsilon).$$

If we set

$$\tilde{Z}_0(s) = \exp\{\sum_{n=1}^{\infty} \frac{1}{n} \sum_{\sigma_A^n \xi = \xi} \exp\, S_n(-s f_0(\xi) + h_0(\xi))\},$$

$\tilde{Z}_0(s)$ is a zeta function of the symbolic flow on (Σ_C^+, σ_C). Thus the above fact suggests us that $Z_\varepsilon(s)$ should be regarded as a perturbation of $\tilde{Z}_0(s)$. But when we compare these, not only the function $-f_0(\xi) + h_0(\xi)$ but also the structure matrix C are perturebed. Thus we should call it singular perturbation.

In the rest of this section we shall give only a sketch of the proof of Theorem 3.1. For the detailed proof, see [Ik5].

3.2. The Perron-Frobenius operators.

In order to find a pole of $Z_\varepsilon(s)$ it is important to examine the spectrum of the Perron-Frobenius operator associated with $Z(s;\varepsilon)$ defined by

$$\mathcal{L}_{\varepsilon,s} = \sum_{\sigma_A \eta = \xi} \exp(r_\varepsilon(\eta, s))\, u(\eta) \quad \text{for} \quad u \in C(\Sigma_A^+).$$

For the proof of the existence of poles of $Z(s;\varepsilon)$, if we use the results of [Po] or [H], it suffices to show the existence s for which $\mathcal{L}_{\varepsilon,s}$ has 1 as an eigenvalue.

Remark that it is difficult to consider directly the spectrum of $\mathcal{L}_{\varepsilon,s}$ since $r_\varepsilon(\xi, s)$ is of the form rather complex for $\varepsilon > 0$. Thus, it is important to find its nice approximations. As the first approximation, we introduce an operator $\mathcal{L}'_s$ in Σ_A^+ by

$$\mathcal{L}'_s = \begin{cases} \sum_{B(\eta_1,\xi_1)=1} \exp(r_\varepsilon(\eta, s))\, u(\eta) & \text{for} \quad \xi \in \Sigma(1), \\ 0 & \text{for} \quad \xi \in \Sigma(2), \end{cases} \tag{3.11}$$

where

$$r_0(\xi; s) = -s f_0(\xi) + h_0(\xi),$$

$\sum_{B(\eta_1,\xi_1)=1}$ indicates the summation taken over all $\eta \in \Sigma_A^+$ such that $\sigma_A \eta = \xi$ and $B(\eta_1, \xi_1) = 1$, and

$$\Sigma(1) = \{\xi \in \Sigma_A^+; B(l, \xi_1) = 1 \quad \text{for some } 1 \le l \le K\},$$
$$\Sigma(2) = \{\xi \in \Sigma_A^+; B(l, \xi_1) = 0 \quad \text{for all } 1 \le l \le K\}.$$

Since $r_0(\xi, s)$ is not necessarily real even for $\varepsilon = 0$ and real s, we have to introduce an approximation $\tilde{\mathcal{L}}_s$ of $\mathcal{L}'_s$ defined by

$$\tilde{\mathcal{L}}_s\, v(\xi) = \sum_{\sigma_C \eta = \xi} \exp(r_\varepsilon(\eta, s))\, u(\eta) \quad \text{for} \quad v \in C(\Sigma_C^+). \tag{3.12}$$

Now $r_0(\xi, s)$ is real valued for all $\xi \in \Sigma_C^+$ and real s and we can apply the generalized Perron-Frobenius theorem and find $s_0 \in \mathbf{R}$ such that $\tilde{\mathcal{L}}_{s_0}$ has 1 as an eigenvalue.

Of course, in using these approximations of $\mathcal{L}_{\varepsilon,s}$, we have to compare the spectra of these operators. In our reasoning, the most crucial step is to give a relationships between spectra of $\tilde{\mathcal{L}}_s$ and $\mathcal{L}'_s$.

3.3. On the decomposition of $\tilde{\mathcal{L}}_s$.

First recall the generalized Perron-Frobenious Theorem of [AS] for symbolic dynamics which is not necessarily mixing. We introduce the following definition of indecomposability of a matrix.

Definition. We say that an $L \times L$ zero-one matrix C is indecomposable when $i \underset{C}{\longrightarrow} j$ for any $i, j \in \{1, 2, \cdots, L\}$.

Then the following theorem holds:

Theorem 3.2. *Suppose that a zero-one matrix C is indecomposable, and r is a real valued function belonging to $\mathcal{F}_\theta(\Sigma_C^+)$. The the operator in $\mathcal{F}_\theta(\Sigma_C^+)$ defined by*

$$\mathcal{L}u(\xi) = \sum_{\sigma_C \eta = \xi} \exp\bigl(r(\eta)\bigr)\, u(\eta)$$

has the following decomposition:

$$\mathcal{L} = \sum_{k=1}^{k_0} \lambda_k\, E_k + S$$

where

$$\begin{gathered} \lambda_1 > 0, \quad \text{and} \quad \lambda_k = \lambda_1 \exp(i(k-1)2\pi/k_0), \quad \text{for } k = 2, \dots, k_0, \\ E_k\, E_l = \delta_{kl} E_k, \quad E_k S = S E_k = 0, \\ \text{dimension of the range } E_k = 1, \\ \text{the spectral radius of } S < \lambda_1(1-\delta) \text{ for some } \delta > 0. \end{gathered}$$

The constant k_0 is the greatest common divisor of all the periods of periodic elements in Σ_C^+

Let us say that i and j are equivalent when $i \underset{B}{\longrightarrow} j$. Then the conditions (3.2) and (3.3) on B imply that this gives an equivalent relation in $\{1, 2, \dots, K\}$. Therefore, by changing the numbering of the elements of $\{1, 2, \dots, K\}$, we may assume that the set $\{1, 2, \dots, K\}$ is decomposed into equivalents classes

$$M_j = \{i_j, i_j + 1, \cdots, i_{j+1} - 1\} \quad (j = 1, 2, \cdots, l).$$

We shall denote by C_j the $(i_{j+1} - i_j) \times (i_{j+1} - i_j)$ matrix $[B(i,j)]_{i,j \in M_j}$. Note that each C_j is indecomposable. We set

$$\Sigma_{C_j}^+ = \{\xi = (\xi_1, \xi_2, \cdots);\ \xi_i \in M_j \text{ and } \ B(\xi_i, \xi_{i+1}) = 1 \ \text{ for all } i\}$$

and

$$\Sigma_C^+ = \{\xi = (\xi_1, \xi_2, \cdots);\ 1 \le \xi_i \le K \text{ and } \ B(\xi_i, \xi_{i+1}) = 1 \ \text{ for all } i\}.$$

Regarding $\Sigma_{C_j}^+$ and Σ_C^+ as subsets of Σ_A^+, we have a decomposition

$$C(\Sigma_C^+) = C(\Sigma_{C_1}^+) \oplus C(\Sigma_{C_2}^+) \oplus \cdots \oplus C(\Sigma_{C_l}^+).$$

For $u \in C(\Sigma_A^+)$ we denote by $[u]$ and $[u]_j$ the restrictions of u to Σ_C^+ and $\Sigma_{C_j}^+$ respectively. Conversely, for functions in Σ_C^+ or in $\Sigma_{C_j}^+$ we shall often treat them as functions defined in Σ_A^+ by extending them by zero in the outside of Σ_C^+ or of $\Sigma_{C_j}^+$.

Let $\tilde{\mathcal{L}}_s$ be the operator in $C(\Sigma_C^+)$ defined by

$$\tilde{\mathcal{L}}_s v(\xi) = \sum_{\sigma_C \eta = \xi} \exp\big(r_0(\eta; s)\big)\, v(\eta) \qquad \text{for } v \in C(\Sigma_C^+),$$

and let $\tilde{\mathcal{L}}_{j,s}$ be the operators in $C(\Sigma_{C_j}^+)$ defined by

$$\tilde{\mathcal{L}}_{j,s}\, v(\xi) = \sum_{\sigma_{C_j} \eta = \xi} \exp\big(r_0(\eta; s)\big)\, v(\eta) \quad \text{for} \quad v \in C(\Sigma_{C_j}^+)$$

where σ_C and σ_{C_j} denote the restrictions of σ_A to Σ_C^+ and $\Sigma_{C_j}^+$ respectively. Then $\tilde{\mathcal{L}}_s$ has a decomposition

$$\tilde{\mathcal{L}}_s = \tilde{\mathcal{L}}_{1,s} \oplus \tilde{\mathcal{L}}_{2,s} \oplus \cdots \oplus \tilde{\mathcal{L}}_{l,s}.$$

By using the notaion introduced in the above, we have for all $u \in \Sigma_A^+$

$$\tilde{\mathcal{L}}_s\,[u] = \tilde{\mathcal{L}}_{1,s}[u]_1 \oplus \tilde{\mathcal{L}}_{2,s}[u]_2 \oplus \cdots \oplus \tilde{\mathcal{L}}_{l,s}[u]_l.$$

Note that the conditions (3.9) and (3.10) imply that r_0 is real valued in $\Sigma_{C_j}^+$ for $s \in \mathbf{R}$. Thus, taking acount of the indecomposability of C_j we can apply the above Theorem 3.2 to $\tilde{\mathcal{L}}_{j,s}$ and get the following

Lemma 3.3. *For $s \in \mathbf{R}$, $\tilde{\mathcal{L}}_{j,s}$ has a decomposition*

$$\tilde{\mathcal{L}}_{j,s} = \sum_{k=1}^{k_j} \tilde{\lambda}_{j,k,s}\, \tilde{E}_{j,k,s} + \tilde{S}_{j,s},$$

with the following properties:

(i) $$\tilde{\mathcal{L}}_{j,s}\, \tilde{E}_{j,k,s} = \tilde{\lambda}_{j,k,s} \tilde{E}_{j,k,s}.$$

(ii) $$\tilde{\lambda}_{j,1,s} > 0 \quad \textit{and} \quad -\frac{d\,\tilde{\lambda}_{j,1,s}}{ds} > 0.$$

(iii) $$|\tilde{\lambda}_{j,k,s}| = \tilde{\lambda}_{j,1,s} \quad \textit{and} \ \ \tilde{\lambda}_{j,k,s} \neq \tilde{\lambda}_{j,k',s} \ \ \textit{if}\ k \neq k'.$$

(iv) $$\tilde{E}_{j,k,s}\, u(\xi) = \nu_{j,k,s}(u)\, p_{j,k,s}(\xi),$$

$$\textit{where } \nu_{j,k,s} \in \cap_{\theta' > 0} \mathcal{F}_{\theta'}(\Sigma_{C_j}^+)^* \textit{satisfying} \ \ \nu_{j,k,s}(p_{j,k,s}) = 1,$$

(v) $$\tilde{E}_{j,k,s} \tilde{E}_{j,k',s} = \delta_{k,k'} \tilde{E}_{j,k,s}, \quad \tilde{E}_{j,k,s} \tilde{S}_{j,s} = \tilde{S}_{j,s} \tilde{E}_{j,k,s} = 0,$$

(vi) $$\textit{the spectral radius of } \ \tilde{S}_{j,s} < \tilde{\lambda}_{j,k,s}.$$

Hereafter, we shall denote often $\tilde{\lambda}_{j,1,s}$ as $\tilde{\lambda}_{j,s}$. Note that we have for each j

$$\tilde{\lambda}_{j,s} \to \infty \qquad \text{as } s \to -\infty,$$
$$\tilde{\lambda}_{j,s} \to 0 \qquad \text{as } s \to \infty.$$

Thus, by changing the numbering of $\tilde{\lambda}_{j,s}$ if necessary, we may suppose that for some $s_0 \in \mathbf{R}$

$$1 = \tilde{\lambda}_{1,s_0} = \tilde{\lambda}_{2,s_0} = \cdots = \tilde{\lambda}_{h,s_0} > \tilde{\lambda}_{h+1,s_0} \geq \cdots \geq \tilde{\lambda}_{l,s_0}.$$

Then, by using the perturbation theory we have immediately the following

Lemma 3.4. *There are a neighborhood D of s_0 in $\mathbf{C}$ and a constant $\delta > 0$ such that for all $s \in D$ we have a decomposition*

$$\tilde{\mathcal{L}}_s = \sum_{j=1}^{h} \sum_{k=1}^{k_j} \tilde{\lambda}_{j,k,s} \tilde{E}_{j,k,s} + \tilde{S}_s$$

with the following properties:

(i) $$\tilde{E}_{j,k,s} u(\xi) = \nu_{j,k,s}([u]_j)\, p_{j,k,s}(\xi),$$

(ii) $$\tilde{E}_{j,k,s} \tilde{E}_{j',k',s} = \delta_{j,j'} \delta_{k,k'} \tilde{E}_{j,k,s}$$

(iii) $$\tilde{E}_{j,k,s} \tilde{S}_s = \tilde{S}_s \tilde{E}_{j,k,s} = 0,$$

(iv) $$|\tilde{\lambda}_{j,s} - 1| < \delta,$$

(v) $$|\tilde{\lambda}_{j,k,s} - 1| > 2\delta, \quad 1 - \delta < |\tilde{\lambda}_{j,k,s}| < 1 + \delta \quad \textit{for } k \geq 2,$$

(vi) $$\textit{the spectral radius of } \tilde{S}_s < 1 - 2\delta.$$

3.4. On eigenvalues of $\mathcal{L}'_s$.

With the aid of the results of the previous subsection, we shall consider the decomposition of $\mathcal{L}'_s$. First remark that for any positive integer m and for $\xi \in \Sigma(1)$ we have an expression

$$\mathcal{L}'^{m}_s u(\xi) = \sum_{\eta_1, \cdots, \eta_m} \exp\left(S_m r_0(\eta_m, \eta_{m-1}, \cdots, \eta_1, \xi; s)\right) \cdot u(\eta_m, \eta_{m-1}, \cdots, \eta_1, \xi), \tag{3.13}$$

where the summation is taken over all $\eta_1, \eta_2, \cdots, \eta_m$ satisfying $B(\eta_1, \xi_1) = 1$, $B(\eta_2, \eta_2) = 1, \cdots, B(\eta_m, \eta_{m-1}) = 1$.

In the expression of (3.13), by using the fact the $r_0 \in \mathcal{F}_\theta(\Sigma_A^+)$ and the decomposition of $\tilde{\mathcal{L}}_s$ shown the the previous subsection, we have the following

Lemma 3.5. *For each pair j, k in Lemma 3.4, there is a function $w_{j,k,s}(\xi) \in \mathcal{F}_\theta(\Sigma_A^+)$ satisfying*

(3.14)
$$|(\tilde{\lambda}_{j,k,s})^{-m} \sum_{\eta_m,\cdots,\eta_2,l} \exp\big(S_q r_0(\eta_m,\cdots,\eta_2,l,\xi)\big)\, p_{j,k,s}(\eta_q,\cdots,l,\eta^{(l)}) \\ - w_{j,k,s}(\xi)| \le C\gamma_1^m \quad \text{for } m = 1,2,\cdots,$$

and

$$\mathcal{L}'_s\, w_{j,k,s} = \tilde{\lambda}_{j,k,s}\, w_{j,k,s}.$$

Here γ_1 is a constant such that $0 \le \gamma_1 < 1$.

Remark that we have from (3.14) and (iv) of Lemma 3.3

$$w_{j,k,s}(\xi) = p_{j,k,s}(\xi) \quad \text{for all } \ \xi \in \Sigma_C^+,$$

from which it follows that

$$\nu_{j,k,s}([w_{j',k',s}]_j) = \delta_{j,j'}\delta_{k,k'}.$$

Define $E'_{j,k,s}$ by

$$E'_{j,k,s}u(\xi) = \nu_{j,k,s}([u]_j)w_{j,k,s}(\xi).$$

Then, we have

$$E'_{j,k,s}\, E'_{j',k',s} = \delta_{j,j'}\delta_{k,k'}.E'_{j,k,s},$$

and

$$\mathcal{L}'_s\, E'_{j,k,s} = \tilde{\lambda}_{j,k,s}E'_{j,k,s}.$$

In the expression (3.13), by using the decomposition of $\tilde{\mathcal{L}}_s$ and Lemma 3.5, we have the following lemma which is crusial for the proof of Theorem 2.1.

Lemma 3.6. *There exist a neighborhood D_1 of s_0 in $\mathbf{C}$ and a positive constant δ_2 such that we have for all $s \in D_1$*

$$1 - \delta_2/2 \le |\tilde{\lambda}_{j,k,s}| \le 1 + \delta_2/2, \tag{3.15}$$

$$|||\mathcal{L}'^m_s u - \sum_{j=1}^{h}\sum_{k=1}^{k_j} (\tilde{\lambda}_{j,k,s})^m E'_{j,k,s}u(\xi)|||_\theta \le C|||u|||_\theta\,(1-2\delta_2)^m. \tag{3.16}$$

3.5. On the decomposition of $\mathcal{L}'_s$.

By using the same argument as in [Ik3], we have the following two estimates concerning $\mathcal{L}'_{s_0}$ for any $u \in \mathcal{F}_\theta(\Sigma_A^+)$

$$\|{\mathcal{L}'_{s_0}}^m u\|_\infty \leq C_1 \|u\|_\infty,$$
$$|||{\mathcal{L}'_{s_0}}^m u|||_\theta \leq C_2\, \theta^m\, |||u|||_\theta + C_3 \|u\|_\infty.$$

Thus, by applying the theorem of [IM] to the pair of the spaces $C(\Sigma_A^+)$ and $\mathcal{F}_\theta(\Sigma_A^+)$, we have from the above inequalities the following decomposition of $\mathcal{L}'_{s_0}$ in $\mathcal{F}_\theta(\Sigma_A^+)$

$$\mathcal{L}'_{s_0} = \sum_{j=1}^{J} c_j E'_j + S' = E' + S',$$

where

$$\begin{gathered} \mathcal{L}'_{s_0} E'_j = c_j E'_j \quad \text{and} \quad |c_j| = 1 \quad \text{for all } \ j, \\ E'_j\, E'_l = \delta_{jl}\, E'_j \quad \text{for all } \ j, \ l, \\ E'_j\, S' = S'\, E'_j = 0 \quad \text{for all } \ j, \\ \text{the spectral radius of } S' < 1. \end{gathered}$$

With the aid of Lemma 3.5 we can show easily that there is no eigenvalue of E' besides $\tilde{\lambda}_{j,k,s_0}$. Now we have the following proposition from the standard perturbation theory:

Proposition 3.7. *There are $s_0 \in \mathbf{R}$, a neighborhood D_2 of s_0 in $\mathbf{C}$ and a positive constant δ_3 such that, for all $s \in D_2$, $\mathcal{L}'_s$ has a decomposition*

$$\mathcal{L}'_s = \sum_{l=1}^{l_0} F'_{l,s} + S'_s$$

satisfying the following:
(1) $F'_{l,s}\, S'_s = S'_s\, F'_{l,s} = 0$, for all $l = 0, 1, \cdots, l_0$.
(2) $F'_{l,s}\, F'_{k,s} = F'_{k,s}\, F'_{l,s} = 0$ for all $l, k = 0, 1, \cdots, l_0$ such that $l \neq k$.
(3) For $0 \leq l \leq l_0$, the dimension of the range of $F'_{l,s} = i_l$ for all $s \in D_2$ and the eigenvalues of $F'_{l,s}$ are $\mu_{(l,i),s}$ $i = 1, 2, \cdots, i_l$, which satisfy

$$|\mu_{(l,i),s} - \mu_l^0| < \frac{1}{3}\delta_3 \quad |\mu_l^0 - \mu_{l'}^0| > \delta_3 \ (l \neq l').$$

Especially, $\mu_0^0 = 1$, $i_0 = h$ and $\mu_{(0,j),s} = \tilde{\lambda}_{j,s}$ $(j = 1, 2, \cdots, h)$.

(4) *the spectral radius of* $S'_s < 1 - 3\delta_3$.

3.6. Spectrum of $\mathcal{L}_{\varepsilon,s}$.

Suppose that Lemmas 3.6 and Proposition 3.7 hold for the open disk $D_2 = \{s; |s - s_0| < \alpha_0\}$ ($\alpha_0 > 0$). Recall that $\tilde{\lambda}_{j,s}$, $j = 1, 2, \cdots, h$ are analytic in D_2, and satisfies

$$\tilde{\lambda}_{j,s_0} = 1, \qquad -\frac{d}{ds}\tilde{\lambda}_{j,s}\Big|_{s=s_0} > 0.$$

Thus, by exchanging α_0 by a smaller one if necessary, we may assume the following:

$$|\tilde{\lambda}_{s,j} - 1| \le \delta_3/3 \qquad \text{for all } s \in D_2,$$
$$|\tilde{\lambda}_{s,j} - 1| \ge c_1|s - s_0| \quad \text{for all } s \in \{s; |s - s_0| \le \alpha_0\} \quad (c_1 > 0).$$

By the same argument as in [Ik3, Section 3] we have

$$|||\mathcal{L}'_{0,s} - \mathcal{L}_{\varepsilon,s}|||_\theta \to 0 \quad \text{uniformly in } \ s \in D_2 \ \text{ as } \ \varepsilon \to 0.$$

Therefore by applying the standard perturbation theory we have

Lemma 3.8. *There are positive constants* ε_0 *and* δ_4 *such that for all* $0 < \varepsilon \le \varepsilon_0$ *and* $s \in D_2$ *we have the following decomposition of* $\mathcal{L}_{\varepsilon,s}$:

$$\text{(i)} \qquad \mathcal{L}_{\varepsilon,s} = \sum_{l=0}^{l_0} \mathcal{E}_{(l),\varepsilon,s} + \mathcal{S}_{\varepsilon,s}$$

where

$$\text{(ii)} \qquad \mathcal{E}_{(l),\varepsilon,s}\,\mathcal{E}_{(k),\varepsilon,s} = \mathcal{E}_{(k),\varepsilon,s}\,\mathcal{E}_{(l),\varepsilon,s} = 0 \quad \text{if } \ l \ne k,$$

$$\text{(iii)} \qquad \mathcal{E}_{(l),\varepsilon,s}\,\mathcal{S}_{\varepsilon,s} = \mathcal{S}_{\varepsilon,s}\,\mathcal{E}_{(l),\varepsilon,s} = 0,$$

$$\text{(iv)} \qquad \text{the spectral radius of } \mathcal{S}_{\varepsilon,s} < 1 - 2\delta_3,$$
$$\dim \operatorname{Range} \mathcal{E}_{(l),\varepsilon,s} = i_l \quad \text{for all } 0 < \varepsilon < \varepsilon_0,$$

$$\text{(v)} \qquad \sum_{\sigma_A^n \xi = \xi} \exp\big(\operatorname{Re} r_\varepsilon(\xi, s)\big) \le C(1 + \delta_3)^n \quad \text{for all } n.$$

Moreover, denoting the eigenvalues of $\mathcal{E}_{(l),\varepsilon,s}$ *by* $\lambda_{l,i}(\varepsilon, s), i = 0, 1, \cdots, i_l,\ l = 1, 2, \cdots, h$, *we have for all* $0 < \varepsilon \le \varepsilon_0$

$$\text{(vi)} \qquad |\lambda_{l,j}(\varepsilon, s) - \mu_l^0| \le \frac{2}{3}\delta_3 \quad \text{for all } s \in D_2, \quad l = 0, 1, \cdots, l_0,$$

$$\text{(vii)} \qquad |\lambda_{0,j}(\varepsilon, s) - 1| > \delta_4 \quad \text{for all } s \in \{s; |s - s_0| = \alpha_0\}.$$

3.7. Proof of Theorem.

Set

$$f_l(\lambda, s; \varepsilon) = \prod_{i=0}^{i_l} (\lambda - \lambda_{l,i}(\varepsilon, s)).$$

It is easy to check that, for each l, $f_l(\lambda, s; \varepsilon)$ is holomorphic in s. With the aid of Rouché's theorem, we can show easily from (vii) of Lemma 3.8 that for each $0 < \varepsilon \leq \varepsilon_0$, $f_0(1, s; \varepsilon) = 0$ has exactly h zeros in $\{s; |s - s_0| < \alpha_0\}$ $(\alpha_0 > 0)$.

Now we apply Theorem 2 of [Po] or Theorem 4 of [H] to $\mathcal{L}_{\varepsilon,s}$. By exchanging ε_0 by a smaller one if necessary we may assume that

$$\theta(1 + \delta_3) < 1.$$

Then, the application of the theorems of [Po, H] to $\mathcal{L}_{\varepsilon,s}$ assures that

$$Z_\varepsilon(s) \text{ is meromorphic in } \operatorname{Re} s > s_0 + \alpha_0$$

and is of the form

$$Z_\varepsilon(s) = \exp(\phi(s, \varepsilon)) \prod_{l=0}^{l_0} f_l(1, s; \varepsilon)^{-1},$$

where $\phi(\cdot, \varepsilon)$ is holomorphic in $\operatorname{Re} s > s_0 + \alpha_0$. Recall that f_0 has h zeros near s_0. Thus Theorem 3.1 is proved.

4. Application to small balls

Let $\mathcal{O}$ be the obstacle defined by (2.2) satisfying (H.1) and (H.2). Now we explain briefly the relationship between symbolic dynamics and bounded rays in the exterior of $\mathcal{O}$.

Let $A = (A(i,j))_{i,j=1,\cdots,L}$ be the $L \times L$ matrix defined by

$$A(i,j) = \begin{cases} 1, & \text{if } i \neq j \\ 0, & \text{if } i = j, \end{cases}$$

and set

$$\Sigma_A = \{\xi = (\cdots, \xi_{-1}, \xi_0, \xi_1, \cdots) \in \prod_{i=-\infty}^{\infty} \{1, 2, \cdots, L\}; \\ A(\xi_j, \xi_{j+1}) = 1 \text{ for all } j\}.$$

Let $X(s)$ $(s \in \mathbf{R})$ be a representation of an orientated broken ray by the arc length such that $X(0) \in \Gamma$ and $X(s)$ moves in the orientation as s increases. When $\{|X(s)|; s \in \mathbf{R}\}$ is bounded, $X(s)$ repeats reflections on the boundary Γ infinitely many times as s tends to $\pm\infty$. Let the j-th reflection point X_j be on Γ_{l_j}. Then a bounded broken ray defines an infinite sequence $\xi = \{\cdots, l_{-1}, l_0, l_1, \cdots\}$, which is called the reflection order of $X(s)$. Remark that, for a bounded broken ray with direction, there is freedom of such representation, that is, the freedom of the choice of $X(0)$. Therefore the correspondance between bounded broken rays and Σ_A is not one to one. We set

$$f(\xi) = |X_0 X_1|$$

where X_j denote the j-th reflection point of the broken ray corresponding to ξ.

For a real valued function $g(\xi) \in \mathcal{F}_\theta(\Sigma_A)$, we define $\zeta(s)$ by

$$\zeta(s) = \exp\left(\sum_{n=1}^{\infty} \frac{1}{n} \sum_{\sigma_A^n \xi = \xi} \exp S_n(-sf(\xi) + g(\xi) + \pi i)\right).$$

Denote by ν_0 the abscissa of convergence of $F_D(s)$, that is,

$$\nu_0 = \inf\{\nu;\ F_D(s) \text{ converges absolutely for } \mathrm{Re}s > \nu\}$$

If we choose $g(\xi)$ in a suitable way, there is $a_2 > 0$, which is a constant determined by $\mathcal{O}$, such that the singularities of $F_D(s)$ and $-\dfrac{d}{ds} \log \zeta(s)$ are coincide in $\{s; \mathrm{Re}\, s \geq \nu_0 - a_2\}$. The function $g(\xi)$ with the above property is determined uniquely by the geometry of $\mathcal{O}$.

Thus, if we can show the existence of poles of $-\frac{d}{ds}\log\zeta(s)$ in $\{s; \mathrm{Re}\, s \geq \nu_0 - a_2\}$, we get the existence of poles of $F_D(s)$.

Now we turn to considerations on the singularities of $\zeta(s)$ corresponding to $\mathcal{O}_\varepsilon$ of in Theorem 3.2. Remark that (A) in Theorem 2.2 implies (H.2) for $\mathcal{O}_\varepsilon$ when ε is small.

We denote $f(\xi), g(\xi)$ and $\zeta(s)$ attached to $\mathcal{O}_\varepsilon$ by $f_\varepsilon(\xi), g_\varepsilon(\xi)$ and $\zeta_\varepsilon(s)$ respectively. It is easy to see that, by setting $f_0(\xi) = |P_{\xi_0}P_{\xi_1}|$,

$$|\log\varepsilon|\ |||f_\varepsilon - f_0|||_\theta \to 0 \qquad \text{as} \quad \varepsilon \to 0. \tag{4.1}$$

By using the relationship between the curvatures of the wave fronts of incident and reflected waves we have

$$|||g_\varepsilon(\xi) - \left(\log\varepsilon + \frac{1}{2}\log\frac{1}{4}(\cos\frac{\Theta(\xi)}{2})\right)|||_\theta \to 0 \qquad \text{as} \quad \varepsilon \to 0,$$

where $\Theta(\xi) = \angle P_{\xi_{-1}}P_{\xi_0}P_{\xi_1}$. Then, by setting $\tilde{g}_\varepsilon(\xi) = g_\varepsilon(\xi) - \log\varepsilon$ and $\tilde{g}_0(\xi) = \frac{1}{2}\log\frac{1}{4}(\cos\frac{\Theta(\xi)}{2})$ we have

$$|||\tilde{g}_\varepsilon - \tilde{g}_0|||_\theta \to 0 \qquad \text{as} \quad \varepsilon \to 0. \tag{4.2}$$

Set

$$d_{\max} = \max_{i \neq j}|P_iP_j|$$

and

$$B(i,j) = \begin{cases} 1 & \text{if } |P_iP_j| = d_{\max}, \\ 0 & \text{if } |P_iP_j| < d_{\max}. \end{cases}$$

By changing the numbering of the points if necessary, we may suppose that

$$\begin{aligned} B(i,j) &= 0 \qquad \text{for all } j \quad \text{if } \ i \geq K+1, \\ B(i,j) &= 1 \qquad \text{for some } j \quad \text{if } \ i \leq K, \end{aligned}$$

holds for some $2 \leq K \leq L$.

Define $k(\xi)$ by

$$k(\xi) = 1 - f_0(\xi)/d_{\max}.$$

By putting $s' = s - (\log\varepsilon + \sqrt{-1}\,\pi)/d_{\max}$ we have

$$-sf_\varepsilon + g_\varepsilon + \sqrt{-1}\,\pi = -s'f_\varepsilon + h_\varepsilon + k\log\varepsilon,$$

where

$$h_\varepsilon = \tilde{g}_\varepsilon + \sqrt{-1}\,\pi\, k + (\log\varepsilon + \sqrt{-1}\,\pi)\frac{(f_0 - f_\varepsilon)}{d_{\max}}.$$

By tending ε to the zero, it follows that

$$h_0 = \tilde{g}_0 + \sqrt{-1}\,\pi\, k,$$

hence we have

$$h_0(\xi) = \tilde{g}_0(\xi) \quad \text{for } \xi \text{ satisfying } B(\xi_0, \xi_1) = 1.$$

Thus $f_\varepsilon, h_\varepsilon, k$ satisfy the conditions required in Theorem 2.1.

Let $Z_\varepsilon(s)$ be the zeta function defined by using these $f_\varepsilon, h_\varepsilon, k$. Note that we have the relation

$$\zeta_\varepsilon(s) = Z_\varepsilon(s - (\log\,\varepsilon + \sqrt{-1}\,\pi)/d_{\max}).$$

On the other hand, Theorem 3.1 says that there exists $\varepsilon_0 > 0, s_0 \in \mathbf{R}$ and D_0 such that $Z_\varepsilon(s)$ has a pole in D_0, which implies that $\zeta_\varepsilon(s)$ is meromorphic in $D_\varepsilon = \{s = z + (\log\,\varepsilon + \sqrt{-1}\,\pi)/d_{\max}; z \in D_0\}$ and has a pole near $s_0 + (\log\,\varepsilon + \sqrt{-1}\,\pi)/d_{\max}$. It is evident that this pole of $\zeta_\varepsilon(s)$ stays in the domain where the singularities of $\zeta_\varepsilon(s)$ and $F_{D,\varepsilon}(s)$ coincide. Thus the existence of singularities of $F_{D,\varepsilon}(s)$ is proved.

References

[AS] T.Adachi and T.Sunada *Twisted Perron-Frobenius theorem and L-functions.* J.Funct.Anal. vol 71 (1987) pages 1-46

BGR] C.Bardos, J.C.Guillot and J.Ralston *La relation de Poisson pour l'équa- -tion des ondes dans un ouvert non borné. Application à la théorie de la diffusion.* Comm.Partial Diff. Equ. vol 7 (1982) pages 905-958

[G] C.Gérard *Asymptotique des poles de la matrice de scattering pour deux obstacles strictement convexes.* Bull.S.M.F. vol Tome 116 Mémoire n° 31 (1989)

[H] N.Hadyn *Meromorphic extension of the zeta function for Axiom A flows* . Ergod.Th.& Dynam.Sys. vol 10 (1990) pages 347-360

[Ik1] M.Ikawa *Trapping obstacles with a sequence of poles of the scattering matrix converging to the real axis.* Osaka J.Math. vol 22 (1985) pages 657-689

[Ik2] M.Ikawa *Singular perturbation of symbolic flows and poles of the zeta functions.* Osaka J.Math vol 27 (1990) pages 281-300

[Ik3] M.Ikawa *On the distribution of poles of the scattering matrix for several convex bodies* . Proceeding of Conference Held in Honor of Prof.T.Kato, "Functional Analytic Methods for Partial Differential Equations" LNM 1450, Springer-Verlag, (1990) pages 210-225

[Ik4] M.Ikawa *On scattering by obstacles.* to appear in Proceeding of ICM-90

Ik5] M.Ikawa *Singular perturbation of symbolic flows and poles of the zeta functions. Addendum.* to appear in Osaka J. Math

[IM] C.T.Ionescu Turcia and C.Marinescu *Théorie ergodique pour des classes d'opérateurs non complètement continus.* Ann.Math.vol 52 (1950) pages 140-147

[K] T.Kato *Perturbation theory of linear operators.* Springer-Verlag Berlin (1976)

[LP] P.D.Lax and R.S.Phillips *Scattering Theory, Revised Edition.* Academic Press, New York (1989)

[P] W.Parry *Bowen's equidistribution theory and the Dirichlet density theorem.* Ergod.Th.& Dynam.Sys. vol 4(1984) pages 117-134

[Po] M.Pollicott *Meromorphic extensions of generalized zeta functions.* Invent.Math. vol 85 (1986) pages 147-164

[S] H.Soga *The behavior of oscillatory integrals with degenerate stationary points.* Tsukuba J.Math. vol 11 (1987) pages 93-100

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Large atoms in large magnetic fields

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LARGE ATOMS IN LARGE MAGNETIC FIELDS

ELLIOTT H. LIEB

I. INTRODUCTION.

In this talk I shall discuss the effect on matter, specifically atoms, of a very strong magnetic field. This turns out to be an interesting exercise in semiclassical analysis. Results obtained in collaboration with J.P. Solovej and J. Yngvason will be summarized and details will appear elsewhere [LSY I, II, III]. The motivation for studying extremely strong magnetic fields of the order of 10^{12} Gauss is that they are supposed to exist on the surface of neutron stars (cf. [FGP]). The heuristic argument usually given to explain these strong fields is that in the collapse, resulting in the neutron star, the magnetic field lines follow the collapse and thus become very dense.

The structure of matter in strong magnetic fields is thus a question of considerable interest in astrophysics.

II. THE PAULI HAMILTONIAN.

To give the quantum mechanical energy of a charged spin-$\frac{1}{2}$ particle in a magnetic field $\mathbf{B}$, we have to make a choice of vector potential $\mathbf{A}(x)$, $x \in \mathbb{R}^3$ satisfying $\mathbf{B} = \nabla \times \mathbf{A}$.

The energy is then given by the Pauli Hamiltonian

$$H_{\mathbf{A}} = \big((\mathbf{p} - \mathbf{A}(x)) \cdot \boldsymbol{\sigma}\big)^2 . \tag{2.1}$$

Here $\mathbf{p} = -i\nabla$ and $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$, where

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} , \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} , \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

are the Pauli matrices. The Pauli Hamiltonian acts in the space $L^2(\mathbb{R}^3; \mathbb{C}^2)$. We can also write $H_{\mathbf{A}} = (\mathbf{p} - \mathbf{A})^2 - \mathbf{B} \cdot \boldsymbol{\sigma}$. In the case $\mathbf{A} = 0$ we get as usual $H_0 = \mathbf{p}^2 = -\Delta$. We shall here concentrate on the case where $\mathbf{B}$ is constant, say $\mathbf{B} = (0, 0, B)$, with $B \geq 0$. We choose $\mathbf{A} = \frac{1}{2}\mathbf{B} \times x$. In this case the spectrum of $H_{\mathbf{A}}$ is described by the socalled Landau bands $\varepsilon_{p\nu} = 2B\nu + p^2$, where p is the momentum along the field and $\nu = 0, \dots$ is the index of the band. The higher bands $\nu = 1, \dots$ are twice as degenerate as the lowest band $\nu = 0$.

As usual in the study of fermionic energies we shall be interested in the sum of the negative eigenvalues of operators of the form $H = H_{\mathbf{A}} - V(x)$, where $V(\geq 0$ for simplicity) is an external potential. In this connection there is an important difference between $H_{\mathbf{A}}$ and the operator $(\mathbf{p} - \mathbf{A})^2$ which has no spin dependence. While the spectrum for $(\mathbf{p} - \mathbf{A})^2$ is (B, ∞) the spectrum for $H_{\mathbf{A}}$ is $(0, \infty)$.

Indeed, one can estimate the sum of the negative eigenvalues of H by $L \int V(x)^{5/2} \, dx$, according to the standard Lieb-Thirring inequality (with a magnetic field the proof of this inequality given in [LT] is still correct if one appeals to the diamagnetic inequality, i.e., that the heat kernel with a magnetic field is pointwise bounded in absolute value by the heat kernel without a magnetic field.) However, in the case of $H_{\mathbf{A}} - V$ the question is somewhat more subtle. In fact, if $V \in L^{3/2}(\mathbb{R}^3)$ the operator $(\mathbf{p} - \mathbf{A})^2 - V$ has a finite number of negative eigenvalues, while the operator $H_{\mathbf{A}} - V$ can have infinitely many negative eigenvalues (compare [I]). We can, however, prove [LSY I,III]

THEOREM 1. *There exist universal constants $L_1, L_2 > 0$ such that if we let $e_j(B, V)$, $j = 1, 2, \dots$ denote the negative eigenvalues of $H_{\mathbf{A}} - V$ with $0 \leq V \in L^{3/2}(\mathbb{R}^3) \cap L^{5/2}(\mathbb{R}^3)$ then*

$$\sum_j |e_j(B, V)| \leq L_1 B \int V(x)^{3/2} \, dx + L_2 \int V(x)^{5/2} \, dx \, . \tag{2.2}$$

We can choose L_1 as close to $2/3\pi$ as we please, compensating with L_2 large.

The first term on the right side is a contribution from the lowest band $\nu = 0$. For large B this is the leading term.

We now ask the question of a semiclassical analog of (2.2). Thus consider the operator

$$\left[(h\mathbf{p} - b\mathbf{a}(x)) \cdot \boldsymbol{\sigma}\right]^2 - v(x) , \tag{2.3}$$

where $\mathbf{a}(x) = \frac{1}{2}\hat{z} \times x$, $\hat{z} = (0,0,1)$ and $0 \leq v$.

If one computes the leading term in h^{-1} of the sum of the negative eigenvalues of (2.3) for fixed b one finds as in [HR] that there is no b dependence. In our case, however, we shall not assume b fixed, or more precisely not assume that b is small compared with h^{-1}. The reason for this is that in the application to neutron stars it is not true, as we shall discuss below that $b \ll h^{-1}$.

The interesting fact is, however, that we can prove ([LSY III]) a semiclassical formula for the sum of the negative eigenvalues of the operator (2.3), which holds uniformly in b (even for large b).

THEOREM 2. *Let $e_j(h,b,v)$, $j = 1,2,\ldots$, denote the negative eigenvalues of the operator (2.3), with $0 \leq v \in L^{3/2}(\mathbb{R}^3) \cap L^{5/2}(\mathbb{R}^3)$. Then*

$$\lim_{h\to 0}\Big(\sum_j |e_j(h,b,v)|/E_{\mathrm{scl}}(h,b,v)\Big) = 1,$$

uniformly in b, where

$$E_{\mathrm{scl}}(h,b,v) = \frac{1}{3\pi^2}h^{-2}b\int\Big(v(x)^{3/2} + 2\sum_{\nu=1}^{\infty}[v(x) - 2\nu bh]_+^{3/2}\Big)\,dx\,. \tag{2.4}$$

Here $[t]_+ = t$ if $t > 0$, zero otherwise.

The formula (2.4) was already implicitly noted in [Y].

For $bh \ll 1$, the right side of (2.4) reduces to the standard semiclassical formula from [HR],

$$\frac{2}{15\pi^2}h^{-3}\int v(x)^{5/2}\,dx\,.$$

(Recall that we are counting the spin which accounts for the 2 in front of the sum in (2.4).) For $bh \gg 1$, the sum in (2.4) is negligible, and we are left with the first term.

Formula (2.4) (with h replaced by 1) can be compared with the Lieb-Thirring inequality (2.2), which holds even outside the semiclassical regime. The two terms in (2.2) correspond to respectively the $b \to \infty$ (first term) and $b \to 0$ (last term) asymptotics of (2.4). A natural question, which is similar to the Lieb-Thirring conjecture, is whether the semiclassical constant $1/3\pi^2$ is the optimal value for L_1 in (2.2) rather than as proved $2/3\pi$.

III. THE ATOMIC HAMILTONIAN.

The Hamiltonian describing an atom with N electrons and nuclear charge Z in a constant magnetic field $\mathbf{B} = (0, 0, B)$ is

$$H_N = \sum_{i=1}^{N} \left(H_{\mathbf{A}}^{(i)} - Z|x_i|^{-1} \right) + \sum_{1 \le i < j \le N} |x_i - x_j|^{-1} , \tag{3.1}$$

acting in $\mathcal{H} = \overset{N}{\wedge} L^2(\mathbb{R}^3; \mathbb{C}^2)$. We shall here give a short sketch of what we call the Thomas-Fermi theory for (3.1). The goal of this theory is to approximate the ground state energy

$$E(N, B, Z) = \inf \mathrm{spec}_{\mathcal{H}} H(N) . \tag{3.2}$$

Furthermore, in the case where $H(N)$ has a (normalized) ground state $\psi \in \mathcal{H}$, i.e., $H(N)\psi = E(N, B, Z)\psi$, we also want to estimate the density

$$\rho_\psi(x) = N \int \|\psi(x, x_2, \ldots, x_N)\|^2_{\wedge \mathbb{C}^2} dx_2 \ldots dx_N . \tag{3.3}$$

The first step in studying (3.1) is to replace the repulsive two-body term, $\sum_{i<j} |x_i - x_j|^{-1}$, by a socalled self-consistent mean field potential of the form $\sum_i \rho * |x_i|^{-1}$. (This replacement is as in standard Thomas-Fermi theory (see [L]) and shall not be discussed here.) The question is how to find the appropriate self-consistent density ρ. It must of course be an approximation to ρ_ψ.

It should be noted that as we replace the two-body potential by a self-consistent one-body potential we must also subtract a term

$$\frac{1}{2} \int \rho(x) |x - y|^{-1} \rho(y) \, dx dy$$

from the Hamiltonian. With this term our new Hamiltonian is

$$\sum_{i=1}^{N}(H_{\mathbf{A}}^{(i)} - V(x_i)) - \frac{1}{2}\int \rho(x)|x-y|^{-1}\rho(y)\,dxdy\ , \tag{3.4}$$

with $V(x) = Z|x|^{-1} - \rho * |x|^{-1}$. The ground state energy of the operator in (3.4) (without the extra term) is the sum of the N first negative eigenvalues of $H_{\mathbf{A}} - V$.

We assume now that V is such that we can estimate the sum of the negative eigenvalues by the semiclassical formula (2.4). We of course have to verify this assumption. Since we will not know the density ρ until the end of the calculation, this verification will have to rely on knowledge of general properties of ρ. This kind of reasoning is typical for self-consistent mean field theories like Thomas-Fermi theory (see [L]).

In Thomas-Fermi theory there is a standard way ([L]) of approximating the expectation value of the kinetic energy operator $\sum_{i=1}^{N} H_{\mathbf{A}}^{(i)}$ by a functional of ρ using semiclassical formulas like (2.4). In our case we replace $\sum_{i=1}^{N} H_{\mathbf{A}}^{(i)}$ by $\int \tau_B(\rho(x))\,dx$, where τ_B is the Legendre transform of the convex function

$$V \mapsto \frac{1}{3\pi^2}B\Big(V^{3/2} + 2\sum_{\nu=1}^{\infty}[V - 2\nu B]_+^{3/2}\Big) \tag{3.5}$$

which is derived from (2.4) (without h). Here we point out that τ_B is convex (by definition) and $\tau_B(t) \sim \dfrac{t^3}{B^2}$ for small t ($t \lesssim B^{3/2}$), $\tau_B(t) \sim t^{5/3}$ for large t ($t \gg B^{3/2}$).

The ground state energy of (3.4) should then be well approximated by

$$\begin{aligned}\mathcal{E}_{MTF}(\rho) &= \int \tau_B(\rho) - \int V(x)\rho(x)\,dx - \frac{1}{2}\int \rho(x)|x-y|^{-1}\rho(y)\,dxdy \\ &= \int \tau_B(\rho) - \int Z|x|^{-1}\rho(x)\,dx + \frac{1}{2}\int \rho(x)|x-y|^{-1}\rho(y)\,dxdy\ .\end{aligned} \tag{3.6}$$

We call this functional the **Magnetic Thomas-Fermi Functional.** It is studied in detail in [LSY III]. The paper [TY] (see also [FGP]) is probably the earliest reference that uses a Thomas-Fermi theory that takes *all* Landau levels into account. This theory was also studied in [FGPY] and put on a rigorous basis in [Y] for the regime $B \sim Z^{4/3}$. We now choose our density ρ to be the unique minimizer for $\mathcal{E}_{\rm MTF}$ constrained to the set $\int \rho \leq N$. We denote

$$E_{\rm MTF}(N,B,Z) = \inf\{\mathcal{E}_{\rm MTF})(\rho) \mid \int \rho \leq N\} .$$

Knowing ρ we can now prove that $E_{\rm MTF}(N,B,Z)$ is really a semiclassical approximation to the true ground state energy for (3.4). To do this one should first realize that it follows from the study of $\mathcal{E}_{\rm MTF}$ with our choice of ρ that the potential $V(x) = Z|x|^{-1} - \rho * |x|^{-1}$ will have the following behavior in Z and B

$$\begin{aligned} V(x) &= Z^{4/3}v(Z^{1/3}x) \ \text{ if } \ B \leq Z^{4/3} \\ V(x) &= Z^{4/5}B^{2/5}v(Z^{-1/5}B^{2/5}x) \ \text{ if } \ B \geq Z^{4/3} , \end{aligned} \tag{3.7}$$

where v is a function which does not depend significantly on B and Z.

Concentrating on the case $B \geq Z^{4/3}$ we see by a simple rescaling that the Hamiltonian $H_{\mathbf{A}} - V(x)$ from (3.4) is unitarily equivalent to the operator

$$Z^{4/5}B^{2/5}\left[\left((h\mathbf{p} - b\mathbf{a}(x))\cdot\boldsymbol{\sigma}\right)^2 - v(x)\right] , \tag{3.8}$$

where

$$h = \left(B/Z^3\right)^{1/5} \ \text{ and } \ b = \left(B^2/Z\right)^{1/5} . \tag{3.9}$$

In the case when $B \leq Z^{4/3}$ we get $Z^{4/3}$ in front of [ ] in (3.8) and

$$h = Z^{-1/3} \ \text{ and } \ b = B/Z . \tag{3.10}$$

When h is small we can study (3.8) by semiclassical methods. Indeed, using (2.4) we can now prove that if Z is sufficiently large and B/Z^3 sufficiently small, $E_{\rm MTF}$ approximates the true ground state energy (3.2) as well as we please.

THEOREM 3. *Let N/Z be fixed and suppose that $B/Z^3 \to 0$ as $Z \to \infty$. Then*

$$E(N,B,Z)/E_{MTF}(N,B,Z) \to 1 \ \text{ as } Z \to \infty . \tag{3.11}$$

Furthermore, if $N/Z \leq 1$, then $H(N)$ has a ground state ψ. The corresponding density ρ_ψ, defined by equation (3.3), is well approximated by the unique minimizer ρ for $\mathcal{E}_{MTF}$ in the following sense. If $\chi \in C_0^\infty(\mathbb{R}^3)$ then

$$Z^{-1} \int \Big(\rho_\psi(x) - \rho(x)\Big)\chi\big((Z^{1/3} + Z^{-1/5}B^{2/5})x\big)dx \to 0 \,. \tag{3.12}$$

(The above scaling of χ should be compared to equation (3.7).) We emphasize that from the uniqueness the minimizer ρ is spherically symmetric.

Notice that from equations (3.9) and (3.10), $hb = 1$ if $B = Z^{4/3}$, which when compared to equation (2.4) explains why the behavior in (3.7) changes at this point. Indeed, when $B \gg Z^{4/3}$ all electrons are in a certain sense confined to the lowest Landau band. This result which is given in the next theorem is completely independent of the semiclassical analysis.

THEOREM 4. *If Π_0^N is the projection in $\mathcal{H} = \bigwedge^N L^2(\mathbb{R}^3;\mathbb{C}^2)$ onto the subspace where all electrons are in the lowest Landau band we define the* **confined energy**

$$E_0(N, B, Z) = \inf \operatorname{spec}_{\mathcal{H}} \Pi_0^N H(N) \Pi_0^N \,. \tag{3.13}$$

Then if $N < \lambda Z$ for some fixed $\lambda > 0$ we get

$$E_0(N, B, Z)/E(N, B, Z) \to 1 \quad \text{if} \quad Z^{4/3}/B \to 0 \,. \tag{3.14}$$

The preceeding analysis gives the following different regimes in B and Z.

1) *$B \ll Z^{4/3}$, Z large (i.e., $hb \ll 1$, h small)*:

The effect of the magnetic field is negligible. We get standard Thomas-Fermi theory with $\tau_B(\rho) \sim \rho^{5/3}$.

2) *$B \sim Z^{4/3}$, Z large (i.e., $hb \sim 1$, h small)*:

The magnetic field becomes important. The function τ_B is complicated because we have a finite number of terms in (3.5). The density is still almost spherical and stable atoms are almost neutral (see [Y]).

3) $Z^{4/3} \ll B \ll Z^3$, *Z large (i.e., $hb \gg 1$, h small).*

The magnetic field is increasingly important. Most electrons will be confined to the lowest Landau band. The function τ_B is simple since there is only one term in (3.5), $\tau_B(\rho) \sim \rho^3/B^2$. The density is almost spherical and stable atoms are almost neutral. Furthermore, the atom is getting smaller. The atomic radius behaves like $Z^{1/5}B^{-2/5}$ (compare (3.7) and (3.12)).

4) $B \sim Z^3$ *(i.e., $h \sim 1$).*

In this regime one can no longer use semiclassics. The functional $\mathcal{E}_{\mathrm{MTF}}$ from (3.6) is not a good approximation to the energy. When this talk was given we had no description of this region, but now we do in terms of a density *matrix* functional. See [LSY I, II].

5) $B \gg Z^3$.

When $B \gg Z^3$ and Z is large we can find a new functional of ρ very different from $\mathcal{E}_{\mathrm{MTF}}$ which approximates the energy. We shall discuss this in the following section. In this super strong case it turns out that the atom becomes very cylindrical in shape.

We end this section by a short discussion of which regime is relevant in the case of neutron stars. Since the natural unit of magnetic field is $(2m)^2e^3c/\hbar^3 = 9.4 \times 10^9$ Gauss. we get in our units where all relevant physical constants have been suppressed that the magnetic field on the surface of a neutron star is in order of magnitude $B \sim 10^2$. Thus for, say, iron with $Z = 26$ we have $bh = (B/Z^{4/3})^{3/5} \sim 1$. To make a quantitative evaluation we would of course have to really estimate error terms in the analysis. Qualitatively, however, (all relevant constants are of order 1) it seems unreasonable to assume $bh \ll 1$ in this case. Thus the magnetic field might have a significant effect.

IV. THE SUPER-STRONG CASE $B \gg Z^3$.

We shall here present the correct energy functional of the density when $B \gg Z^3$, and very briefly indicate what is involved in proving the correctness of the approximation. Note: When this talk was given the super-strong functional was the only description we had of region 5. Since then we were able to simplify this functional even further to the *hyper-strong* functional. See [LSY I, II].

The correct functional is now

$$\mathcal{E}_{SS}(\rho) = \int \left(\frac{\partial}{\partial x_3} \sqrt{\rho} \right)^2 - \int \frac{Z}{|x|} \rho(x) + \frac{1}{2} \int \rho(x) |x-y|^{-1} \rho(y) \, dx \, dy \, , \quad (4.1)$$

with the condition that

$$\int \rho(x) dx_3 \leq \frac{B}{2\pi} \quad \text{for all} \quad (x_1, x_2) \, . \qquad (4.2)$$

The claim is that

$$E_{SS}(N) = \inf\{\mathcal{E}_{SS}(\rho) \mid \int \rho \leq N \, , \; \rho \; \text{ satisfies (4.2)}\} \qquad (4.3)$$

is a good approximation to the energy in a certain regime of B and Z with $B \gg Z^3$.

In understanding this the first step is to recall that from Theorem 4 all electrons are confined to the lowest Landau band. In the lowest band the degeneracy is such that we have $B/2\pi$ states per area perpendicular to the field $\mathbf{B}$. Thus given any infinite cylinder parallel to the field and of base area $2\pi/B$. If there is more than one electron in such a cylinder, they will have to occupy orthogonal states in the parallel direction, but this one can prove costs too much energy if $B \gg Z^3$. This shows that (4.2) must hold. The functional (4.1) now follows because in each infinite cylinder with only one electron, the electron can be treated as a boson, i.e., we can neglect the exclusion principle and that is why $\mathcal{E}_{SS}$ is reminiscent of (bosonic) Hartree theory. (For details see [LSY I, II]).

References

[FGP] Fushiki, I., Gudmundsson, E.H. and Pethick, C.J.: Surface structure of neutron stars with high magnetic fields, Astrophys. Jour., vol 342;pages 958–975 (1989)

[FGPY] Fushiki, I., Gudmundsson, E.H., Pethick, C.J. and Yngvason, J.: Matter in a magnetic field in the Thomas-Fermi and related theories. Annals of Physics, vol 216; pages 29–72 (1992)

[HR] Helffer, B. and Robert, D.:Calcul fonctionel par la transformeé de Mellin et operateurs admissibles; Jour. Func. Anal., vol 53 pages246–268 (1983)

[I] Ivrii, V.: In preparation.

[L] Lieb, E. H.:Thomas-Fermi and related theories of atoms and molecules Rev. Mod. Phys., vol 53, 603-642 (1981). Errata, vol 54; page 311 (1982)

[LSY I] Lieb, E. H., Solovej, J. P. and Yngvason, J.:Heavy atoms in the strong magnetic field of a neutron star. Phys. Rev. Letters, vol 69; pages 749–752 (1992)

[LSY II] Lieb, E. H., Solovej, J. P. and Yngvason, J.:Asymptotics of heavy atoms in high magnetic fields: I. Lowest Landau band regions. Commun. Pure Appl. Math., McKean issue, (in press)

[LSY III] Lieb, E. H., Solovej, J. P. and Yngvason, J.:Asymptotics of heavy atoms in high magnetic fields: II. Semiclassical regions (in preparation)

[LT] Lieb, E. H. and Thirring, W. E.:A bound for the moments of the eigenvalues of the Schrödinger Hamiltonian and their relation to Sobolev inequalities, in Studies in Mathematical Physics: Essays in Honor of Valentine Bargmann
-E. H. Lieb, B. Simon and A. S. Wightman, Princeton Press (1976)

[TY] Tomishima, Y. and Yonei, K.:Thomas-Fermi theory for atoms in strong magnetic field. Progr. Theor. Phys. vol 59 pages 683–696 (1978)

[Y] Yngvason, J.:Thomas-Fermi theory for matter in a magnetic field as a limit of quantum mechanics. Lett. Math. Phys., vol 22 pages107–117 (1991)

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Resolvent Estimates and Time-Decay in the Semiclassical Limit

SHU NAKAMURA

1. Introduction.

In this note we study the Schrödinger operator :

$$H = -(\hbar^2/2)\Delta + V(x), \qquad \text{on} \quad L^2(\mathbf{R}^d), \quad \hbar > 0$$

in the semiclassical limit: $\hbar \to 0$. In particular, we are interested in the scattering theory and long time behaviors of the time evolution: $e^{-itH/\hbar}\varphi$. Boundary value of the resolvent: $\lim_{\varepsilon \to +0} (H - \lambda \pm i\varepsilon)^{-1} = (H - \lambda \pm i0)^{-1}$ plays essential roles in the scattering theory, and various observable quantities, e.g., scattering amplitude, time-delay, etc., are represented by it ([RS]). In studying the boundary value of the resolvent, the theory of Mourre is quite powerful and has been applied to many problems (e.g., [M], [PSS], [CFKS]). Jensen, Mourre and Perry extended the theory using multiple commutators, and proved the existence of boundary values of *powers* of the resolvent ([JMP]). Using the result they also obtained time-decay results (see also [J1]).

In a series of papers [RT1]–[RT4], Robert and Tamura systematically studied the semiclassical limit of the scattering process for nontrapping energies. In their arguments, an estimate of the form:

$$\left\| \langle x \rangle^{-\alpha} (H - \lambda \pm i0)^{-1} \langle x \rangle^{-\alpha} \right\| \leq C_\alpha \hbar^{-1}, \qquad \hbar > 0, \alpha > 1/2,$$

which is called *semiclassical resolvent estimate*, plays a crucial role. Here we have used the standard notation: $\langle x \rangle = \left(1 + |x|^2\right)^{1/2}$. They proved it using a parametrix for the time evolution. The proof was simplified and generalized by several authors with the aid of the Mourre theory ([GM], [HN], [G], [W2], etc.). Moreover, Wang proved semiclassical estimates for powers of the resolvent ([W1], [W2]):

$$\left\| \langle x \rangle^{-\alpha} (H - \lambda \pm i0)^{-n} \langle x \rangle^{-\alpha} \right\| \leq C_\alpha \hbar^{-n}, \qquad \hbar > 0, \alpha > n - 1/2.$$

We also want to mention works on semiclassical resolvent estimates for high energies ([Y], [J2]).

On the other hand, motivated by works on the barrier top resonances ([BCD], [S]), the author generalized the semiclassical resolvent estimate to the simplest trapping energy, namely the barrier top energy ([N1]). In this case, the estimate has the form:

$$\left\| \langle x\rangle^{-\alpha} (H-\lambda \pm i0)^{-1} \langle x\rangle^{-\alpha} \right\| \le C_\alpha \hbar^{-2}, \qquad \hbar>0, \alpha>1/2,$$

where λ is the barrier top energy.

The aim of this note is to construct a semiclassical analogue of the multiple commutator method of Jensen, Mourre and Perry, and apply it to the barrier top energy and nontrapping energies. We note that for the nontrapping energy case, this was done by Wang ([W2]). Roughly speaking, our abstract result is as follows: Let A and H be a pair of self-adjoint operators satisfying certain regularity conditions (cf. (H1)–(H4) in Section 2). If, in addition, they satisfy

$$E_\Delta(H)[H, iA]E_\Delta(H) \ge c\hbar^\beta E_\Delta(H), \qquad \hbar > 0,$$

for some $1 \le \beta \le 2$, where Δ is a neighborhood of an energy E, then we can show

$$\left\| \langle A\rangle^{-\alpha} (H-E \pm i0)^{-n} \langle A\rangle^{-\alpha} \right\| \le C_\alpha \hbar^{-n\beta}, \qquad \hbar>0, \alpha>n-1/2.$$

$\beta = 1$ corresponds to the nontrapping case, and $\beta = 2$ to the barrier top case. We don't know any concrete examples with $1 < \beta < 2$. Even though the restriction $\beta \le 2$ doesn't seem crucial, our proof dosn't work for the case $\beta > 2$. Time-decay results in the semiclassical limit follow from the above result (Theorem 3). In particular, it follows that if $f \in C_0^\infty(\mathbf{R})$ is supported in a small neighborhood of the barrier top energy, then

$$\left\| \langle x\rangle^{-s} e^{-itH} f(H) \langle x\rangle^{-s} \right\| \le C\hbar^{-s} \langle t\rangle^{-s'}, \qquad t \in \mathbf{R},$$

for $s > s' > 0$.

This note is organized as follows: In Section 2 we state the abstract results, and it is proved in Section 4. Applications to Schrödinger operators are discussed in Section 3.

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2. Abstract Results.

Let H and A be $\hbar$-dependent self-adjoint operators on a Hilbert space $\mathcal{H}$ ($\hbar \in (0,\infty)$). We first suppose

(H1) $D(A) \cap D(H)$ is dense in $D(H)$ with respect to the graph norm.

Let $B_0 = H$. We wish to define B_j inductively by

$$B_j = [B_{j-1}, iA], \qquad j = 1, 2, \cdots,$$

at least formally. In order that we suppose

(H2) $B_1 = [H, iA]$, defined as a form on $D(H) \cap D(A)$, is extended to a bounded operator from $D(H)$ to $\mathcal{H}$. Inductively, $B_{j+1} = [B_j, iA]$, defined as a form on $D(H) \cap D(A)$, is extended to a bounded operator from $D(H)$ to $\mathcal{H}$ for any $j \geq 1$.

In this sense, H is C^∞-smooth with respect to A. We suppose the following $\hbar$-dependence of these commutators:

(H3) For each $j \geq 1$ there is $C_j > 0$ such that

$$\left\| B_j(H+i)^{-1} \right\| \leq C_j \hbar^j, \qquad \hbar > 0.$$

(H4) There is $C > 0$ such that

$$\left\| (H+i)^{-1}[H,[H,iA]](H+i)^{-1} \right\| \leq C\hbar^2, \qquad \hbar > 0.$$

In applications, (H1)–(H4) follow easily from the symbol calculus. See Section 3.

Now let us fix an energy $E_0 \in \mathbf{R}$. The next inequality, a semiclassical variation of the Mourre estimate, is essential. Let $\beta \geq 1$.

(H5:β) There is an interval $\Delta \ni E_0$ and $C > 0$ such that

$$E_\Delta(H)[H, iA]E_\Delta(H) \geq C\hbar^\beta E_\Delta(H), \qquad \hbar > 0,$$

where $E_\Delta(H)$ is the spectral projection of H and Δ.

We prove the next theorem in Section 4.

THEOREM 1. *Suppose (H1)–(H5:β) with $1 \leq \beta \leq 2$. Then there is an interval $\Delta \ni E_0$ satisfying the following: Let $n \geq 1$ an integer, and let $s > n - 1/2$, then for any $\lambda \in \Delta$,*

$$\lim_{\delta \to +0} \langle A \rangle^{-s} (H - \lambda \pm i\delta)^{-n} \langle A \rangle^{-s} \equiv \langle A \rangle^{-s} (H - \lambda \pm i0)^{-n} \langle A \rangle^{-s}$$

exists and satisfies

$$\left\| \langle A \rangle^{-s} (H - \lambda \pm i0)^{-n} \langle A \rangle^{-s} \right\| \leq C\hbar^{-n\beta}, \qquad \hbar > 0, \lambda \in \Delta. \tag{1}$$

REMARK: Condition (H4) is missing in Lemma 2.3 of [N2], but we need it even for $n = 1$ if $\beta > 1$. On the other hand, it is not necessary if $\beta = 1$ (cf. Proof of Lemma 6).

The next result on time-decay is a direct consequence of Theorem 1.

THEOREM 2. *Suppose (H1)–(H5:β) with $1 \leq \beta \leq 2$. Then there is an interval $\Delta \ni E_0$ such that for any $f \in C_0^\infty(\Delta)$ and for any constants $s > s' > 0$, $s'' > s'(\beta - 1)$,*

$$\left\| \langle A \rangle^{-s} e^{-itH/\hbar} f(H) \langle A \rangle^{-s} \right\| \leq C\hbar^{-s''} \langle t \rangle^{-s'}, \qquad \hbar > 0, t \in \mathbf{R}. \tag{2}$$

PROOF: We follow the argument of Theorem 4.2 in [JMP]. Since

$$\begin{aligned} \left(\frac{d}{d\lambda}\right)^j E'_\lambda(H) &= \frac{1}{2\pi i}\left(\frac{d}{d\lambda}\right)^j \left((H-\lambda-i0)^{-1} - (H-\lambda+i0)^{-1}\right) \\ &= \frac{j!}{2\pi i}\left((H-\lambda-i0)^{-j-1} - (H-\lambda+i0)^{-j-1}\right), \end{aligned}$$

it follows from Theorem 1 that

$$\left\| \langle A \rangle^{-s} \left(\frac{d}{d\lambda}\right)^j E'_\lambda \langle A \rangle^{-s} \right\| \leq C\hbar^{-\beta(j+1)}$$

if $s > j + 1/2$. By integration by parts and the functional calculus, we have

$$\begin{aligned} t^j e^{-itH/\hbar} f(H) &= \int_{-\infty}^{\infty} \left(t^j e^{-it\lambda/\hbar}\right) f(\lambda) E'_\lambda d\lambda \\ &= \int_{-\infty}^{\infty} e^{-it\lambda/\hbar} \left(-it\hbar\frac{d}{d\lambda}\right)^j (f(\lambda)E'_\lambda)\, d\lambda. \end{aligned}$$

Thus

$$t^j \left\| \langle A \rangle^{-s} e^{-itH/\hbar} f(H) \langle A \rangle^{-s} \right\| \leq C\hbar^{-\beta}\hbar^{-(\beta-1)j},$$

and hence

$$\left\| \langle A \rangle^{-s} e^{-itH/\hbar} f(H) \langle A \rangle^{-s} \right\| \leq C \langle t \rangle^{-j} \hbar^{-\beta}\hbar^{-(\beta-1)j}$$

if $s > j + 1/2$. Now (2) follows by interpolation. ∎

3. Applications.

Here we apply the results of Section 2 to Schrödinger operators:

$$H = -\frac{1}{2}\hbar^2\Delta + V(x) \qquad \text{on} \quad \mathcal{H} = L^2(\mathbf{R}^d)$$

with $d \geq 1$, $\hbar > 0$. Throughout this section we assume the potential $V(x)$ satisfies the following condition:

(P) $V \in C^\infty(\mathbf{R}^d)$ and for any multi-index α,

$$\left| \left(\frac{d}{dx}\right)^\alpha V(x) \right| \leq C_\alpha \langle x \rangle^{-|\alpha|}, \qquad x \in \mathbf{R}^d.$$

Let $h(x,p) = \frac{1}{2}p^2 + V(x)$ be the corresponding classical Hamiltonian. We denote the solutions of the Newton equation:

$$x'(t) = p(t), \qquad p'(t) = -\frac{\partial V}{\partial x}(x(t))$$

with the initial condition: $x(0) = x_0$, $p(0) = p_0$ by $x(x_0, p_0; t)$ and $p(x_0, p_0; t)$. We write the ω-limit set as

$$\omega\text{-}\lim(x_0, p_0) = \bigcap_{M=1}^{\infty} \overline{\{(x(x_0, p_0; t), p(x_0, p_0; t)) \,|\, t \geq M\}}.$$

Now we fix an energy $E_0 \in \mathbf{R}$. E_0 is called *nontrapping* if the following condition is satisfied:

(NT) There is $\varepsilon > 0$ such that for any $(x,p) \in \mathbf{R}^d \times \mathbf{R}^d$ satisfying $h(x,p) \in [E_0 - \varepsilon, E_0 + \varepsilon]$, $\omega\text{-}\lim(x,p) = \emptyset$.

We also suppose that $V(x)$ satisfies the virial condition near $x = \infty$, i.e.,

(V) There are $R > 0$ and $\delta > 0$ such that

$$(E_0 - V(x)) - \frac{1}{2}x \cdot \frac{\partial V}{\partial x}(x) \geq \delta \qquad \text{for} \quad |x| \geq R.$$

THEOREM 3. *Suppose (P), (NT) and (V). Then there is Δ : a neighborhood of E_0, such that:*

(i) *For any $n \geq 1$ and $s > n - 1/2$, the limit*

$$\lim_{\delta \to +0} \langle x \rangle^{-s} (H - \lambda \pm i\delta)^{-n} \langle x \rangle^{-s} \equiv \langle x \rangle^{-s} (H - \lambda \pm i0)^{-n} \langle x \rangle^{-s}$$

exists for $\lambda \in \Delta$ and sufficiently small $\hbar > 0$. Moreover it satisfies

$$\left\| \langle x \rangle^{-s} (H - \lambda \pm i0)^{-n} \langle x \rangle^{-s} \right\| \leq C\hbar^{-n}, \qquad \lambda \in \Delta, \hbar > 0. \tag{3}$$

(ii) *For any $f \in C_0^\infty(\Delta)$ and $s > s' > 0$, $\varepsilon > 0$,*

$$\left\| \langle x \rangle^{-s} e^{-itH/\hbar} f(H) \langle x \rangle^{-s} \right\| \leq C\hbar^{-\varepsilon} \langle t \rangle^{-s'}, \qquad t \in \mathbf{R}, \hbar > 0. \tag{4}$$

REMARK: Theorem 3 was first proved by Wang ([W1] Theorem 2) using different methods. See also [W2], where the estimate (3) is proved for N-body Schrödinger operators. We note (4) is not optimum. In fact Wang showed that if $V(x)$ is short range then the estimate holds with $s = s'$ and $\varepsilon = 0$ ([W1]

Theorem 1). It seems difficult to obtain such an estimate from (3). We expect that the optimum estimate can be proved by more direct method.

Now we turn to the barrier top energy case. If V attain its maximum at a point, then $E_0 = \sup V$ is clearly trapping energy in the classical sense. We call it the *barrier top energy*, and we suppose:

(BT-i) The origin is the unique nondegenerate maximum of $V(x)$, i.e.,

$$E_0 = \sup_x V(x) = V(0), \qquad \det\left(\frac{\partial^2 V}{\partial x \partial x}(0)\right) \neq 0.$$

(BT-ii) There is $\varepsilon > 0$ such that any classical particle with the energy in $[E_0 - \varepsilon, E_0 + \varepsilon]$ has no ω-limit set except for $(0,0)$, i.e.,

$$\bigcup_{h(x,p)\in[E_0-\varepsilon,E_0+\varepsilon]} \omega\text{-}\lim(x,p) = \{(0,0)\}.$$

(BT-iii) There are no homoclinic orbits with the energy E_0, i.e., if $x(t) \to 0$ as $t \to \pm\infty$ then $x(t) \equiv 0$.

THEOREM 4. *Let E_0 be the barrier top energy and suppose (P), (V) and (BT). Then there is Δ : a neighborhood of E_0, such that:*

(i) *For any $n \geq 1$ and $s > n - 1/2$, the limit*

$$\lim_{\delta\to+0} \langle x\rangle^{-s} (H - \lambda \pm i\delta)^{-n} \langle x\rangle^{-s} \equiv \langle x\rangle^{-s} (H - \lambda \pm i0)^{-n} \langle x\rangle^{-s}$$

exists for $\lambda \in \Delta$ and sufficiently small $\hbar > 0$. Moreover it satisfies

$$\left\| \langle x\rangle^{-s} (H - \lambda \pm i0)^{-n} \langle x\rangle^{-s} \right\| \leq C\hbar^{-2n}, \qquad \lambda \in \Delta, \hbar > 0. \tag{5}$$

(ii) *For any $f \in C_0^\infty(\Delta)$ and $s > s' > 0$,*

$$\left\| \langle x\rangle^{-s} e^{-itH/\hbar} f(H) \langle x\rangle^{-s} \right\| \leq C\hbar^{-s} \langle t\rangle^{-s'}, \qquad t \in \mathbf{R}, \hbar > 0. \tag{6}$$

REMARK: (6) implies that it takes at most time of order $O(\hbar^{s/s'})$ for a quantum particle with the energy near E_0 to escape from a bounded region. As in Theorem 3, we expect that (6) holds with $s = s'$.

In the proof, we use the symbol class $S(m,g)$ with $m = m(\hbar; x, \xi)$, $g = dx^2/\langle x\rangle^2 + d\xi^2/\langle \xi\rangle^2$. $S(m,g)$ is the set of functions: $f(\hbar; x, \xi) \in C^\infty(\mathbf{R}^n \times \mathbf{R}^n)$ with a parameter $\hbar > 0$ such that for any α and β,

$$\left| \left(\frac{\partial}{\partial x}\right)^\alpha \left(\frac{\partial}{\partial \xi}\right)^\beta f(\hbar; x, \xi) \right| \leq C_{\alpha\beta}\, m(\hbar; x, \xi) \langle x\rangle^{-|\alpha|} \langle \xi\rangle^{-|\beta|}, \quad x, \xi \in \mathbf{R}^d.$$

The Weyl operator with the symbol $b(\hbar; x, \xi)$ (or the $\hbar$-pseudodifferential operator with the Weyl symbol $b(\hbar; x, \xi)$) is defined (formally) by

$$b^w(\hbar; x, \hbar D)\psi(x) = (2\pi\hbar)^{-n} \int e^{i(x-y)\xi/\hbar}\, b\left(\hbar; \frac{x+y}{2}, \xi\right) \psi(y)\, dy d\xi.$$

Conversely, we denote the Weyl symbol of an $\hbar$-pseudodifferential operator by $\sigma^w(\cdot)$, i.e., $\sigma^w\,(b^w(\hbar; x, \hbar D)) = b(\hbar; x, \xi)$. (cf. [H]; see also [R], [G], [N1] for the calculus of $\hbar$-pseudodifferential operators.)

It is easy to see that $h(x, \xi) = \frac{1}{2}\xi^2 + V(x) \in S(\langle\xi\rangle^2, g)$ is the symbol of H.

LEMMA 1. *Let $a \in S(\langle x\rangle \langle\xi\rangle, g)$ and suppose $A = a^w(\hbar; x, \hbar D)$ is essentially self-adjoint on the Schwartz space $\mathcal{S}$. Then the pair of operators H and A satisfies the conditions (H1)–(H4).*

PROOF: (H1) is clear since $\mathcal{S}$ is dense in $D(H) = H^2(\mathbf{R}^d)$. For any $B = b^w(\hbar; x, \hbar D)$, $b \in S(\langle\xi\rangle^2, g)$, we have

$$\sigma^w([B, iA]) \in S(\langle x\rangle \langle\xi\rangle \cdot \langle\xi\rangle^2 \cdot \hbar \langle x\rangle^{-1} \langle\xi\rangle^{-1}, g) = S(\hbar \langle\xi\rangle^2, g),$$

and hence $\left\|[B, iA](H+i)^{-1}\right\| \leq C\hbar$. In particular,

$$\sigma^w(B_1) = \sigma^w([H, iA](H+i)^{-1}) \in S(\hbar \langle\xi\rangle^2, g); \qquad \left\|B_1(H+i)^{-1}\right\| \leq C\hbar.$$

Inductively, we have

$$\sigma^w(B_j) = \sigma^w([B_{j-1}, iA]) \in S(\hbar^j \langle\xi\rangle^2, g); \qquad \left\|B_j(H+i)^{-1}\right\| \leq C\hbar^j,$$

for $j \geq 2$. This proves (H2) and (H3). Similarly, we have

$$\sigma^w([H, [H, iA]]) \in S(\hbar^2 \langle x\rangle^{-1} \langle\xi\rangle^3, g),$$

and hence

$$\left\|(H+i)^{-1}[H, [H, iA]](H+i)^{-1}\right\| \leq C\hbar^2. \qquad ∎$$

In order to prove Theorems 3 and 4, it remains to show that there is $a \in S(\langle x\rangle \langle\xi\rangle, g)$ such that (H5:β) holds with $\beta = 1$ and 2, respectively. For the nontrapping case, such $a(x, \xi)$ was constructed by Gérard and Martinez [GM]:

LEMMA 2. *Suppose (P), (NT) and (V). Then there is a real-valued symbol: $a \in C_0^\infty(\mathbf{R}^d \times \mathbf{R}^d)$ such that:*

(i) $a(x, \xi) - x \cdot \xi \in C_0^\infty(\mathbf{R}^d \times \mathbf{R}^d)$;

(ii) *There are* $\varepsilon > 0$ *and* $\delta > 0$ *such that for any* $(x, \xi) \in \mathbf{R}^d \times \mathbf{R}^d$ *with* $h(x, \xi) \in [E_0 - \varepsilon, E_0 + \varepsilon]$,

$$\{h, a\}(x, \xi) \geq \delta, \tag{7}$$

where $\{\cdot, \cdot\}$ *is the Poisson bracket:*

$$\{a, b\} \equiv \sum_{i=1}^{d} \left(\frac{\partial a}{\partial \xi_i} \frac{\partial b}{\partial x_i} - \frac{\partial a}{\partial x_i} \frac{\partial b}{\partial \xi_i} \right).$$

Let $a_0(x, \xi) = x \cdot \xi$. then $A_0 = a_0^w(x, \hbar D)$ is the generator of the dilation group, and hence it is essentially self-adjoint on $\mathcal{S}$. It follows from Lemma 2-(i) that $a \in S(\langle x\rangle \langle \xi\rangle, g)$ and $A = a^w(x, \hbar D)$ is also essentially self-adjoint. Thus A satisfies the conditions of Lemma 1. The next lemma follows from (7) and the functional calculus:

LEMMA 3. *Let* $a(x, \xi)$, ε *and* δ *as in Lemma le:a2. Then for any* $\delta > \delta' > 0$ *and* $f \in C_0^\infty(E_0 - \varepsilon, E_0 + \varepsilon)$,

$$f(H)[H, iA]f(H) \geq \delta' \hbar f(H)^2, \qquad \hbar > 0. \tag{8}$$

For the detail, we refer [GM]. See [G] for the 3-body case, and [W2] for the N-body case. See also [HN] and [N2] for similar discussions.

PROOF OF THEOREM 3: By these lemmas, H and A satisfy (H1)–(H5:1). Thus Theorems 1 and 2 apply to obtain (3) and (4), respectively, with the weight $\langle A\rangle^{-s}$ instead of $\langle x\rangle^{-s}$. We note that

$$\left\| \langle x\rangle^{-s} (H + i)^{-n} \langle A\rangle^{s} \right\| \leq C$$

if $s \leq 2n$. If $s = 2n$, the above estimate follows from the observation:

$$\sigma^w \left(\langle x\rangle^{-2n} (H + i)^{-n} \langle A\rangle^{2n} \right) \in S\left(\langle x\rangle^{-2n} \cdot \langle \xi\rangle^{-2n} (\langle x\rangle \langle \xi\rangle)^{2n}, g \right) = S(1, g),$$

and it is extended to $0 \leq s \leq 2n$ by complex interpolation (cf. [PSS], Lemma 8.2). Combining these we obtain the conclusion. ∎

For the barrier top energy case, such $a(x, \xi)$ was constructed in [N2]:

LEMMA 4. *Suppose (P), (V) and (BT). Then there is a real-valued symbol:* $a(x, \xi) \in C^\infty(\mathbf{R}^d \times \mathbf{R}^d)$ *such that:*

(i) $a(x, \xi) - x \cdot \xi \in C_0^\infty(\mathbf{R}^d \times \mathbf{R}^d)$;

(ii) *There are* $\varepsilon, \alpha, \beta > 0$ *such that for any* $(x, \xi) \in \mathbf{R}^d \times \mathbf{R}^d$ *with* $h(x, \xi) \in [E_0 - \varepsilon, E_0 + \varepsilon]$,

$$\{h, a\}(x, \xi) \geq \min\left(\alpha(|x|^2 + |\xi|^2), \beta \right). \tag{9}$$

The next lemma follows from (9) analogously to Lemma 3:

LEMMA 5. *Let $a(x,\xi)$, ε as in Lemma 4. Then for any $f \in C_0^\infty(E_0-\varepsilon, E_0+\varepsilon)$, there is $c>0$ such that*

$$f(H)[H,iA]f(H) \geq c\hbar^2 f(H)^2, \qquad \hbar > 0. \tag{10}$$

For the detail, we refer [N2]. Now Theorem 4 follows from Lemmas 1 and 5, analogously to Theorem 3.

4. Proof of Theorem 1.

Throughout this section we assume (H1)–(H5:β) hold with $1 \leq \beta \leq 2$. We trace arguments in [JMP] and [CFKS], Section 4.3. Let $f \in C_0^\infty(\mathbf{R})$ be supported in Δ of (H5:β), and $f=1$ in a neighborhood of E_0. Then (H5:β) implies

$$f(H)[H,iA]f(H) \geq c\hbar^\beta f(H)^2. \tag{11}$$

We often write $f=f(H)$ and $\widetilde{f}=1-f$ for simplicity. We also write $\rho = \langle A\rangle^{-1}$. For $\varepsilon \geq 0$ and $z \in \mathbf{C}\setminus\mathbf{R}$, we let

$$G_\varepsilon^M(z) = G_\varepsilon^M = (H - i\varepsilon M^2 - z)^{-1}; \qquad M^2 = f(H)[H,iA]f(H) \geq 0.$$

We fix a neighborhood of E_0: $\Delta' \subset\subset \{\lambda | f(\lambda)=1\}$, and let

$$\Omega_\pm = \{z \in \mathbf{C} | \mathrm{Re}\ z \in \Delta', \pm \mathrm{Im}\ z > 0\}.$$

LEMMA 6. *For $\varepsilon \geq 0$, $Im\ z > 0$, $(H - i\varepsilon M^2 - z)$ is invertible. The inverse is continuous in ε for $\varepsilon \geq 0$ and smooth for $\varepsilon > 0$. Moreover, there are $\varepsilon_0 > 0$ and $C > 0$ such that*

$$\left\| f G_\varepsilon^M \varphi \right\| \leq C\hbar^{-\beta/2}\varepsilon^{-1/2} \left|\langle \varphi, G_\varepsilon^M \varphi\rangle\right|^{1/2}, \tag{12}$$

$$\left\| f G_\varepsilon^M \right\| + \left\| H f G_\varepsilon^M \right\| \leq C\hbar^{-\beta}\varepsilon^{-1}, \tag{13}$$

$$\left\| \widetilde{f} G_\varepsilon^M \right\| + \left\| H \widetilde{f} G_\varepsilon^M \right\| \leq C \tag{14}$$

for $0 < \varepsilon \leq \varepsilon_0$, $0 < \hbar \leq 1$ and $z \in \Omega_\pm$.

PROOF: For $z = \mu + i\delta$, $\mu \in \Delta'$, $\delta > 0$,

$$\begin{aligned} \left\| \left(H - i\varepsilon M^2 - z\right)\varphi \right\|^2 &= \left\| \left(H - i\varepsilon M^2 - \mu\right)\varphi \right\|^2 + \delta^2 \|\varphi\|^2 + 2\varepsilon\delta \|M\varphi\|^2 \\ &\geq \delta^2 \|\varphi\|^2, \qquad \varphi \in D(H). \end{aligned}$$

Hence $G_\varepsilon^M(z)$ exists and it is easy to see that it is smooth in ε if $\varepsilon > 0$ because M^2 is bounded. Now we use the Mourre estimate (11):

$$\begin{aligned}\left\|fG_\varepsilon^M\varphi\right\|^2 &= \langle\varphi, G_\varepsilon^{M*}f^2G_\varepsilon^M\varphi\rangle\\ &\le C\hbar^{-\beta}\langle\varphi, G_\varepsilon^{M*}M^2G_\varepsilon^M\varphi\rangle\\ &\le C\hbar^{-\beta}\varepsilon^{-1}\langle\varphi, G_\varepsilon^{M*}\left(2\varepsilon M^2+2\mathrm{Im}\ z\right)G_\varepsilon^M\varphi\rangle\\ &= C\hbar^{-\beta}\varepsilon^{-1}\langle\varphi, i\left(G_\varepsilon^{M*}-G_\varepsilon^M\right)\varphi\rangle\\ &\le 2C\hbar^{-\beta}\varepsilon^{-1}\left|\langle\varphi, G_\varepsilon^M\varphi\rangle\right|.\end{aligned}$$

This proves (12). Estimate (12) implies

$$\left\|fG_\varepsilon^M\right\| \le C\hbar^{-\beta/2}\varepsilon^{-1/2}\left\|G_\varepsilon^M\right\|^{1/2}. \tag{15}$$

Now we decompose G_ε^M as

$$\begin{aligned}\left\|G_\varepsilon^M\right\| &\le \left\|fG_\varepsilon^M\right\| + \left\|\widetilde{f}G_\varepsilon^M\right\|\\ &\le C\hbar^{-\beta/2}\varepsilon^{-1/2}\left\|G_\varepsilon^M\right\|^{1/2} + \left\|\widetilde{f}(H-z)^{-1}\right\| + \left\|\widetilde{f}(H-z)^{-1}\varepsilon M^2G_\varepsilon^M\right\|\\ &\le C\hbar^{-\beta/2}\varepsilon^{-1/2}\left\|G_\varepsilon^M\right\|^{1/2} + C\left(1+\hbar\varepsilon\left\|G_\varepsilon^M\right\|\right).\end{aligned}$$

By solving the quadratic inequality in $\left\|G_\varepsilon^M\right\|^{1/2}$, we obtain

$$\left\|G_\varepsilon^M\right\| \le C\hbar^{-\beta}\varepsilon^{-1} \tag{16}$$

if $\hbar\varepsilon$ is sufficiently small. We set $\varepsilon_0 > 0$ so small that it holds for any $0 < \hbar \le 1$. (13) follows immediately from (16).

In order to prove (14), we first note that by the resolvent equation,

$$\begin{aligned}\left\|\widetilde{f}G_\varepsilon^M\right\| &\le \left\|\widetilde{f}(H-z)^{-1}\right\| + \left\|\widetilde{f}(H-z)^{-1}\left(i\varepsilon M^2\right)G_\varepsilon^M\right\|\\ &\le C\left(1+\hbar\varepsilon\cdot C\hbar^{-\beta}\varepsilon^{-1}\right) \le C\hbar^{1-\beta}.\end{aligned} \tag{17}$$

We take $\widetilde{g} \in C_0^\infty(\mathbf{R})$ so that $\widetilde{g} = 0$ in a neighborhood of Δ' and $\widetilde{g}\widetilde{f} = \widetilde{f}$. Then (17) holds for $\widetilde{g}G_\varepsilon^M$ also. We decompose $\widetilde{f}G_\varepsilon^M$ as

$$\widetilde{f}G_\varepsilon^M = \widetilde{f}(H-z)^{-1}\left(i\varepsilon M^2\right)\widetilde{g}(H)G_\varepsilon^M + \widetilde{f}(H-z)^{-1}\left[\widetilde{g}(H), i\varepsilon M^2\right]G_\varepsilon^M.$$

Since (H4) implies

$$\begin{aligned}\left\|\left[\widetilde{g}, i\varepsilon M^2\right]\right\| &= \varepsilon\left\|f\left[\widetilde{g},[H,iA]\right]f\right\|\\ &\le \varepsilon\left\|\left[(1-\widetilde{g}),[H,iA]\right]\right\| \le C\hbar^2\varepsilon,\end{aligned}$$

and $\beta \le 2$, we have

$$\left\|\widetilde{f}G_\varepsilon^M\right\| \le C + C\hbar\varepsilon\cdot C\hbar^{1-\beta} + C\hbar^2\varepsilon\cdot\hbar^{-\beta}\varepsilon^{-1} \le C\left(1+\hbar^{2-\beta}\right) \le C.$$

$\left\|H\widetilde{f}G_\varepsilon^M\right\| \le C$ easily follows from this. ∎

LEMMA 7. *Let ε_0 as in Lemma 6. Then*

$$\left\|\rho G_\varepsilon^M \rho\right\| \leq C\hbar^{-\beta}, \tag{18}$$

$$\left\|G_\varepsilon^M \rho\right\| \leq C\hbar^{-\beta}\varepsilon^{-1/2} \tag{19}$$

for $0 < \varepsilon \leq \varepsilon_0$, $0 < \hbar \leq 1$ and $z \in \Omega_\pm$.

PROOF: Let $F_\varepsilon^M = \rho G_\varepsilon^M \rho$. Substituting $\varphi = \rho\psi$ to (12) and using (14), we obtain

$$\begin{aligned}\left\|G_\varepsilon^M \rho\psi\right\| &\leq \left\|\widetilde{f} G_\varepsilon^M \rho\psi\right\| + \left\|f G_\varepsilon^M \rho\psi\right\| \\ &\leq C\left\|\psi\right\| + C\hbar^{-\beta/2}\varepsilon^{-1/2}\left|\langle\psi, \rho G_\varepsilon^M \rho\psi\rangle\right|^{1/2} \\ &\leq C\left(1 + \hbar^{-\beta/2}\varepsilon^{-1/2}\left\|F_\varepsilon^M\right\|^{1/2}\right)\left\|\psi\right\|.\end{aligned}$$

Thus

$$\left\|G_\varepsilon^M \rho\right\| \leq C\left(1 + \hbar^{-\beta/2}\varepsilon^{-1/2}\left\|F_\varepsilon^M\right\|^{1/2}\right). \tag{20}$$

On the other hand, as in the proof of Lemma 4.15 of [CFKS], we have

$$\begin{aligned}\frac{1}{i}\frac{d}{d\varepsilon}F_\varepsilon^M &= \rho G_\varepsilon^M M^2 G_\varepsilon^M \rho = Q_1 + Q_2 + Q_3, \\ Q_1 &= -\rho G_\varepsilon^M \widetilde{f} B_1 \widetilde{f} G_\varepsilon^M \rho, \\ Q_2 &= -\rho G_\varepsilon^M \widetilde{f} B_1 f G_\varepsilon^M \rho - \rho G_\varepsilon^M f B_1 \widetilde{f} G_\varepsilon^M \rho, \\ Q_3 &= \rho G_\varepsilon^M [H, iA] G_\varepsilon^M \rho.\end{aligned}$$

By (13), (14) and (20), Q_1 and Q_2 are estimated as follows:

$$\begin{aligned}\left\|Q_1\right\| &\leq \left\|G_\varepsilon^M \widetilde{f}\right\|\left\|B_1(H+i)^{-1}\right\|\left\|(H+i)\widetilde{f} G_\varepsilon^M\right\| \leq C\hbar, \\ \left\|Q_2\right\| &\leq 2\left\|G_\varepsilon^M \widetilde{f}\right\|\left\|B_1(H+i)^{-1}\right\|\left\|(H+i)f\right\|\left\|G_\varepsilon^M \rho\right\| \\ &\leq C\hbar\left(1 + \hbar^{-\beta/2}\varepsilon^{-1/2}\left\|F_\varepsilon^M\right\|^{1/2}\right).\end{aligned}$$

We decompose $Q_3 = Q_4 + Q_5$ where

$$\begin{aligned}Q_4 &= \rho G_\varepsilon^M \left[H - i\varepsilon M^2 - z, iA\right] G_\varepsilon^M \rho, \\ Q_5 &= \rho G_\varepsilon^M \left[i\varepsilon M^2, iA\right] G_\varepsilon^M \rho.\end{aligned}$$

Using (20) again, we have

$$\left\|Q_4\right\| \leq 2\left\|\rho G_\varepsilon^M A\rho\right\| \leq 2\left\|\rho G_\varepsilon^M\right\| \leq C\left(1 + \hbar^{-\beta/2}\varepsilon^{-1/2}\left\|F_\varepsilon^M\right\|\right).$$

Since

$$\| [M^2, iA] \| \leq 2 \|[f, iA]\| \, \|[H, iA]f\| + \|[[H, iA], iA]f\| \leq C\hbar^2,$$

Q_5 is estimated as

$$\|Q_5\| \leq 2\varepsilon \left\|\rho G_\varepsilon^M\right\|^2 \cdot C\hbar^2 \leq C\hbar^{2-\beta} \left\|F_\varepsilon^M\right\| \leq C \left\|F_\varepsilon^M\right\|.$$

Combining these, we obtain

$$\left\| \frac{d}{d\varepsilon} F_\varepsilon^M \right\| \leq \left(1 + \hbar^{-\beta/2} \varepsilon^{-1/2} \left\|F_\varepsilon^M\right\|^{1/2} + \left\|F_\varepsilon^M\right\|\right). \tag{21}$$

By (13) and (14), we learn

$$\left\|F_\varepsilon^M\right\| \leq \left\|G_\varepsilon^M\right\| \leq C\hbar^{-\beta}\varepsilon^{-1}. \tag{22}$$

(21) and (22) imply $\left\|\frac{d}{d\varepsilon} F_\varepsilon^M\right\| \leq C\left(1 + \hbar^{-\beta}\varepsilon^{-1}\right)$. Integrating this, we obtain

$$\begin{aligned} \left\|F_\varepsilon^M\right\| &\leq C\hbar^{-\beta}\varepsilon_0^{-1} + C\int_\varepsilon^{\varepsilon_0} \left(1 + \hbar^{-\beta}\nu^{-1}\right) d\nu \\ &\leq C\hbar^{-\beta}(1 + |\log \varepsilon|). \end{aligned}$$

We substitute this to (21) and integrate again:

$$\left\|F_\varepsilon^M\right\| \leq C\hbar^{-\beta} + C\hbar^{-\beta} \int_0^{\varepsilon_0} (1 + |\log \varepsilon|) d\varepsilon \leq C\hbar^{-\beta}.$$

This proves (18) and (19) follows from (18) and (20). ∎

For $m \geq 2$ we set

$$C_m(\varepsilon) = \sum_{j=1}^{m} \frac{(-i\varepsilon)^j}{j!} B_j, \qquad \varepsilon > 0,$$

which is bounded from $D(H)$ to $\mathcal{H}$.

LEMMA 8. *There is $\varepsilon_0 > 0$ such that $(H + C_m(\varepsilon) - z)$ has a bounded inverse $G_\varepsilon(z)$ for $0 \leq \varepsilon \leq \varepsilon_0$ and $z \in \Omega_\pm$. $G_\varepsilon(z)$ is continuous in ε for $0 \leq \varepsilon \leq \varepsilon_0$ and smooth for $0 < \varepsilon \leq \varepsilon_0$. Moreover, it satisfies*

$$\|G_\varepsilon\| + \|HG_\varepsilon\| \leq C\hbar^{-\beta}\varepsilon^{-1}, \tag{23}$$

$$\|G_\varepsilon\rho\| + \|HG_\varepsilon\rho\| \leq C\hbar^{-\beta}\varepsilon^{-1/2}. \tag{24}$$

PROOF: We construct G_ε following [JMP]. (14) implies $\left\|\varepsilon B_1 f G_\varepsilon^M \tilde{f}\right\| \leq C\hbar\varepsilon$. Hence

$$G_\varepsilon^0(z) = G_\varepsilon^M - G_\varepsilon^M \tilde{f}\left(1 - i\varepsilon B_1 f G_\varepsilon^M \tilde{f}\right)^{-1}(-i\varepsilon B_1) f G_\varepsilon^M$$

is bounded, and it is an inverse to $(H - i\varepsilon B_1 f)$ if ε is sufficiently small. Moreover, by (13), (14) and (19), we learn that estimates (23)–(24) hold for G_ε^0 and

$$\left\|\tilde{f}G_\varepsilon^0\right\| + \left\|H\tilde{f}G_\varepsilon^0\right\| \leq C. \tag{25}$$

Now (25) implies $\left\|\varepsilon\tilde{f}G_\varepsilon^0 B_1\right\| \leq C\hbar\varepsilon$, and hence

$$G_\varepsilon^1 = G_\varepsilon^0 - G_\varepsilon^0(-i\varepsilon B_1)\left(1 + \tilde{f}G_\varepsilon^0(-i\varepsilon B_1)\right)^{-1}\tilde{f}G_\varepsilon^0$$

is bounded, and it is an inverse to $(H - i\varepsilon B_1 - z)$. Moreover, estimates (23)–(25) hold for G_ε^1.

At last, noting

$$\begin{aligned}\|(C_m(\varepsilon) - (-i\varepsilon)B_1)\,G_\varepsilon^1\| &\leq \|(C_m - (-i\varepsilon)B_1)(H+i)^{-1}\|\;\|(H+i)G_\varepsilon^1\| \\ &\leq C\hbar^2\varepsilon^2 \cdot C\hbar^{-\beta}\varepsilon^{-1} \leq C\hbar^{2-\beta}\varepsilon \leq C\varepsilon,\end{aligned}$$

we learn that

$$G_\varepsilon = G_\varepsilon^1 - G_\varepsilon^1\left(1 + (C_m - (-i\varepsilon)B_1)\,G_\varepsilon^1\right)^{-1}(C_m - (-i\varepsilon)B_1)\,G_\varepsilon^1$$

is bounded and it is an inverse to $(H + C_m - z)$. Now (23)–(24) follow easily from the corresponding estimates for G_ε^1. The smoothness in $\varepsilon > 0$ follows from the H-boundedness of B_j. ∎

LEMMA 9. *Let $G_\varepsilon(z)$ as in Lemma 8. Then*

$$\frac{d}{d\varepsilon}G_\varepsilon = (-i)\,[G_\varepsilon, iA] + i\frac{(-i\varepsilon)^m}{m!}G_\varepsilon B_{m+1}G_\varepsilon. \tag{26}$$

PROOF: We first note $\frac{d}{d\varepsilon}G_\varepsilon = -G_\varepsilon\left(\frac{d}{d\varepsilon}C_m(\varepsilon)\right)G_\varepsilon$, and

$$\begin{aligned}\frac{d}{d\varepsilon}C_m(\varepsilon) &= \frac{d}{d\varepsilon}\sum_{j=1}^m \frac{(-i\varepsilon)^j}{j!}B_j = (-i)\sum_{j=1}^m \frac{(-i\varepsilon)^{j-1}}{(j-1)!}B_j \\ &= -iB_1 + (-i)\sum_{j=1}^m \frac{(-i\varepsilon)^j}{j!}B_{j+1} - (-i)\frac{(-i\varepsilon)^m}{m!}B_{m+1} \\ &= (-i)\,[H + C_m - z, iA] + i\frac{(-i\varepsilon)^m}{m!}B_{m+1}.\end{aligned}$$

(23) follows from this and $[G_\varepsilon, iA] = -G_\varepsilon[H + C_m - z, iA]G_\varepsilon$. ∎

PROOF OF THEOREM 1: Since the case $n = 1$ is already known, we may suppose $n \geq 2$ and hence $s > n - 1/2 > 1$. Let $m \geq \beta(n+1) - 1$ and let $G_\varepsilon = (H - C_m - z)^{-1}$, $F_\varepsilon = \rho^s (G_\varepsilon)^n \rho^s$. We compute its derivative in ε:

$$\begin{aligned}
\frac{d}{d\varepsilon} F_\varepsilon &= \rho^s \frac{d}{d\varepsilon} (G_\varepsilon)^n \rho^s = \rho^s \sum_{j=0}^{n-1} G_\varepsilon{}^j \left(\frac{d}{d\varepsilon} G_\varepsilon\right) G_\varepsilon{}^{n-j-1} \rho^s \\
&= -i \sum_{j=0}^{n-1} \rho^s G_\varepsilon{}^j [G_\varepsilon, iA] G_\varepsilon{}^{n-1-j} \rho^s + i \frac{(-i\varepsilon)^m}{m!} \sum_{j=0}^{n-1} \rho^s G_\varepsilon{}^{j+1} B_{m+1} G_\varepsilon{}^{n-j} \rho^s \\
&= -i\rho^s \left[G_\varepsilon{}^n, iA\right] \rho^s + i \frac{(-i\varepsilon)^m}{m!} \sum_{j=0}^{n-1} \rho^s G_\varepsilon{}^{j+1} B_{m+1} G_\varepsilon{}^{n-j} \rho^s \\
&\equiv I + II.
\end{aligned}$$

We estimate II using Lemma 8:

$$\begin{aligned}
\|II\| &\leq C\varepsilon^m \sum_{j=0}^{n-1} \|\rho G_\varepsilon\| \left\|G_\varepsilon{}^j\right\| \left\|B_{m+1}(H+i)^{-1}\right\| \left\|(H+i) G_\varepsilon{}^{n-j-1}\right\| \|G_\varepsilon \rho\| \\
&\leq C\varepsilon^m \sum_{j=1}^{n-1} \hbar^{-\beta} \varepsilon^{-1/2} \left(\hbar^{-\beta}\varepsilon^{-1}\right)^j \hbar^{m+1} \left(\hbar^{-\beta}\varepsilon^{-1}\right)^{n-j-1} \hbar^{-\beta}\varepsilon^{-1/2} \\
&\leq C\hbar^{(m+1)-(n+1)\beta} \varepsilon^{m-n} \leq C.
\end{aligned}$$

In the last step we have used the condition: $m + 1 \geq (n+1)\beta$. The other term is

$$\begin{aligned}
\|I\| &\leq 2 \left\|\rho^s G_\varepsilon{}^n A \rho^s\right\| \leq 2 \left\|\rho^{s-1} G_\varepsilon{}^n \rho^s\right\| \leq 2 \left\|\rho^s G_\varepsilon{}^n \rho^s\right\|^{1-1/s} \left\|G_\varepsilon{}^n \rho^s\right\|^{1/s} \\
&\leq C \|F_\varepsilon\|^{1-1/s} \left(\left(\hbar^{-\beta}\varepsilon^{-1}\right)^{n-1} \left(\hbar^{-\beta}\varepsilon^{-1/2}\right)\right)^{1/s} \\
&\leq C\hbar^{-n\beta/s} \varepsilon^{-(n-1/2)/s} \|F_\varepsilon\|^{1-1/s}.
\end{aligned}$$

Combining these we have

$$\left\|\frac{dF_\varepsilon}{d\varepsilon}\right\| \leq C \left(1 + \hbar^{-n\beta/s} \varepsilon^{-(n-1/2)/s} \|F_\varepsilon\|^{1-1/s}\right). \tag{27}$$

On the other hand, Lemma 8 implies

$$\|F_\varepsilon\| \leq C \|\rho G_\varepsilon\| \|G_\varepsilon\|^{n-2} \|G_\varepsilon \rho\| \leq C\hbar^{-n\beta} \varepsilon^{-(n-1)}.$$

If we substitute $\|F_\varepsilon\| \leq C\hbar^{-n\beta}\varepsilon^{-\gamma}$, $\gamma > 0$, to (27), by integration by parts we obtain

$$\|F_\varepsilon\| \leq C\hbar^{-n\beta}\varepsilon^{-\gamma(1-1/s)-(n-1/2)/s+1} \leq C\hbar^{-n\beta}\varepsilon^{-\gamma+(1-(n-1/2)/s)}.$$

Since $1 > (n-1/2)/s$, finitely many iterations give us $\|F_\varepsilon\| \leq C\hbar^{-n\beta}$ for any $0 < \varepsilon \leq \varepsilon_0$. Hence

$$\sup_{z\in\Omega_\pm} \left\|\rho^s(H-z)^{-n}\rho^s\right\| \leq \sup_{z\in\Omega_\pm} \sup_{\varepsilon\in(0,\varepsilon_0]} \|\rho^s G_\varepsilon{}^n \rho^s\| \leq C\hbar^{-n\beta}.$$

Since the existence of the boundary value is proved in [JMP], this completes the proof. ∎

References.

[BCD] Briet, Ph., Combes, J. M., Duclos, P.: On the location of resonances for Schrödinger operators in the semiclassical limit. II. Barrier top resonances. Comm. P. D. E. **12**, 201–222 (1987).

[CFKS] Cycon, H. L., Froese, R. G., Kirsch, W., Simon, B.: Schrödinger Operators, with Applications to Quantum Mechanics and Global Geometry. 1987, Springer-Verlag.

[G] Gérard, Ch.: Semiclassical resolvent estimates for two- and three-body Schrödinger operators. Comm. P. D. E. **15**, 1161–1178 (1990)

[GM] Gérard, Ch., Martinez, A.: Principe d'absorption limite pour des opérateurs de Schrödinger à longue portée. C. R. Acad. Sci. Paris **306**, 121–123 (1989).

[H] Hörmander, L.: The Analysis of Partial Differential Operators. Vol. 3. 1985, Springer Verlag.

[HN] Hislop, P. D., Nakamura, S.: Semiclassical resolvent estimates. Ann. Inst. H. Poincaré **51**, 187–198 (1989).

[J1] Jensen, A.: Propagation estimates for Schrödinger-type operators. Trans. A. M. S. **291**, 129–144 (1985).

[J2] Jensen, A.: High energy estimates for generalized many-body Schrödinger operators. Publ. R. I. M. S., Kyoto Univ. **25**, 155–167 (1989).

[JMP] Jensen, A., Mourre, E., Perry, P.: Multiple commutator estimates and resolvent smoothness in quantum scattering theory, Ann. Inst. H. Poincaré **41**, 207–225 (1984).

[N1] Nakamura, S.: Shape resonances for distortion analytic Schrödinger operators. Comm. P. D. E. **14**, 1383–1419 (1989).

[N2] Nakamura, S.: Semiclassical resolvent estimates for the barrier top energy, Comm. P. D. E. **16**, 873–883 (1991).

[M] Mourre, E.: Absence of singular continuous spectrum for certain self-adjoint operators. Comm. Math. Phys. **78**, 391–408 (1981).

[PSS] Perry, P., Sigal, I. M., Simon, B.: Spectral analysis of N-body Schrödinger operators. Ann. Math. **114**, 519–567 (1981).

[R] Robert, D.: Autour de l'approximation semiclassique. 1983, Birkhauser.

[RS] Reed, M., Simon, B.: Methods of Modern Mathematical Physics. Vol. 3. Scattering Theory. Academic Press, 1979.

[RT1] Robert, D., Tamura, H.: Semiclassical bounds for resolvents for Schrödinger operators and asymptotics for scattering phases, Comm. P. D. E. **9**, 1017–1058 (1984).

[RT2] Robert, D., Tamura, H.: Semiclassical bounds for resolvents and asymptotics for total cross-sections. Ann. Inst. H. Poincaré **46**, 415–442 (1987).

[RT3] Robert, D., Tamura, H.: Semiclassical asymptotics for local spectral density and time-delay problems in scattering processes. J. Funct. Anal. **80**, 124–147 (1988).

[RT4] Robert, D., Tamura, H.: Asymptotic behavior of scattering amplitudes in semi-classical and low energy limits. Ann. Inst. Fourier, Grenoble **39**, 124–147 (1989).

[S] Sjöstrand, J.: Semiclassical resonances generated by non-degenerate critical points. Springer Lecture Notes in Math. **1256**, 402–429 (1987).

[W1] Wang, X. P.: Time-decay of scattering solutions and resolvent estimates for semiclassical Schrödinger operators, J. Diff. Eq. **71**, 348–395 (1988).

[W2] Wang, X. P.: Semiclassical resolvent estimates for N-body Schrödinger operators. J. Funct. Anal. **97**, 466–483 (1991).

[Y] Yafaev, D. R.: The eikonal approximation and the asymptotics of the total cross-section for the Schrödinger equations. Ann. Inst. H. Poincaré **44**, 397–425 (1986).

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Magnetic breakdown

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Magnetic Breakdown

James Ralston

This paper treats a problem in quantum mechanics by what might be called the "classical" method of semi-classical analysis. One makes an *Ansatz* and solves eichonal and transport equations to determine phases and amplitudes. However, the problem has some nonclassical aspects. First, the small parameter in the problem is not Planck's constant but the magnetic field strength, ε. When one scales variables so that powers of ε appear where they should in semi-classical analysis, the electric potential becomes a periodic function of x/ε. This complicates the *Ansatz*, and makes the wave function one is trying to construct vector-valued rather than scalar. In most regions one can uncouple the components and construct the wave function one component at a time. That case was discussed in [2] and [4].

In the situation called "magnetic breakdown" one can only uncouple a two component system, and the matrix of the zero magnetic field operator on this system has a codimension two eigenvalue crossing of the form discussed in [5]. The eichonal equation becomes one treated by Horn in [7], and, after several reductions, the transport equations become a 2×2 first order hyperbolic system which degenerates on the set where the eigenvalues cross and uncoupling is impossible. Much of the analysis here is devoted to deriving that system and showing that it has solutions. However, the solutions do not add much to one's qualitative understanding of magnetic breakdown. Perhaps the oddest feature of the ultimate transport equations is that one cannot solve the initial value problem for them. Their solutions are uniquely determined by the inhomogeneous terms. Fortunately, since it would be embarassing to devote so much effort to constructing the zero function, one can prescribe nonzero inhomogeneous terms for the top order transport.

I should emphasize that the constructions here are time-dependent. One could construct asymptotic solutions to the time-independent Schrödinger equation by suppressing the time dependence in the *Ansatz* as was done in the construction of quasimodes in [2], [4] and [7]. However, for questions related to the spectral density an approach like that of Helffer and Sjöstrand [6], [9] would be more effective.

I. Hypotheses and Preliminaries

We consider the Schrödinger equation for a single electron in a crystal lattice of ions in a constant magnetic field. That is, we consider the Schrödinger equation with a smooth, periodic electric potential $V(x)$ and a linear magnetic potential $\varepsilon A(x)$:

$$i\varepsilon\frac{\partial u}{\partial t} = \left(i\frac{\partial}{\partial x} + \varepsilon A(x)\right)^2 u + V(x)u, \quad x \in \mathbb{R}^3. \tag{1}$$

Here $A(x) = \frac{\omega\times x}{2}$, $|\omega| = 1$, and the magnetic field is given by $B = \nabla\times\varepsilon A = \varepsilon\omega$. The periodicity condition on V is $V(x+\ell) = V(x)$ for all ℓ in a three-dimensional lattice L. The Schrödinger equation takes the form (1) in suitable distance, energy and time scales - Ångstroms for distance and roughly electron volts for energy. These units make $\varepsilon = 1.5 \times 10^{-9}g$, where g is the magnetic field strength in gauss. Thus ε is the natural small parameter here. In what follows we will put (1) in the form

$$i\varepsilon\frac{\partial u}{\partial t} = \left(i\varepsilon\frac{\partial}{\partial y} + A(y)\right)^2 u + V\left(\frac{y}{\varepsilon}\right)u, \tag{2}$$

by making the change of variables $y = \varepsilon x$.

The article [4] discussed asymptotic solutions of (2) of the form

$$u = e^{-i\varphi(y,t)/\varepsilon} m(y/\varepsilon,\ y,\ t,\ \varepsilon) \tag{3}$$

where $m(x,\ y,\ t,\ \varepsilon) = m(x+\ell,\ y,\ t,\ \varepsilon)$, $\forall \ell \in L$, and $m = m_0(x,\ y,\ t) + \varepsilon m_1(x,\ y,\ t) + \cdots$. Substituting the *Ansatz* (3) into (2), equating coefficients of powers of ε to zero and solving the resulting equations, one constructs asymptotic solutions to all orders in ε. The leading amplitude is given by

$$m_0(x,\ y,\ t) = h(y,\ t)\psi_n\left(x,\ \frac{\partial\varphi}{\partial y} + A(y)\right),$$

where $\psi_n(x,\ k)$ is an eigenfunction of the operator

$$L(k) = \left(i\frac{\partial}{\partial x} + k\right)^2 + V(x)$$

with the lattice periodicity condition, belonging to the eigenvalue $E_n(k)$. The phase φ must be a solution of the Hamilton-Jacobi equation

$$\frac{\partial\varphi}{\partial t} = E_n\left(\frac{\partial\varphi}{\partial y} + A(y)\right). \tag{4}$$

The only hypothesis needed to solve the transport equations and carry out the construction to all orders in ε is that $E_n(k)$ must be a *simple* eigenvalue of $L(k)$ for the values of $k = \frac{\partial\varphi}{\partial y}(y,\ t) + A(y)$ which arise from propagating the support of $h(y,\ 0)$ along the trajectories of the Hamiltonian $E_n(p + A(y)) - \tau$ associated with (4).

In this article I want to consider the situation when $E_n(k)$ is not simple on one of those trajectories. In this case the wave packets $u(y,\ t,\ \varepsilon)$ can no longer just propagate along the trajectories of $E_n(p + A(y)) - \tau$, and one is in the situation called "interband magnetic breakdown" in the physics literature. This terminology refers to the way that packets can now "tunnel" to trajectories of $E_{n+1}(p+A(y))-\tau$, an effect that becomes more evident as the magnetic field strength increases. I should mention that there is also a phenomenon known as "intraband magnetic breakdown" associated with k_0 such that $E_n(k_0)$ is simple, but $\nabla E_n(k_0)\times\omega=0$. The construction of time-dependent wave packets in this situation is included in the preceding, but when one studies the spectrum near $E_n(k_0)$ there are effects caused by tunnelling between the branches of the curve $\{E_n(k)=E_n(k_0),\ \omega\cdot(k-k_0)=0\}$. Quasimodes for this case were constructed in Horn [7], using the same *Ansatz* we will use for interband magnetic breakdown here. The effect of such points on the spectral density (they turn out to be negligible) was analyzed by Sjöstrand in [9]. Closely related spectral problems are discussed in [2], [2a], [3] and [8].

I am going to make a number of assumptions to simplify the constructions. First E_n is only a double eigenvalue, i.e.

$$E_{n-1}(k_0)<E_n(k_0)=\tau_0=E_{n+1}(k_0)<E_{n+2}(k_0).$$

The point k_0 is going to be the base point in what follows. Since $L(k)$ is analytic in k, this implies that, for δ sufficiently small, when $|k-k_0|<\delta$, the span, $R(k)$, of the eigenvectors of $L(k)$ belonging to eigenvalues in $|\tau-\tau_0|<\delta$ has a basis $\{\psi_1(x,k),\ \psi_2(x,k)\}$ which is orthonormal and real analytic in k. The restriction of $L(k)$ to $R(k)$ has the matrix

$$\begin{pmatrix} a(k) & b(k) \\ \bar{b}(k) & c(k)\end{pmatrix} \tag{5}$$

in terms of this basis, where the entries are real-analytic and a and c are real.

Next the potential is assumed to have the symmetry $V(x)=V(-x)$. This symmetry is typical of metals. With this symmetry $L(k)$ commutes with the involution $[If](x)=\bar{f}(-x)$. The 1-eigenspace of I, considered as a real-linear transformation of

$R(k)$, must be two dimensional, and it depends analytically on k. Thus one can assume that ψ_1 and ψ_2 belong to this subspace, and this forces $b(k)$ in (5) to be real-valued. This consequence of $V(x) = V(-x)$ is well-known (it is used in [10]), but I am grateful to J. Sjöstrand for explaining it to me. The symmetry has the effect of changing the set of k where $E_n(k) = E_{n+1}(k)$ from just k_0, as it would be for a generic matrix of the form (5), to a curve through k_0 in the generic case.

Next I assume that we *are* in the generic case.[1] For this I simply assume that a, b and c have linearly independent gradients at k_0. Since

$$D \equiv \det \begin{pmatrix} a(k) - \tau & b(k) \\ b(k) & c(k) - \tau \end{pmatrix} = \left(\frac{a+c}{2} - \tau\right)^2 - \left(\frac{a-c}{2}\right)^2 - b^2,$$

we see that $E_n(k) = E_{n+1}(k)$ on the analytic curve $\Gamma = \{k : a - c = b = 0\}$ through k_0, and the surfaces $D = 0$ have conic singularities on Γ (see Figure 1). Here we consider τ as a parameter.

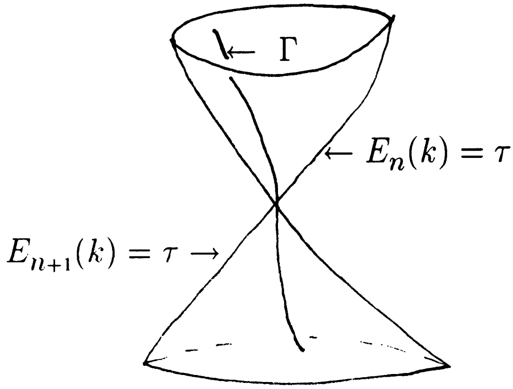

Figure 1. The Cone $D(\cdot,\ \tau) = 0$

The final hypothesis will insure that we are in the situation where magnetic breakdown occurs. One checks easily that on the trajectories of the Hamiltonian $E_n(p + A(y)) - \tau$ the function $k = p + A(y)$

[1] Note that generic here means generic among symmetric real 2×2 matrices scalar at k_0.

satisfies

$$\dot{k} = \omega \times \frac{\partial E_n}{\partial k}(k).$$

Hence k moves on the intersection of the surfaces $D = 0$ with a plane $k \cdot \omega = c$. To get magnetic breakdown we need to choose ω so that these planes cut both nappes of the cone $D = 0$. Thus we assume that the plane $k \cdot \omega = k_0 \cdot \omega$ cuts both nappes of $D(k, \tau_0) = 0$ nontangentially.

With these hypotheses we can put our problem in a standard form. We translate and rotate coordinates in k-space so that the vertex of $D(\cdot, \tau) = 0$ is the origin for all τ, $\omega = \hat{e}_3$ and the Hessian matrix of D in $(k_1, \ k_2)$ is diagonal at the origin with $\frac{\partial^2 D}{\partial k_1^2}(0) > 0$. This is possible because the magnetic breakdown hypothesis implies that the Hessian is indefinite. Then, using the Weierstrass preparation theorem (trivially) in k_1, we have

$$D = ((k_1 - r)^2 - q)Q_0$$

where $r = r(k_2, \ k_3, \ \tau)$, $q = q(k_2, \ k_3, \ \tau)$ and $Q_0(0, \ \tau_0) > 0$. Moreover, the preceding choices of coordinates imply $r = \frac{\partial r}{\partial k_2} = q = \frac{\partial q}{\partial k_i} = 0$ at $(0, \tau_0)$, and the Hessian of q is positive definite. Since $\omega = \hat{e}_3$, it will be convenient to choose $A(y) = y_1 \hat{e}_2$ instead of $\frac{1}{2}\omega \times y$ from here on.

II. The Basic Ansatz and the Eichonal

We are now ready to construct asymptotic solutions to (2) in the magnetic breakdown case. We will use the general *Ansatz*

$$u = \int_C e^{\frac{-i}{\varepsilon}\varphi} m dz, \tag{6}$$

where $\varphi = \varphi_0(y_1, \ z) + \tau t + \xi_2 y_3 + \xi_3 y_3$ and C is a contour to be determined. Thus we assume linear dependence of the phase on all space-time variables except y_1. However, the construction will be uniform in the parameters (ξ_2, τ) on a neighborhood of $((k_0)_2, \tau_0)$ so that one can construct more general wave packets with (crystal) momentum localized around k_0 by superposition in these parameters.

At this point I could simply write out the rest of the *Ansatz* in detail, but I would like to try to motivate the choices. When one substitutes (6) into (2), one does not need to set coefficients of powers of ε in the integrand to zero. As long as the coefficients are equal to smooth multiples of $\frac{\partial \varphi}{\partial z}$ one sees by integration by parts that they contribute to terms with an additional power of ε. Since we assume that $m = m_0 + \varepsilon\, m_1 + \cdots$ with

$$\begin{aligned} m_0 = {}& \alpha(y,\ t,\ z)\psi_1\left(\frac{y}{\varepsilon},\ \frac{\partial \varphi}{\partial y} + y_1 \hat{e}_1\right) \\ & + \beta(y,\ t,\ z)\psi_2\left(\frac{y}{\varepsilon},\ \frac{\partial \varphi}{\partial y} + y_1 \hat{e}_1\right), \end{aligned} \tag{7}$$

the analog for (6) of the eichonal equation (4) is

$$D\left(\frac{\partial \varphi}{\partial y_1},\ \xi_2 + y_1,\ \xi_3,\ \tau\right) = \frac{\partial \varphi}{\partial z} R \tag{8}$$

where R is analytic in z. This condition merely says that $D(\partial\varphi/\partial y_1, \xi_2{+}y_1, \xi_3, \tau)$ and $\partial\varphi/\partial z$ have the same zeros as functions of z, which is implied by

$$\begin{aligned} 0 = {}& \left(\frac{\partial \varphi_0}{\partial y_1} - r(\xi_2 + y_1,\ \xi_3,\ \tau)\right)^2 \\ & - q(\xi_2 + y_1,\ \xi_3,\ \tau) \quad \Longleftrightarrow \quad \frac{\partial \varphi_0}{\partial z} = 0. \end{aligned} \tag{9}$$

A simple way to achieve (9) is to choose φ_0 so that $\partial\varphi_0/\partial y_1$ is linear in z and $\partial\varphi_0/\partial z$ has the zero set of a quadratic function of z. A choice with these properties is

$$\varphi_0 = \frac{z^2}{4} - f z - \frac{h}{2}\log z + g,$$

where $f = f(\xi_2 + y_1, \ \xi_3, \ \tau)$, $h = h(\xi_3, \ \tau)$ and $g = g(y_1 + \xi_2, \ \xi_3, \ \tau)$. This reduces (9) to

$$\frac{\partial f}{\partial k_2}\sqrt{f^2 + h} = \sqrt{q} \tag{10}$$

to be solved with h independent of k_2 and $\frac{\partial f}{\partial k_2}(k_0, \ \tau_0) > 0$. This problem has been treated in a similar setting by Gérard and Grigis in [3] and solved in exactly this setting by Horn [7]. One sees that (10) implies

$$h(k_3, \ \tau) = \frac{1}{\pi i}\int_\gamma \sqrt{q(\zeta, k_3, \tau)}d\zeta,$$

where γ encloses the (two) zeros of $q(\zeta, \ k_3, \ \tau)$ near $\zeta = 0$. From this it follows that

$$h(k_3, \ \tau) = \frac{2\sqrt{2}\det(\mathrm{Hess}D(0, \ \tau))}{(-\det(\mathrm{Hess}D|_{\hat{e}_3\cdot k=0}(0, \ \tau)))^{3/2}}k_3^2 + O(k_3^3). \tag{11}$$

As we will see, h determines the strength of the magnetic breakdown. The formula (11) (with a few typographic errors) was already given by Slutskin in [10].

The function f is assumed to be real-valued here. However, if one takes

$$\varphi_0 = \frac{z^2}{4} + i\tilde{f}z + \frac{\tilde{h}}{2}\log z + \tilde{g},$$

one is again lead to (10) for $\tilde{f}$ and $\tilde{h}$. This gives another family of asymptotic solutions which we will not discuss here (see Horn [7]).

We will take $\{te^{3i\pi/4},\ t > 0\}$ as the branch cut in the definition of $\log z$ and choose $C = \{se^{3i\pi/4} - 1,\ s \in \mathbb{R}\}$ with the orientation in Figure 2

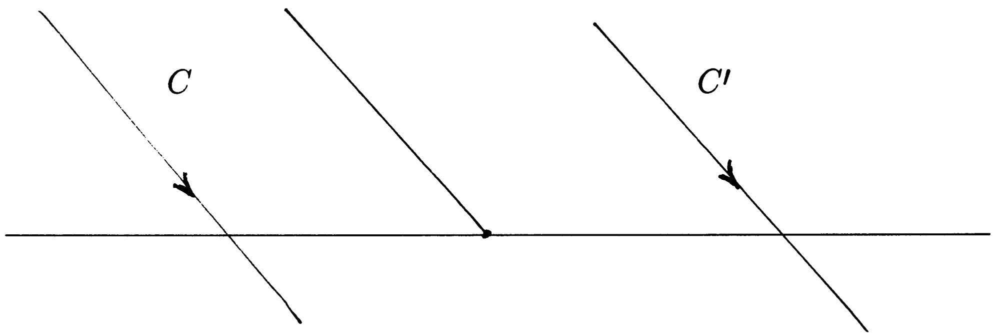

Figure 2

To see how this *Ansatz* incorporates the tunnelling effect of magnetic breakdown one can (when $h > 0$) use the method of steepest descents. Denoting the two zeros of $\frac{\partial\varphi}{\partial z}$ as $z_{\pm} = f \pm \sqrt{f^2 + h}$, one has for $f < 0$ the steepest descent curves $Re\{\varphi(z)\} = Re\{\varphi(z_+)\}$ and $Re\{\varphi(z)\} = Re\{(\varphi(z_-)\}$ as shown in Figure 3.

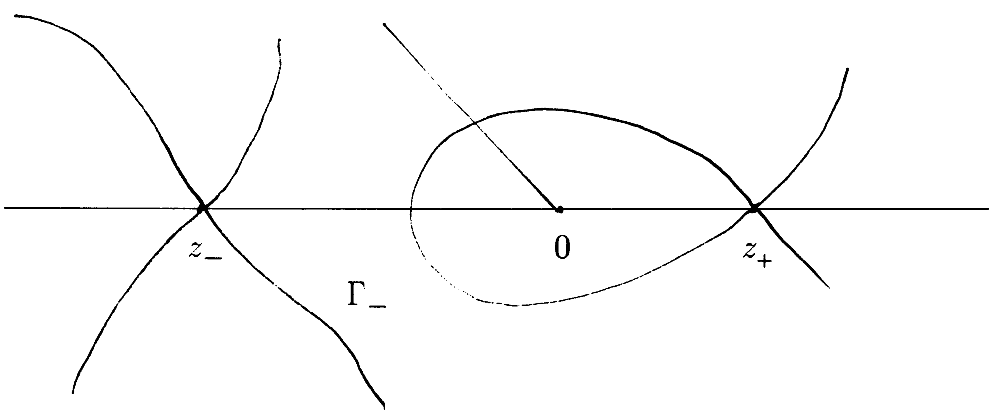

Figure 3

Since C can be deformed to Γ_-, the method of steepest descent shows that for $f < 0$, (6) reduces to (3) with $\varphi(y, t) = \varphi(z_-)$. However, when $f > 0$ the steepest descent curves become those shown in Figure 4.

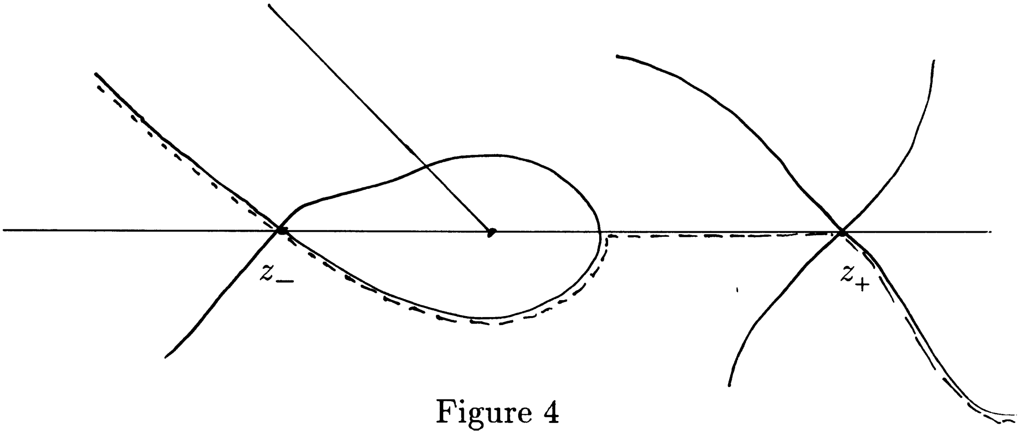

Figure 4

Now C cannot be deformed to a steepest descent curve. One can only deform C to the curve Γ indicated by dots in Fig. 4. Now in addition to the contribution from z_- there is a contribution from z_+. Since $Im\{\varphi(z)\}$ decreases by $\frac{\pi}{2}h$ as one goes along the lower half of the loop, the latter contribution is weaker by a factor of $\exp\left(-\frac{\pi h}{2\varepsilon}\right)$. This is the tunnelling term, and it explains the earlier remark that h measures the strength of magnetic breakdown. Since we are not claiming to construct solutions valid with exponentially small errors, the only rigorous results here on magnetic breakdown will follow from showing that the asymptotics just described hold uniformly for h in $[0, h_0]$. This was carried out in Horn [7]. One notes that

$$F(x) = \int_C e^{-\frac{i}{\varepsilon}\left(\frac{z^2}{4} - xz - \frac{h}{2}\log z\right)} dz$$

is a solution of a second order ordinary differential equation for which one can construct two bases of solutions having simple asymptotics for $h \in [0, h_0]$ when $x > 0$ and when $x < 0$ respectively. Using the explicit computation of these basis functions at $x = 0$ to match them across $x = 0$, one computes the asymptotics of F for $x > 0$, uniformly on $(0, h_0)$. The key step is expressing F, properly normalized, in terms of the basis with simple asymptotics for $x > 0$.

The result of this computation is the identity (with $\gamma = h/2\varepsilon$)
(11′)
$$W_1(x) = e^{-\pi\gamma} Y_1(x) + (1 - e^{-2\pi\gamma})^{1/2} e^{i(\frac{\pi}{4} - \gamma \log \gamma + \gamma + \operatorname{Arg}\Gamma(i\gamma))} W_2(x),$$

where

$$W_1(x) = e^{-\pi\gamma}(\varepsilon h)^{-1/2} \int_C e^{\frac{-i}{\varepsilon}(\frac{z^2}{4} - xz - \frac{h}{2}\log z)} dz$$
$$Y_1 = (\varepsilon h)^{-1/2} \int_{C'} e^{\frac{-i}{\varepsilon}(\frac{z^2}{4} - xz - \frac{h}{2}\log z)} dz, \quad \text{and}$$
$$W_2(x) = \varepsilon^{-1/2} e^{\frac{\pi\gamma}{2}} e^{i(\gamma \log h - \gamma - \frac{\pi}{2})} \int_C e^{\frac{-i}{\varepsilon}(\frac{z^2}{4} + ixz + \frac{h}{2}\log z - x^2)} dz.$$

Here $C' = \{se^{3i\pi/4} + 1,\ s \in R\}$ with the orientation in Figure 2. The choice of normalizing factors here makes the asymptotics of W_1 as $\varepsilon \to 0$ with $h > 0$ fixed and $x < 0$ match the asymptotics of W_2 as $\varepsilon \to 0$ with $h > 0$ fixed and $x > 0$. These asymptotics give terms of order zero as do the asymptotics of Y_1. Since modulo terms of order ε one can assume m is of the form $a+bz$ in (6), the function u in our *Ansatz* can be expressed in terms of $W_1(f)$ and $W_1'(f)$. Thus the identity (11′) is a computation of magnetic breakdown: note that the coefficient of Y_1 is the tunnelling coefficient, and by Stirling's formula the coefficient of W_2 tends to 1 as $\gamma \to \infty$. Once again this formula appears in Slutskin [10, formula (32)]. The computation of tunnelling strength is also related to that given by Hagedorn in [5]. Since we do not justify exponentially small terms here, (11′) gives information to us when $\frac{h}{2\varepsilon} = 0(1)$, i.e. in the regime where $k_3 = O(\varepsilon^{1/2})$ and tunnelling is significant.

The functions W_1, W_2 and Y_1 are related to parabolic-cylinder or Weber functions, but I feel that the integral representation is more transparent.

III. The Transport Equations

If one makes the choice in (7) for m_0, the terms of order ε^0 in the integrand resulting from substituting (6) into (2) will contribute terms of order ε after integration by parts provided

$$\begin{pmatrix} a & b \\ b & c \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \tau \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \tag{12}$$

at $z_\pm$. Here, as always from here on, the entries $a,\ b,\ c$ are evaluated at $k = \frac{\partial\varphi}{\partial y} + y_1\hat{e}_2$. We will need to solve such equations systematically in this section. One way to do this is as follows. For any analytic function $g(z)$ we set

$$g^s = \frac{1}{2}g(z_+) + \frac{1}{2}g(z_-) \quad \text{and} \quad g^a = \frac{g(z_+) - g(z_-)}{(z_+ - z_-)}.$$

Then g^s and g^a are analytic functions of f and h, $g(z_\pm) = g^s \pm \sqrt{f^2 + h}\,g^a$, and

$$g(z) = g^s + (z - f)g^a \quad \operatorname{mod} z\frac{\partial\varphi}{\partial z}.$$

Using the same notation for matrices and setting $A_0 = \begin{pmatrix} a-\tau & b \\ b & c-\tau \end{pmatrix}$, one sees that (12) holds at $z_\pm$, if and only if

$$0 = \begin{pmatrix} A_0^s & (f^2 + h)A_0^a \\ A_0^a & A_0^s \end{pmatrix}\begin{pmatrix} \alpha^s \\ \beta^s \\ \alpha^a \\ \beta^a \end{pmatrix}.$$

Setting

$$U = \begin{pmatrix} I & 0 \\ -\frac{1}{2}(f^2 + h)^{-1/2}I & I \end{pmatrix}\begin{pmatrix} I & (f^2 + h)^{1/2}I \\ 0 & I \end{pmatrix}$$

and $M_0 = \begin{pmatrix} A_0^s & (f^2+h)A_0^a \\ A_0^a & A_0^s \end{pmatrix}$, we have $\begin{pmatrix} A_0(z_+) & 0 \\ 0 & A_0(z_-) \end{pmatrix} = UM_0U^{-1}$. Hence M_0 has rank at most 2. However, when $f = h = 0$ and $\tau = \tau_0$

$$A_0^a = \begin{pmatrix} \frac{\partial a}{\partial k_1}(k_0) & \frac{\partial b}{\partial k_1}(k_0) \\ \frac{\partial b}{\partial k_1}(k_0) & \frac{\partial c}{\partial k_1}(k_0) \end{pmatrix}$$

and, since $\frac{\partial^2 D}{\partial k_1^2}(k_0, \tau_0) > 0$, it follows that A_0^a is nonsingular at the base point. Thus M_0 has rank exactly 2 near the base point and (12) holds if and only if

$$A_0^a \begin{pmatrix} \alpha^s \\ \beta s \end{pmatrix} + A_0^s \begin{pmatrix} \alpha^a \\ \beta a \end{pmatrix} = 0.$$

In other words for each choice of $\binom{\alpha^a}{\beta a}$ there is a unique $\binom{\alpha}{\beta}$ mod $z\frac{\partial \varphi}{\partial z}$ satisfying (12). One checks easily that a convenient basis for these solutions is

$$v_1 = \begin{pmatrix} -b \\ a-\tau \end{pmatrix}, \qquad v_2 = \begin{pmatrix} c-\tau \\ -b \end{pmatrix},$$

and hence the general choice for m_0 is $m_0 = (-b\delta + (c-\tau)\gamma)\psi_1 + ((a-\tau)\delta - b\gamma)\psi_2$, where γ and δ are arbitrary functions of (y, t, z). With this choice of m_0 we assume that m in (6) has the form $m = m_0(y/\varepsilon, y, t, z) + \varepsilon m_1(y/\varepsilon, y, t, z) + \cdots$ where $m_1(x, y, z) = \alpha_1\phi_1\left(x, \frac{\partial \varphi}{\partial y} + y_1\hat{e}_2\right) + \beta_1\psi_2\left(x, \frac{\partial \varphi}{\partial y} + y_1\hat{e}_2\right) + \tilde{m}_1(x, y, z)$. The function $\tilde{m}_1$ is assumed to be orthogonal to $\psi_1\left(x, \frac{\partial \varphi}{\partial y} + y_1\hat{e}_2\right)$ and $\psi_2\left(x, \frac{\partial \varphi}{\partial y} + y_1\hat{e}_2\right)$ in x over a fundamental domain in the lattice.

The "transport" equations arise as follows. When we substitute (6) into (2) and eliminate terms of order ε^0 from the integrand by integration by parts, we need to solve inhomogeneous problems $L(k)\tilde{m}_1 - \tau\tilde{m}_1 = g$ to eliminate the terms of order ε. The condition that the inhomogeneous terms be orthogonal to ψ_1 and ψ_2 over a fundamental domain leads to the transport equations

$$\begin{pmatrix} \frac{\partial a}{\partial k_1} & \frac{\partial b}{\partial k_1} \\ \frac{\partial b}{\partial k_1} & \frac{\partial c}{\partial k_1} \end{pmatrix} \left[\begin{pmatrix} c-\tau & -b \\ -b & a-\tau \end{pmatrix}\begin{pmatrix}\gamma \\ \delta\end{pmatrix}\right]_{y_1} - \left[\begin{pmatrix} c-\tau & -b \\ -b & a-\tau \end{pmatrix}\begin{pmatrix}\gamma \\ \delta\end{pmatrix}\right]_t$$

$$\begin{aligned} (13) \qquad & - R\begin{pmatrix}\gamma \\ \delta\end{pmatrix}_z + D\begin{pmatrix}\gamma \\ \delta\end{pmatrix} + \begin{pmatrix} a-\tau & b \\ b & c-\tau \end{pmatrix}\begin{pmatrix}\gamma_0 \\ \delta_0\end{pmatrix} \\ & = \begin{pmatrix}0 \\ 0\end{pmatrix} \mod z\frac{\partial\varphi}{\partial z}. \end{aligned}$$

Here R is from (8), D is a very complicated (but real-analytic) matrix, and $(\gamma_0, \delta_0) = (i\alpha_1, i\beta_1) + (f_1, f_2)$, where (f_1, f_2) are determined by (γ, δ). Hence we can treat (γ_0, δ_0) as an arbitrary vector which determines $A_0\binom{\alpha_1}{\beta_1}$. Thus, solving (13), determines (α_1, β_1) up to a solution of (12). Expanding this solution in terms of v_1 and v_2, we get higher order transport equations for the resulting coefficients when we try to eliminate the terms of order ε^2. Thus provided we can solve (13) and the analogous inhomogeneous equation we will be able to eliminate terms of all orders in ε.

To reduce (13) to an equation for γ^s, δ^s, γ^a and δ^a we set

$$B = \begin{pmatrix} \frac{\partial a}{\partial k_1} & \frac{\partial b}{\partial k_1} \\ \frac{\partial b}{\partial k_1} & \frac{\partial c}{\partial k_1} \end{pmatrix} \quad \text{and} \quad A_1 = \begin{pmatrix} c-\tau & -b \\ -b & a-\tau \end{pmatrix},$$

and we assume that γ and δ are linear in z, so that $R\binom{\gamma}{\delta}_z \mod z\frac{\partial\varphi}{\partial z}$ does not bring in new terms. This is no loss of generality in the *Ansatz* since one can always reduce γ and δ to linear functions in z by integration by parts, changing m_1. With these definitions we have

$$(14)\qquad \begin{pmatrix} B^s & (f^2+h)B^a \\ B^a & B^s \end{pmatrix} \left[\begin{pmatrix} A^s_1 & (f^2+h)A^a_1 \\ A^a_1 & A^s_1 \end{pmatrix} \begin{pmatrix} \gamma^s \\ \delta^s \\ \gamma^a \\ \delta^a \end{pmatrix} \right]_{y_1}$$

$$- \left[\begin{pmatrix} A^s_1 & (f^2+h)A^a_1 \\ A^a_1 & A^s_1 \end{pmatrix} \begin{pmatrix} \gamma^s \\ \delta^s \\ \gamma^a \\ \delta^a \end{pmatrix} \right]_t + E \begin{pmatrix} \gamma^s \\ \delta^s \\ \gamma^a \\ \delta^a \end{pmatrix}$$

$$+ \begin{pmatrix} A^s_0 & (f^2+h)A^a_0 \\ A^a_0 & A^s_0 \end{pmatrix} \begin{pmatrix} \gamma^s_0 \\ \delta^s_0 \\ \gamma^a_0 \\ \delta^a_0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}.$$

Here E is a new complicated matrix. Since $A_1 = JA_0J^{-1}$ for $J = \left(\begin{smallmatrix} 0 & 1 \\ -1 & 0 \end{smallmatrix}\right)$, the coefficient

$$M_1 = \begin{pmatrix} A^s_1 & (f^2+h)A^a_1 \\ A^a_1 & A^s_1 \end{pmatrix}$$

has the properties of M_0. In particular it has rank 2 near the base point and A^a_1 is nonsingular.

Making the change of variables

$$\begin{pmatrix} \gamma^s \\ \delta^s \\ \gamma^a \\ \delta^a \end{pmatrix} = \begin{pmatrix} I \\ 0 \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} + \begin{pmatrix} (A^a_1)^{-1}A^s_1 \\ -I \end{pmatrix} \begin{pmatrix} w \\ x \end{pmatrix},$$

the transport equation (14) becomes

(15)
$$\begin{pmatrix} B^s & (f^2+h)B^a \\ B^a & B^s \end{pmatrix} \left[\begin{pmatrix} A_1^s \\ A_1^a \end{pmatrix}\begin{pmatrix} u \\ v \end{pmatrix}\right]_{y_1} - \left[\begin{pmatrix} A_1^s \\ A_1^a \end{pmatrix}\begin{pmatrix} u \\ v \end{pmatrix}\right]_t$$
$$+ F\begin{pmatrix} u \\ v \end{pmatrix} + G\begin{pmatrix} w \\ x \end{pmatrix} = 0 \mod \begin{pmatrix} A_0^s \\ A_0^a \end{pmatrix},$$

where F and G are 4×2 matrices. Finally, since A_0^a is invertible, we can simply eliminate the last two components in (15) to get the fully reduced transport equations

$$\hat{B}\begin{pmatrix} u \\ v \end{pmatrix}_{y_1} - \hat{A}\begin{pmatrix} u \\ v \end{pmatrix}_t + \hat{F}\begin{pmatrix} u \\ v \end{pmatrix} = \hat{G}\begin{pmatrix} w \\ x \end{pmatrix} \tag{16}$$

where

$$\hat{A} = A_1^s - A_0^s(A_0^a)^{-1}A_1^a \quad \text{and}$$
$$\hat{B} = B^s A_1^s + (f^2+h)B^a A_1^a - A_0^s(A_0^a)^{-1}(B^a A_1^s + B^s A_1^a).$$

Restricted to $h = 0$, i.e. to the plane $k_3 = 0$ passing through the vertex in Figure 1, the matrix A_0^s and hence A_1^s must be divisible by f. This makes the transport system (16) Fuchsian on $k_3 = 0$. Since $k_2 = \xi_2 + y_1$ and $\frac{\partial f}{\partial k_2} > 0$, we can use f in place of y_1 as a coordinate in (16) so that on $k_3 = 0$ (16) takes the form

$$f\left(\tilde{B}\begin{pmatrix} u \\ v \end{pmatrix}_f - \tilde{A}\begin{pmatrix} u \\ v \end{pmatrix}_t\right) + \hat{F}\begin{pmatrix} u \\ v \end{pmatrix} = H \tag{17}$$

where $\tilde{B} = 2\frac{\partial A_0}{\partial k_1}\frac{\partial A_1}{\partial k_2} + O(f)$. Since $\partial^2 D/\partial k_2^2 < 0$, $\det \frac{\partial A_0}{\partial k_2} < 0$, and hence $\tilde{B}$ is invertible. Moreover, $f\tilde{B}(A_1^s)^{-1}$ is symmetric with positive determinant near $f = 0$ and $\tilde{A}(A_1^s)^{-1}$ is symmetric. Hence, an analytic change of dependent variables makes (17) into a Fuchsian symmetric hyperbolic system.

The equation (17) has a unique analytic solution for given analytic H, provided the matrix

$$\tilde{B}^{-1}(k_0,\ \tau_0)\hat{F}(k_0,\ \tau_0)$$

has no nonpositive integer eigenvalues (this is the "indicial" condition, see Baouendi and Goulaouic [1]). In addition, since (17) can be made symmetric hyperbolic, the work of Tahara [11] (see particularly Theorem 4.1 of part II and the Introduction of III) shows that under the same indicial condition (17) has a unique C^∞ solution for a given C^∞ function $H(f,t)$. Thus to exhibit packets undergoing magnetic breakdown we may proceed as follows. Choosing $\hat{G}\left(\begin{smallmatrix} w \\ x \end{smallmatrix}\right)$ supported in $f<0$ with support near $t=0$ and assuming the indicial condition, we construct $\left(\begin{smallmatrix} u \\ v \end{smallmatrix}\right)$ depending smoothly on k_3 so that (16) holds to order k_3^∞. Since we are only interested in $k_3 = O(\varepsilon^{1/2})$, the errors in solving (16) are $O(\varepsilon^\infty)$. As mentioned in the introduction, $\left(\begin{smallmatrix} u \\ v \end{smallmatrix}\right)$ and all its k_3-derivatives at $k_3=0$ are uniquely determined by $\hat{G}\left(\begin{smallmatrix} w \\ x \end{smallmatrix}\right)$.

To complete this analysis we need to see what form the term $\hat{G}\left(\begin{smallmatrix} w \\ x \end{smallmatrix}\right)$ can have. The terms which contribute to $G\left(\begin{smallmatrix} w \\ x \end{smallmatrix}\right)$ come from

$$(\langle\psi_1,\ -(R\gamma\psi_1 + R\delta\psi_2)_z\rangle,\ \langle\psi_1,\ -(R\gamma\psi_1 + R\delta\psi_2)_z\rangle)$$

where $\langle\ ,\ \rangle$ denotes the L^2-inner product over a fundamental domain in the lattice. From (8) on sees that

$$R = 2z\left(\frac{\partial f}{\partial k_2}\right)^2 Q_0\left(\frac{\partial\varphi}{\partial y_1}\cdot\ \xi_2 + y_1,\ \xi_3,\ \tau\right),$$

and, hence $R = zP$ where P is analytic in z and positive at the base point. From this one concludes that

$$G = -\begin{pmatrix} P^sI + (zM)^s & (f^2+h)(P^aI + (zM)^a) + zPI^s \\ P^aI + (zM)^a & P^sI + (zM)^s + (zP)^aI \end{pmatrix}\begin{pmatrix} (A_1^a)^{-1}A_1^s \\ -I \end{pmatrix},$$

where M is the matrix

$$P\begin{pmatrix} \langle\psi_1, \psi_{1z}\rangle & \langle\psi_1, \psi_{2z}\rangle \\ \langle\psi_2, \psi_{1z}\rangle & \langle\psi_2, \psi_{2z}\rangle \end{pmatrix}.$$

Since $(zC)^s = fC^s + (f^2+h)C^a$ and $(zC)^a = fC^a + C^s$ for any C, this leads to

$$\begin{aligned}\hat{G} = &- P^s((A^a_1)^{-1}A^s_1 + 2A^s_0(A^a_0)^{-1} - fI) \\ &- P^a(fA^s_0(A^a_0)^{-1} - (f^2+h)I) \\ &- (fM^s + (f^2+h)M^a)(A^a_1)^{-1}A^s_1 + (f^2+h)(fM^a + M^s) \\ &+ A^s_0(A^a_0)^{-1}(fM^a + M^s)(A^a_1)^{-1}A^s_1.\end{aligned}$$

Since $A^s_i = f\tilde{A}_i + k_3\tilde{B}_i$, $\tilde{A}_i$ and $\tilde{B}_i$ analytic,

$$\begin{aligned}\hat{G} = &-P^s((A^a_1)^{-1}A^s_1 + 2A^s_0(A^a_0)^{-1} - fI) \\ &+ fk_3H + f^2L + k_3^2N\end{aligned}$$

where K, L and N are analytic matrix functions. To understand the leading term, $\hat{G}_0 = -P^s((A^a_1)^{-1}A^s_1 + 2A^s_0(A^a_0)^{-1} - fI)$, one can use the following. Choosing $v_\pm$ such that $A_0(z_\pm)v_\pm = 0$, and $\|v_\pm\| = 1$, one has

$$A^s_0(A^a_0)^{-1}v_\pm = \pm\sqrt{f^2+h}\,v_\pm.$$

Also one checks $A^s_0(A^a_0)^{-1}(A^a_1)^{-1}A^s_1 = -(f^2+h)I$. Using these facts, it is easy to compute

$$\hat{G}_0 v_\pm = -P^s(-f \pm \sqrt{f^2+h})v_\pm.$$

Note that by (11) $h = k_3^2\tilde{h}$, where $\tilde{h}$ is analytic and nonzero at $k_3 = 0$.

To see how $\hat{G}$ degenerates on $k_3 = 0$ one begins by noting that v_+ and v_- are discontinuous on $h = 0$ at $f = 0$. However, since $f^{-1}A_0^s(A_0^a)^{-1}$ is analytic on $h = 0$ with eigenvalues ± 1, we can choose $\tilde{v}_\pm$ analytic such that $A_0^s(A_0^a)^{-1}\tilde{v}_\pm = \pm f\tilde{v}_\pm$. Therefore, up to order $f^2, \hat{G}$ is the projection onto $\tilde{v}_-$ along $\tilde{v}_+$ multiplied by $-2fP^s$ on $h = 0$. Thus one can choose $(w,\ x)$ so that $\hat{G}\binom{w}{x}$ is approximately $f\tilde{v}_-$ near $f = k_3 = 0$.

References

[1] M. S. Baouendi and C. Goulaouic, "Cauchy problems with characteristic initial hypersurface," *CPAM* **26** (1973), 455-475.

[2] V. Buslaev, "The quasi-classical approximation for equations with periodic coefficients," *Uspekhi Mat. Nauk* **42** (1987), 77-98.

[2a] V. Buslaev, "On spectral properties of adiabatically perturbed Schrödinger operators with periodic potentials," *Seminaire EDP* 1990-91, *Ecole Polytechnique, Exposé* **23**, April 1991.

[3] C. Gerard and A. Grigis, "Precise estimates of tunnelling and eigenvalues near a potential barrier," *J. Diff. Eq.* **72** (1988), 149-177.

[4] J.-C. Guillot, J. Ralston and E. Trubowitz, "Semi-classical asymptotics in solid state physics," *Commun. Math. Phys.* **116** (1988), 401.

[5] G. A. Hagedorn, "Electron energy level crossings in the time-dependent Born-Oppenheimer approximation," *Theoretica Chimica Acta* **77** (1990), 163-190.

[6] B. Helffer and J. Sjöstrand, "On diamagnetism and de Haas-van Alphen effects," *Ann. Inst. H. Poincaré* **52** (1990), 303-375.

[7] W. Horn, "Semi-classical constructions in solid state physics," *Comm. in P.D.E.* **16** (1991), 255-290.

[8] C. März, "Spectral asymptotics for Hill's equation near the potential maximum," to appear *Asymptotic Analysis.*

[9] J. Sjöstrand, "Density of states oscillations for magnetic Schrödinger operators," preprint Orsay, 1991.

[10] A. A. Slutskin, "Dynamics of conduction electrons under magnetic breakdown conditions," *Soviet Physics JETP* **26** (1968), 474-482.

[11] H. Tahara, "Singular hyperbolic systems I, II, III," *J. Fac. Sci.* Tokyo, Sec. IA Math. **26** (1979), 213-238, **26** (1979), 391-412, **27** (1980), 465-507.

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NEAR—COHOMOLOGY OF HILBERT COMPLEXES AND TOPOLOGY OF NON—SIMPLY CONNECTED MANIFOLDS.

M.Gromov,M.A.Shubin

Introduction

In an earlier paper [5] we introduced some new homotopy invariants of compact non–simply connected manifolds (possibly with boundary) or finite CW–compexes. In terms of these invariants the heat kernel invariants of closed non–simply connected manifolds [9] (see also [4]) can be expressed and thus their homotopy invariance can be proved.

Note that both invariants in [5] and [9] are expressed in terms of L^2–de Rham complex on the universal covering, using the deck transformation action of the fundamental group in differential forms. The use of the combinatorial Laplacians leads to the same invariants as was proved by A. Efremov [3].

In this paper we follow the abstract setting from [5] and give a refined formulation of the abstract result there. This leads to a new notion of near–cohomology for Hilbert complexes. We take a special family of quadric cones depending on a small positive parameter and consisting of cochains which have coboundaries which are small with respect to the distance of the cochains to the space of all cocycles. Heuristically this means that we take cochains with small coboundaries modulo cochains close to cocycles. (Instead of cochains close to cocycles we could also take cochains close to coboundaries which would remind cohomology more but it just adds cohomology as a direct summand.) Near–cohomology are germs of such families of quadric cones modulo an equivalence relation which naturally arises if we consider homotopy equivalence of Hilbert complexes with morphisms given by bounded linear operators. Then near–cohomology becomes a homotopy invariant.

Adding a von Neumann algebra structure to the Hilbert complex we can transform near–cohomology to a set of positive–valued functions of the small parameter up to an equivalence. These functions are defined as maximal von Neumann dimensions of linear spaces which belong to the cones. The equivalence is given by estimates of these functions with dilatated arguments.

Applying these constructions to the de Rham L^2–complex on the universal covering of a compact manifolds (with the von Neumann algebras consisting of operators commuting with deck transformations on differential forms) we obtain invariants which were introduced and studied in [5].

Note that the idea that there may be topology invariants lying near cohomology was first formulated in [8].

1. Hilbert complexex and their near–cohomology.

A. Let us consider a sequence

$$E : 0 \longrightarrow E_0 \xrightarrow{d_0} E_1 \longrightarrow \ldots \longrightarrow E_k \xrightarrow{d_k} E_{k+1} \longrightarrow \ldots \xrightarrow{d_{N-1}} E_N \longrightarrow 0,$$

where E_k is a Hilbert space and the differential $d_k : E_k \longrightarrow E_{k+1}$ is a closed densely defined linear operator (with the domain $D(d_k)$). This sequence is called a *Hilbert complex* if $d_{k+1} \circ d_k = 0$ on $D(d_k)$ or, equivalently, Im $d_k \subset$ Kerd_{k+1}. Note that Ker d_k is always a closed linear subspace in E_k.

Let E' be another Hilbert complex of the same length N (if the lengths differ then we can always formally extend the shorter complex by adding zero spaces in the end; so for the sake of simplicity we shall always suppose that all complexes have the same length N). The corresponding spaces and differentials will be denoted E'_k and d'_k.

Definition 1.1. A *morphism* $f : E \longrightarrow E'$ of the Hilbert complexes is a collection of *bounded* linear operators $f_k : E_k \longrightarrow E'_k$ such that

$$f_{k+1}d_k \subset d'_k f_k,$$

which means that $f_{k+1}d_k = d'_k f_k$ on $D(d_k)$. In particular we require that $f_k(D(d_k)) \subset D(d'_k)$.

If $f : E \longrightarrow E'$ and $g : E' \longrightarrow E''$ are two morphisms of Hilbert complexes then their composition $g \circ f : E \longrightarrow E''$ is a morphism defined as the collection of compositions $g_k \circ f_k$, $k = 0, 1, \dots, N$.

Definition 1.2. Let $f, g : E \longrightarrow E'$ be two morphisms of the same Hilbert complexes. A *homotopy* (between f and g) is a collection T of *bounded* linear operators $T_k : E_k \longrightarrow E'_{k-1}$ such that

$$f_k - g_k - T_{k+1}d_k \subset d'_{k-1}T_k, \; k = 0, 1, \dots, N,$$

or equivalently, $f_k - g_k = T_{k+1}d_k + d'_{k-1}T_k$ on $D(d_k)$ (in particular this means that $T_k(D(d_k)) \subset D(d'_{k-1})$). If there exists a homotopy between morphisms f and g then f and g are called *homotopic* and we denote it as $f \sim g$. (It is easy to check that being homotopic is really an equivalence relation between morphisms.)

Hilbert complexes E, E' are called *homotopy equivalent* if there exists morphisms $f : E \longrightarrow E'$ and $g : E' \longrightarrow E$ such that $g \circ f \sim \mathrm{Id}_E$, $f \circ g \sim \mathrm{Id}_{E'}$ where Id_E and $\mathrm{Id}_{E'}$ are identity morphisms of the corresponding Hilbert complexes. We shall denote the homotopy equivalence between E and E' as $E \sim E'$.

Definition 1.3. E is called a *retract* of E' if there exist morphisms $f : E \longrightarrow E'$ and $g : E' \longrightarrow E$ such that $g \circ f \sim \mathrm{Id}_E$. In this case f (resp. g) is called a *homotopy inclusion* (resp. *homotopy retraction*) map.

Remark. Cohomology spaces $H^k(E) = \mathrm{Ker}\ d_k / \mathrm{Im}\ d_{k-1}$ and reduced cohomology spaces $\overline{H}^k(E) = \mathrm{Ker}\ d_k / \overline{\mathrm{Im}\ d_{k-1}}$ are homotopy functors in the category of Hilbert complexes with morphisms and homotopy as before.

B. Now let us introduce the following quadric cones, depending on the degree k and on a positive parameter λ:

$$B_\lambda^{(k)} = \{\omega|\omega \in E_k/\text{Ker } d_k, \| d_k\omega \| \leq \lambda \| \omega \|_{\text{mod Ker } d}\},$$

where $\| \omega \|_{\text{mod Ker } d}$ is the norm in the quotient space $E_k/\text{Ker } d_k$, $\| d_k\omega \|$ means the norm of $d_k\omega$ in E_{k+1}. It is understood that in this definition we should only take co-sets in $E_k/\text{Ker } d_k$ defined by elements $\omega \in D(d_k)$ to make $d_k\omega$ well defined. So $B_\lambda^{(k)}$ becomes a conic set in the Hilbert space $E_k/\text{Ker } d_k$ which can also be identified with $(\text{Ker } d_k)^\perp$ (the orthogonal complement of Ker d_k in E_k).

Lemma 1.4. Let $\mathcal{H}_1, \mathcal{H}_2$ be Hilbert spaces, $A : \mathcal{H}_1 \to \mathcal{H}_2$ be a closed linear operator with the domain $D(A)$. Then for every $\lambda > 0$ the set

$$C_{\lambda,A} = \{x|x \in D(A), \| Ax \| \leq \lambda \| x \|\}$$

is closed in $\mathcal{H}_1$.

Proof. Suppose that x is in the closure of $\mathcal{C}_{\lambda,A}$. Without loss of generality we may assume that $\| x \| = 1$. Then we easily obtain that there exist $x_\gamma \in C_{\lambda,A}$ such that

$$\lim_\Gamma \| x_\gamma - x \| = 0, \| Ax_\gamma \| \leq \lambda \| x_\gamma \|, \gamma \in \Gamma,$$

where Γ is a directed set. Taking a cofinal subset of Γ we may further suppose that $\| x_\gamma \| \leq 1+\varepsilon$ whatever fixed $\varepsilon > 0$. Changing Γ again we may suppose that there exists $w - \lim_\Gamma Ax_\gamma = y$ (weak limit is taken in $\mathcal{H}_2$). Then we have

$$\| y \| \leq \liminf_\Gamma \| Ax_\gamma \| \leq \lambda \liminf_\Gamma \| x_\gamma \| \leq \lambda \| x \|$$

Now the pair $\{x, y\}$ is in the weak closure of the graph of the operator A in $\mathcal{H}_1 \times \mathcal{H}_2$. The graph is a closed linear subspace, hence it is weakly closed. Therefore $x \in D(A)$ and $y = Ax$. Hence $x \in C_{\lambda,A}$ as required. $\square$

Applying Lemma 1.4 to $\mathcal{H}_1 = E_k/\text{Ker } d_k$, $\mathcal{H}_2 = E_{k+1}$ and $A = d_k$ we see that $B_\lambda^{(k)}$ is a closed cone in $E_k/\text{Ker } d_k$ for every

$\lambda > 0$. Now let us look what happens to these cones when we apply morphisms of Hilbert complexes.

Let us consider a morphism of Hilbert complexes $f : E \longrightarrow E'$ defined by a collection of bounded linear operators $f_k : E_k \longrightarrow E'_k$, $k = 0, \dots, N$. Then $f_k(\text{Ker } d_k) \subset \text{Ker } d'_k$ so f_k naturally defines a bounded linear operator

$$\hat{f}_k : E_k/\text{Ker } d_k \longrightarrow E'_k/\text{Ker } d'_k.$$

Theorem 1.5. Let a Hilbert complex E be a retract of E' and $f : E \longrightarrow E'$, $g : E' \longrightarrow E$ be corresponding homotopy inclusion and retraction maps. Let $B_\lambda^{(k)}$, $'B_\lambda^{(k)}$ be families of cones defined as before in E, E' respectively. Then there exist $C > 0$ and $\lambda_0 > 0$ such that for every $\lambda \in (0, \lambda_0)$

(i) $$\hat{f}_k(B_\lambda^{(k)}) \subset {}'B_{C\lambda}^{(k)};$$

(ii) $$\| \omega \| \le C \| \hat{f}_k \omega \| \ \text{ if } \omega \in B_\lambda^{(k)}.$$

Proof. Let us consider $\omega \in B_\lambda^{(k)}$ and let $\omega_1 \in (\text{Ker } d_k)^\perp$ represent ω i.e. $\omega_1 \mod \text{Ker } d_k = \omega$. Then $\| d_k\omega_1 \| \le \lambda \| \omega_1 \|$. It follows that $f_k\omega_1 \in D(d'_k)$, $d'_k f_k \omega_1 = f_{k+1} d_k \omega_1$ and

$$\| d'_k(f_k\omega_1) \| = \| f_{k+1}(d_k\omega_1) \| \le \| f_{k+1} \| \| d_k\omega_1 \| \le \lambda \| f_{k+1} \| \| \omega_1 \|$$

Now we should estimate $\| \omega_1 \|$ by $C_1 \| f_k\omega_1 \|_{\text{mod Ker } d'}$ provided $\lambda \in (0, \lambda_0)$ with a small $\lambda_0 > 0$ with a constant C_1 which does not depend on ω_1 or λ. Then (i) and (ii) will follow. Let us split $f_k\omega_1$ into the sum

$$f_k\omega_1 = \omega'_1 + \omega'_2$$

with $\omega'_2 \in \text{Ker } d'_k, \omega'_1 \perp \text{Ker } d'_k$. Hence

$$\| f_k\omega_1 \|_{\text{mod Ker } d'} = \| \omega_1' \| \ .$$

Now let us use a homotopy T between $g \circ f$ and Id_E. In particular we have

$$\mathrm{Id}_E - g_k \circ f_k = T_{k+1}d_k + d_{k-1}T_k \text{ on } D(d_k).$$

hence

$$\begin{aligned}\omega_1 =& g_k(f_k\omega_1) + T_{k+1}d_k\omega_1 + d_{k-1}T_k\omega_1 = \\ & g_k(\omega_1' + \omega_2') + T_{k+1}d_k\omega_1 + d_{k-1}T_k\omega_1.\end{aligned}$$

Clearly $g_k\omega_2' \in \text{ Ker } d_k$, hence

$$\omega_1 \equiv g_k\omega_1' + T_{k+1}d_k\omega_1 \text{ mod Ker } d_k.$$

It follows that

$$\begin{aligned}\| \omega_1 \| \leq \| g_k\omega_1' + T_{k+1}d_k\omega_1 \| \leq \| g_k \| \| \omega_1' \| + \| T_{k+1} \| \| d_k\omega_1 \| \leq \\ \leq \| g_k \| \| \omega_1' \| + \lambda \| T_{k+1} \| \| \omega_1 \|,\end{aligned}$$

hence

$$\| \omega_1 \| \leq \frac{\| g_k \| \| \omega_1' \|}{1 - \lambda \| T_{k+1} \|} \leq 2 \| g_k \| \| \omega_1' \|,$$

if $\lambda \in (0, \lambda_0)$ where $\lambda_0 = (2 \| T_{k+1} \|)^{-1}$. This gives the required estimate that proves the Theorem. □

Corollary 1.6. Suppose that Hilbert complexes E, E' are homotopy equivalent and this equivalence is given by the morphisms $f : E \longrightarrow E'$ and $g : E' \longrightarrow E$. Then there exist constants $C > 0$, $\lambda_0 > 0$ such that for every $\lambda \in (0, \lambda_0)$ and for every $k = 0, \dots, N$

(i) $$\hat{f}(B_\lambda^{(k)}) \subset {}'B_{C\lambda}^{(k)};\ \hat{g}({}'B_\lambda^{(k)}) \in B_{C\lambda}^{(k)};$$

(ii) $\| \omega \| \leq C \| \hat{f}\omega \|,\ \omega \in B_\lambda^{(k)};\ \| \omega' \| \leq C \| \hat{g}\omega' \|,\ \omega' \in {}'B_\lambda^{(k)}.$

Now we can introduce an appropriate notion of near–cohomology of a Hilbert complex. This will be done along the lines that can be traced in Corollary 1.6.

Definition 1.7. *Special family of quadric cones* in a Hilbert space E is a family of closed subsets $B_\lambda \subset E$ defined for all $\lambda > 0$ as follows:

$$B_\lambda = \{x \mid x \in D(A), \| Ax \| \leq \lambda \| x \|\},$$

where $A: \ E \longrightarrow E_1$ is a closed densely defined linear operator (E_1 is another Hilbert space) with the domain $D(A)$, the norms $\| Ax \|$ and $\| x \|$ are taken in E_1 and E respectively.

Two such families $B_\lambda \subset E$ and $'B_\lambda \subset E'$ are called *equivalent* if there exist two bounded linear operators: $f: \ E \longrightarrow E'$, $g: E' \longrightarrow E$ and positive constants $C > 0$, $\lambda_0 > 0$ such that for every $\lambda \in (0, \lambda_0)$

(i) $$f(B_\lambda) \subset {}'B_{C\lambda}, \ g({}'B_\lambda) \subset B_{C\lambda};$$

(ii) $$\| x \| \leq C \| fx \|, \ x \in B_\lambda; \ \| x' \| \leq C \| gx' \|, \ x' \in {}'B_\lambda.$$

So in fact up to the equivalence only the germ of the family B_λ near 0 is important.

Definition 1.8. Let E be a Hilbert complex. Its *near cohomology* $NH^k(E)$ of degree k is the equivalence class of the special family of quadric cones $B_\lambda^{(k)}$.

Corollary 1.6 means then that the near–cohomology is a homotopy invariant of the Hilbert complex if the homotopy equivalence is defined as a chain homotopy equivalence with bounded morphisms and homotopy operators as in Definitions 1.1 and 1.2.

Remark. All results of this Section can be easily extended to complexes of reflexive Banach spaces.

2. Von Neumann structure

Von Neumann structure on a Hilbert complex allows to transform near–cohomology to some simpler invariants: to make the same kind of transfer from homotopy to the Betti numbers.

First we shall recall some necessary definitions (see e.g. [2]). Let $\mathcal{H}$ be a Hilbert space, $\mathcal{B}(\mathcal{H})$ be the algebra of all bounded linear operators in $\mathcal{H}$. A *von Neumann algebra* of operators in $\mathcal{H}$ is a subalgebra $\mathcal{A} \subset \mathcal{B}(\mathcal{H})$ satisfying the following conditions:

(i) $A \ni \mathrm{Id}_{\mathcal{H}}$, $\mathcal{A}$ is a $*$–algebra (i.e. $A \in \mathcal{A} \Rightarrow A^* \in \mathcal{A}$),
(ii) $\mathcal{A}$ is closed in the weak operator topology.

Let $\mathcal{A}^+ = \{A \mid A \in \mathcal{A},\ A \geq 0\}$. A *trace* $\mathrm{Tr}_{\mathcal{A}}$ on $\mathcal{A}$ is a map $\mathrm{Tr}_{\mathcal{A}} : \mathcal{A}^+ \longrightarrow [0, +\infty]$ satisfying the following conditions:

(i) $\mathrm{Tr}_{\mathcal{A}}(\lambda_1 A_1 + \lambda_2 A_2) = \lambda_1 \mathrm{Tr}_{\mathcal{A}} A_1 + \lambda_2 \mathrm{Tr}_{\mathcal{A}} A_2$ if $\lambda_i \in [0, +\infty]$, $A_i \in \mathcal{A}^+$, $i = 1, 2$,
(ii) $\mathrm{Tr}_{\mathcal{A}}(AA^*) = \mathrm{Tr}_{\mathcal{A}}(A^*A)$ for every $A \in \mathcal{A}$,
(iii) If $A_\gamma \in \mathcal{A}^+$ and $A_\gamma \nearrow A$ then $\mathrm{Tr}_{\mathcal{A}} A_\gamma \longrightarrow \mathrm{Tr}_{\mathcal{A}} A$ (normality);
(iv) $\mathrm{Tr}_{\mathcal{A}} A = \sup\{\mathrm{Tr}_{\mathcal{A}} B | 0 \leq B \leq A, B \in \mathcal{A}, \mathrm{Tr}_{\mathcal{A}} B < \infty\}$ for every $A \in \mathcal{A}^+$ (semi–finiteness);
(v) $\mathrm{Tr}_{\mathcal{A}} A = 0$, $A \in \mathcal{A}^+ \Rightarrow A = 0$ (faithfulness).

If a trace $\mathrm{Tr}_{\mathcal{A}}$ is given on $\mathcal{A}$ then we can define *von Neumann dimension* $\dim_{\mathcal{A}}$. It is defined on all closed subspaces $L \subset \mathcal{H}$ which are *affiliated* with $\mathcal{A}$ i.e. such that $P_L \in \mathcal{A}$ where P_L is the orthogonal projection in $\mathcal{H}$ with the image L. Then we write $L \eta \mathcal{A}$ and $\dim_{\mathcal{A}} L = \mathrm{Tr}_{\mathcal{A}} P_L$.

Definition 2.1. Let E be a Hilbert complex. A *von Neumann structure on* E is a collection of von Neumann algebras $\mathcal{A}_k \subset \mathcal{B}(E_k)$ for all $k = 0, \dots, N$, and a trace $\mathrm{Tr}_{\mathcal{A}}$ on every algebra $\mathcal{A}_k$ (we denote all the traces $\mathrm{Tr}_{\mathcal{A}}$ for all k for simplicity of notations because it does not lead to a confusion), provided $\mathrm{Ker}\, d_k$ is affiliated with $\mathcal{A}_k$ for every k.

Now modelling the well known variational principle (Glazman's Lemma) for the operators $d_k^* d_k$ we can introduce the following functions which will imitate the eigenvalue distribution function of the discrete spectrum.

Definition 2.2.
$$F_k(\lambda) = \sup_{L \subset B_\lambda^{(k)}} \dim_{\mathcal{A}} L$$

Here it is convenient to identify $E_k/\mathrm{Ker}\ d_k$ with $(\mathrm{Ker}\ d_k)^\perp$ so L can be considered as a closed linear subspace in E_k (such that in fact $L \subset (\mathrm{Ker}\ d_k)^\perp$), hence $\dim_{\mathcal{A}} L$ makes sense.

Since the cones $B_\lambda^{(k)}$ increase with λ the function $F_k(\lambda)$ is an increasing function on $(0, \infty)$. If $F_k(\lambda_0) < \infty$ for some $\lambda_0 > 0$ then $F_k(+0) = 0$.

Now let us introduce morphisms and homotopy equivalence for Hilbert complexes with von Neumann structure.

Definition 2.3. Let E, E' be Hilbert complexes with von Neumann structures,
$f : E \longrightarrow E'$ a morphism of Hilbert complexes. Then f is called *compatible* with von Neumann structures if the following condition is satisfied:

(C) *Suppose that* $L \subset E_k, L\eta\mathcal{A}_k$ *and there exists* $C > 0$ *such that*

$$\| x \| \le C \| f_k x \|, \ x \in L.$$

Then $f_k(L)\eta\mathcal{A}'_k$ *and* $\dim_{\mathcal{A}'} f_k(L) = \dim_{\mathcal{A}} L$.

Roughly speaking this means that the morphism f conserves the von Neumann dimension of a subspace provided this subspace is mapped by f isomorphically (in topological sense).

Definition 2.4. Let E, E' be Hilbert complexes with von Neumann structures. They are called *homotopy equivalent* if there exist morphisms of Hilbert complexes compatible with von Neumann structure $f : E \longrightarrow E'$, $g : E' \longrightarrow E$, such that $f \circ g \sim \mathrm{Id}_{E'}$, $g \circ f \sim \mathrm{Id}_E$. (Here homotopy between morphisms is understood as in Sect. 1 without any additional compatibility conditions). E is called a *retract* of E' if there exist morphisms (again compatible with von Neumann structure) $f : E \longrightarrow E'$, $g : E' \longrightarrow E$ such that $g \circ f \sim \mathrm{Id}_E$. The following theorem is an immediate corollary of Theorem 1.5.

Theorem 2.5. Let E, E' be Hilbert complexes with von Neumann structures and E a retract of E'. Denote by F_k, F'_k the functions defined for E, E' according to Definition 2.2. Then there exist $C > 0, \lambda > 0$ such that for every $k = 0, \dots, N$

$$F_k(\lambda) \leq F'_k(C\lambda), \ \lambda \in (0, \lambda_0).$$

Corollary 2.6. Suppose that Hilbert complexes E, E' with von Neumann structure are homotopy equivalent. Then there exist $C > 0, \lambda_0 > 0$ such that

$$F_k(C^{-1}\lambda) \leq F'_k(\lambda) \leq F_k(C\lambda), \ \lambda \in (0, \lambda_0).$$

This corollary tells that the asymptotics of F_k and F'_k near zero coincide in a weak sense. In particular let us introduce

$$\beta_k = \liminf_{\lambda \downarrow 0} \frac{\log F_k(\lambda)}{\log \lambda}$$

and let β'_k mean the same number for F'_k.

Corollary 2.7. If E, E' are as in Corollary 2.6 then $\beta_k = \beta'_k$ for all $k = 0, \dots, N$.

Hence β_k is a homotopy invariant of the Hilbert complex E with the von Neumann structure. We can also introduce an equivalence relation between functions F_k, F'_k given by the inequalities in Corollary 2.6. Then the equivalence class of F_k will be a homotopy invariant of the Hilbert complex E with the von Neumann structure.

3. Geometric examples.

Let X be a compact Riemannian manifold (possibly with a piecewise smooth boundary), M its universal covering with the lifted from X Riemannian metric. Then let us take $E_k = L^2 \wedge^k (M)$, the Hilbert space of all square integrable exterior differential forms of degree k on M. Let us define d_k as the de Rham exterior differential on E_k with the maximal domain i.e.

$$D(d_k) = \{\omega | \omega \in L^2 \wedge^k (M), \ d\omega \in L^2 \wedge^{k+1} (M)\},$$

where $d\omega$ is understood in the sense of distributions. Thus we obtain a Hilbert de Rham complex $L^2 \wedge^\bullet (M)$. Its near–cohomology are homotopy invariants of X if homotopy invariance is understood already in the usual topology sense (for the proof see reasoning given in [5], Sect. 5). Note that the group $\Gamma = \pi_1(X)$ acts on M by deck transformations and a more general example can be obtained if we consider a more general discrete group Γ acting without fixed points as a discrete group of isometries of a Riemannian manifold M (with boundary) so that the orbit space $X = M/\Gamma$ is compact. Then similarly defined near–cohomology will be homotopy invariants in the homotopy category of Γ–manifolds and Γ–maps.

The action of Γ by isometries on the spaces $L^2 \wedge^k (M)$ (induced by the change–of–variable maps on differential forms) allows to introduce a von Neumann structure on $L^2 \wedge^\bullet (M)$ if we define

$$\mathcal{A}_k = \{A | A \in \mathcal{B}(L^2 \wedge^k (M)),\ A\gamma^* = \gamma^* A \text{ for every } \gamma \in \Gamma\}$$

(where γ^* is the change–of–variable map on $L^2 \wedge^k (M)$ given by γ) and take $\mathrm{Tr}_{\mathcal{A}} = \mathrm{Tr}_\Gamma$, the Γ–trace introduced by M. Atiyah in [1]. It is shown in [5] that the heat–kernel invariants introduced in [9] (see also [4]) for the case of manifolds without boundary can be expressed in terms of the functions F_k and the numbers β_k, and in this way the homotopy invariance of the heat–kernel invariants can be proved. Note that the result of A. Efremov [3] means really the coincidence of the near–cohomology of a closed manifold and its simplicial approximation.

Another geometrical example naturally arises if we consider a foliation with a transverse measure on a compact manifold. The arguments from [3] can be applied here too. This fact was independently noticed by J.L.Heitsh and C. Lazarov.

Note finally that some calculations of heat–kernel invariants made by J. Lott (see [6],[7]) allow to make some conclusions about the numbers β_k (and sometimes even calculate them, e.g. for the case when M is the hyperbolic space).

REFERENCES

[1] M. Atiyah, *Elliptic operators, discrete groups and von Neumann algebras*, Asterisque, 32–33 (1976), 43–72.

[2] J. Dixmier, *Les algèbres d'opérateurs dans l'espace Hilbertien (Algèbres de von Neumann)*, 2nd ed. Gauthier–Villars, Paris (1969).

[3] A.V. Efremov, *Combinatorial and analytic Novikov–Shubin invariants*, Preprint.

[4] D.V. Efremov, M.A. Shubin, *Spectrum distribution function and variational principle for automorphic operators on hyperbolic space*, Seminaire Équations aux Derivees Parielles. École Polytechnique. Centre de mathematiques. 1988–1989, Expose VIII.

[5] M. Gromov, M.A. Shubin, *Von Neumann spectra near zero*, Geometric Analysis and Functional Analysis, v. 1, no. 4.

[6] J. Lott, *Heat kernels on covering spaces and topological invariants*, Preprint, IHES/M/90/47, Juin 1990.

[7] J. Lott, *Heat kernels on covering spaces and topological invariants*, Proc. of 1990 Summer Institute on Differential Geometry.

[8] S.P. Novikov, M.A. Shubin, *Morse inequalities and von Neumann II_1-factors*, Doklady Akad. Nauk SSSR **289** (1986), 289–292.

[9] S.P. Novikov, M.A. Shubin, *Morse theory and Neumann invariants of non–simply connected manifolds*, Uspekhy Matem. Nauk **41** (1986), no. 5, 222–223.

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The Scott correction and the quasi-classical limit

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The Scott Correction and the Quasi-classical Limit

Barry Simon[1]

The Scott correction is the second term in a large Z asymptotic expansion of the total binding energy of an atom with nuclear charge Z. The atom is a complicated system with multiparticle correlations among the electrons. Nevertheless, the proof of the Scott correction can be reduced to the study of the semi-classical limit of a one-body system where the electron-electron interaction is replaced by an averaged self-consistent potential.

This reduction is more or less well-known to the experts in the field, so this paper is unabashedly pedagogic. However, previous discussions have so intertwined the reduction to the classical limit with the control of that limit that the simplicity of the reduction has been hidden.

Basically, we will compare a quantum Hamiltonian, H, with a quasi-classical Hamiltonian, H^{QC}, with responding energies E and E^{QC}, and ground states Ψ and Ψ^{QC} and we will show (modulo a fact about the quasi-classical limit) that:

$$E \leq (\Psi^{QC}, H\Psi^{QC}) = E^{QC} + O(Z^{5/3})$$

$$E^{QC} \leq (\Psi, H^{QC}\Psi) = E + O(Z^{5/3})$$

where $E \sim Z^{7/3}$ and the Scott correction is $O(Z^2)$.

To be precise, the N-electron charge Z atomic Hamiltonian acts on $L^2_a\mathbb{R}^{3N}$ by

$$H = \sum_{i=1}^{N}\Big(-\Delta_i - \frac{Z}{|x_i|}\Big) + \sum_{i<j}\frac{1}{|x_i - x_j|} \tag{1}$$

where a point in R^{3N} is written as $(x_1, \ldots, x_N)$ with $x_i \in \mathbb{R}^3$ and L^2_a means those functions $\Psi(x_1, \ldots, x_N)$ in L^2 which are antisymmetric under interchanges of coordinates.

The Hamiltonian H has several simplifications. We ignore electron spin which affects the statistics. It can be easily accommodated by changing the

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constants in the discussion below. We ignore corrections due to a finite nuclear mass. We ignore relativistic corrections.

What will concern us is the total binding energy:

$$E(N,Z) \equiv \inf_{\Psi}(\Psi, H\Psi) = \inf \operatorname{spec}(H)$$

and

$$E(Z) \equiv E(N=Z,Z)$$

We will henceforth take $N = Z$ without further comment.

To describe the quasi-classical problems, we describe the Thomas-Fermi model (invented by Thomas [16] and Fermi [3]). This posits an electron gas with density $\rho(x)$ obeying

$$\int \rho(x)dx = Z \tag{2a}$$

and energy given by

$$\mathcal{E}_{TF}(\rho) = d\int \rho^{5/3}(x)dx - \int \rho(x)|x|^{-1}Z + \frac{1}{2}\int \frac{\rho(x)\rho(y)}{|x-y|} \tag{2b}$$

where d is the universal constant $\frac{3}{5}\left(\frac{3}{4\pi}\right)^{5/3}$ defined so that the sum of the first N eigenvalues of the Dirichlet Laplacian in a cubic region of volume V is asymptotic as $N \to \infty$ to

$$dV(N/V)^{5/3}$$

Thus, the first term is a quasi-classical limit of the kinetic energy term in (1) and the other terms are clearly the nuclear attraction and electron-electron repulsion.

According to Lieb-Simon [7,8], there is a unique ρ, call it ρ_Z^{TF}, minimizing

$$E^{TF}(Z) = \inf\{\mathcal{E}_{TF}(\rho) \mid \text{(2a) holds; } \rho \in L^1 \cap L^{5/3}\}$$

and moreover,

$$E(Z)/E^{TF}(Z) \to 1 \tag{3}$$

as $Z \to \infty$.

It is fairly easy to determine the Z dependence of TF theory:

$$\rho_Z^{TF}(x) = Z^2 \rho_1^{TF}(Z^{1/3}x)$$

$$E^{TF}(Z) = Z^{7/3}E^{TF}(1) \equiv Z^{7/3}e_{TF}$$

In what follows, a critical role will be played by the TF potential

$$\varphi_Z^{TF}(x) \equiv \frac{Z}{|x|} - \int |x-y|^{-1}\rho_Z^{TF}(y)dy$$

Note that the Euler-Lagrange equations for minimizing $\mathcal{E}$ read

$$\frac{5}{3}d\rho^{2/3} = \varphi \tag{4}$$

Equation (3) says that $E(Z) \sim e_{TF}Z^{7/3}$ as $Z \to \infty$. There has been work on the next two terms in the asympototic series. Scott [11] looked at the situation where the electron repulsion is dropped and the N-body problem reduces to a one-body problem (Hydrogen atom), which can be exactly solved. He noted the leading corrections to the Thomas-Fermi analog for this model of order Z^2 came from the inner shells where the electron repulsion shouldn't matter; so he posited that the $O(Z^2)$ term was the same for the true atomic case. That

$$E(Z) = e_{TF}Z^{7/3} + e_{\text{Scott}}Z^2 + o(Z^2) \tag{5}$$

was proven recently by Hughes [4] and Siedentop-Weikard [13]. A recent preprint of Ivrii-Sigal [5] provides a new proof and extends the result to the molecular case.

Fefferman-Seco [2] have announced control of the $Z^{5/3}$ term, which has a contribution due to electron exchange (computed originally by Dirac [1]) and one from the higher order classical limit (computed by Schwinger [10]). Actually Fefferman-Seco study $\inf_N E(Z, N)$, not $E(Z)$ but they should be the same to $O(Z^{5/3})$.

These proofs are all over 100 pages and one of our goals here is to hope for a proof of the Scott correction on one foot.

The quasi-classical problem we will relate to H is given by

$$H^{QC} = \sum_{i=1}^{Z}\Big(-\Delta_i - \varphi_Z^{TF}(x)\Big) - \frac{1}{2}\int \frac{\rho_Z^{TF}(x)\rho_Z^{TF}(y)}{|x-y|}\, d^3x\, d^3y \tag{6}$$

The final term in H^{QC} is a number (constant), which needs to be there because φ_Z overcounts the energy of interaction. In fact, the constant is exactly ([8]),

$$-\frac{1}{3}e_{TF}Z^{7/3}$$

By scaling $\varphi_Z^{TF} = Z^{4/3}\varphi_1^{TF}(Z^{1/2}x)$ so $-\Delta_i - \varphi_Z^{TF}(t)$ is unitarily equivalent to $Z^{4/3}h_Z^{QC}$ where

$$h_Z^{QC} = -Z^{-2/3}\Delta - \varphi_1^{TF}(x)$$

Thus, h^{QC} is a one-body Hamiltonian with $\hbar = Z^{-1/3}$ and $Z \to \infty$ is the $\hbar \to 0$ limit. Let

$$e_1^{QC}(Z) \leq e_2^{QC}(Z) \leq \cdots$$

be the eigenvalues of h_Z^{QC} with eigenfunction $\eta_1^{QC;Z}$, $\eta_2^{QC;Z}$, ... Then

$$E^{QC}(Z) \equiv \text{ inf spec}(H^{QC}) = Z^{4/3}\sum_{i=1}^{Z} e_i^{QC}(Z) - \frac{1}{3}e_{TF}Z^{7/3}$$

and the one electron density for H^{QC} is

$$\rho_Z^{QC}(x) = Z\sum_{i=1}^{Z} \left|\eta_i^{QC;Z}(Z^{1/3}x)\right|^2$$

Our goal is to prove:

THEOREM.

$$\left|E(Z) - E^{QC}(Z)\right| \le cZ^{5/3} + \frac{1}{2}\int \frac{\delta\rho(x)\delta\rho(y)}{|x-y|}\, d^3x\, d^3y$$

where

$$\delta\rho(x) = \left[\rho_Z^{TF}(x) - \rho_Z^{QC}(x)\right]$$

The point is that the $\delta\rho$ Coulomb energy is

$$Z^{7/3}\frac{1}{2}\int \frac{\delta\tilde{\rho}(x)\,\delta\tilde{\rho}(y)}{|x-y|}$$

with

$$\delta\tilde{\rho} = \left[\frac{1}{Z}\sum_{i=1}^{Z} |\eta_i(x)|^2\right] - \rho_1^{TF}(x)$$

The leading order for $\frac{1}{Z}\sum \eta_i^2$ is ρ_1 by (4), so good control of the classical limit should imply that $\delta\tilde{\rho} \sim Z^{-1/3}$ so one expects that

$$\frac{1}{2}\int \frac{\delta\rho(x)\delta\rho(y)}{|x-y|} = O(Z^{5/3}) \tag{7}$$

or less (Seco [12] tells us that it is less). Thus, the Scott correction (5) would follow from control of E^{QC}, a one-body problem, to $O(Z^2)$ and a proof of (7).

We now turn to the proof of the Theorem. We will show that

$$E(Z) \le E^{QC}(Z) + \frac{1}{2}\int \frac{\delta\rho(x)\delta\rho(y)}{|x-y|}\, d^3x\, d^3y \tag{8a}$$

and

$$E^{QC}(Z) \le E(Z) + cZ^{5/3} \tag{8b}$$

To prove (8a), let Ψ^{QC} be the ground state of H^{QC}, so

$$\Psi^{QC}(x_1,\dots,x_N) = (Z!)^{-1/2}\det\big(\xi_i^{QC}(x_j)\big)$$

with $\xi_i^{QC}(x) = Z^{1/2}\eta_i^{QC;Z}(Z^{1/3}x)$. Then

$$\begin{aligned} E(Z) &= \big(\Psi^{QC}, H\Psi^{QC}\big) \\ &= E^{QC}(Z) + \big(\Psi^{QC}, (H - H^{QC})\Psi^{QC}\big) \end{aligned}$$

Now $H - H^{QC}$ has three terms:

(a) $\big(\Psi^{QC}, \sum_i\big[\varphi_Z^{TF}(x_i) - Z|x_i|^{-1}\big]\Psi^{QC}\big) = -\int \frac{\rho^{TF}(y)\rho^{QC}(x)}{|x-y|}\, d^3x\, d^3y$ since $(\Psi^{QC}, (\sum_i W(x_i))\Psi^{QC}) = \int W(x)\rho^{QC}(x)dx$ for any W.

(b) $\big(\Psi^{QC}, \sum_{i<j} \frac{1}{|x_i - x_j|}\Psi^{QC}\big) \equiv \frac{1}{2}\int \frac{\rho^{QC}(x)\rho^{QC}(y)}{|x-y|}\, d^3x\, d^3y - Ex(\Psi^{QC})$ where the exchange energy, $Ex(\Psi)$ is defined for any Ψ as:

$$Ex(\Psi) = -\Big(\Psi, \sum_{i<j}\frac{1}{|x_i - x_j|}\Psi\Big) + \frac{1}{2}\int\frac{\rho_\Psi(x)\rho_\Psi(y)}{|x-y|}\, d^3x\, d^3y \qquad (9)$$

where

$$\rho_\Psi(x) = Z\int |\Psi(x, x_2, \dots, x_N)|^2 d^3x_2 \dots d^3x_N$$

is the one particle density. For determinantal Ψ one can compute $Ex(\Psi)$ explicitly and see that

$$Ex(\Psi) \ge 0$$

using the positive definiteness of the kernel $|x-y|^{-1}$. Thus, this term is $\le \int \frac{\rho^{QC}(x)\rho^{QC}(y)}{|x-y|}\, d^3x\, d^3y$.

(c) The explicit term $\frac{1}{2}\int \frac{\rho^{TF}(x)\rho^{TF}(y)}{|x-y|}\, d^3x\, d^3y$ in the definition of H^{QC}.

Putting these three terms together yields (8a).

To prove (8b), let Ψ be the true ground state of the quantum Hamiltonian and let ρ^Q be its one particle density. Then

$$\begin{aligned} E^{QC}(Z) &\equiv (\Psi, H^{QC}\Psi) \\ &= E(Z) + \big(\Psi, (H^{QC} - H)\Psi\big) \end{aligned}$$

The calculation of the second term is identical to the one done for $(\Psi^{QC}, (H - H^{QC})\Psi^{QC})$, viz

$$(\Psi, (H^{QC} - H)\Psi) = Ex(\Psi) - \frac{1}{2}\int \frac{(\delta_1\rho)(x)(\delta_1\rho)(y)}{|x-y|}\, d^3x\, d^3y$$

where

$$(\delta_1\rho)(x) = \rho^Q(x) - \rho^{TF}(x)$$

By the positive definiteness of $|x-y|^{-1}$, the second term is negative. Now we need to pull a rabbit out of our hat, namely, an inequality of Lieb [6]:

$$Ex(\Psi) \le c\int \rho_\Psi(x)^{4/3} d^3x$$

for any Ψ. Thus, by the Schwartz inequality:

$$E^{QC}(Z) \le E(Z) + c\Big(\int \rho(x)d^3x\Big)^{1/2}\Big(\int \rho^{5/3}(x)d^3x\Big)^{1/2}$$

Now by definition of ρ:

$$\int \rho(x)d^3x = Z$$

and by the Lieb-Thirring inequality and the virial theorem:

$$\begin{aligned}\int \rho^{5/3}(x)d^3x &\le c(\Psi, -\Delta\Psi)\\ &\le c[-E(Z)]\\ &\le dZ^{7/3}\end{aligned}$$

by an elementary estimate on the quantum binding energy (for example, drop the Coulomb repulsion and use Hydrogen eigenvalues). Thus

$$E^{QC}(Z) \le E(Z) + c'Z^{1/2}(Z^{7/3})^{1/2} = E(Z) + c'Z^{5/3}$$

proving (8b) and so the Theorem. □

We close with several remarks about the proof:

(1) If one proves that $E - E^{QC} = O(Z)^{5/3}$ (i.e., if one proves that $\int \frac{(\delta\rho)(x)(\delta\rho)(y)}{|x-y|}\, d^3x\, d^3y = O(Z^{5/3})$), then the proof shows that

$$\int \frac{(\delta_1\rho)(x)(\delta_1\rho)(y)}{|x-y|}\, d^3x\, d^3y = O(Z^{5/3})$$

so we get some control on the approach of ρ^Q to ρ^{TF}.

(2) To use these ideas to go to the $Z^{5/3}$ term, we would need to show that the $\delta\rho$ Coulomb energies are $o(Z^{5/3})$, control E^{QC} to $O(Z^{5/3})$ and get control of $Ex(\Psi)$ and $Ex(\Psi^{QC})$. Control of $Ex(\Psi^{QC})$ should be possible as Dirac did his calculation. $Ex(\Psi)$ is a full many-body question.

(3) To prove the Lieb-Simon result on leading order for $E(Z)$, one only proves some leading order results on the quasi-classical limit. For energy, this can be done via path integrals [14], coherent states [15] or Dirichlet-Neumann bracketing [9]. The $\delta\rho$ Coulomb energy should be accessible via L^1 bounds and local L^q convergence of ρ.

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REFERENCES

[1] P.A.M. Dirac, Note on exchange phenomena in the Thomas atom, *Proc. Camb. Philos. Soc.* **26** (1930), 376–385.
[2] C.L. Fefferman and L. Seco, On the energy of a large atom, *Bull. Amer. Math. Soc.* **23** (1990), 525–530.
[3] E. Fermi, Un metodo statistico per la determinazione di alcune priorietà dell'atomo, *Rend. Accad. Naz. Lincei* **6** (1927), 602–607.
[4] W. Hughes, *Advances in Math.* (to appear).
[5] V. Ja. Ivrii and I.M. Sigal, Asymptotics of the ground state energies of large Coulomb systems (to appear).
[6] E.H. Lieb, A lower bound for Coulomb Energies, *Phys. Lett. A* **70** (1979), 444–446.
[7] E.H. Lieb and B. Simon, Thomas-Fermi theory revisited, *Phys. Rev. Lett.* **31** (1973), 681–683.
[8] E.H. Lieb and B. Simon, The Thomas-Fermi theory of atoms, molecules and solids, *Advances in Math.* **23** (1977), 22–116.
[9] M. Reed and B. Simon, *Methods of Modern Mathematical Physics. IV. Analysis of Operators*, Academic Press, 1978.
[10] J. Schwinger, Thomas-Fermi model: The second correction, *Phys. Rev. A* **24** (1981), 2353–2361.

[11] J.M.C. Scott, The binding energy of the Thomas-Fermi atom, *Philos. Mag.* **43** (1952), 859–867.
[12] L. Seco, *private communication.*
[13] H. Siedentop and R. Weikard, On the leading energy correction for the statistical model of the atom: Interacting case, *Comm. Math. Phys.* **112** (1987), 471–490.
[14] B. Simon, *Functional Integration and Quantum Physics*, Academic Press, 1979.
[15] W. Thirring, A lower bound with the best possible constant for Coulomb Hamiltonians, *Comm. Math. Phys.* **79** (1981), 1–7.
[16] L.H. Thomas, The calculation of atomic fields, *Proc. Camb. Philos. Soc.* **23** (1927), 542–548.

Astérisque

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Exponential convergence of the first eigenvalue divided by the dimension, for certain sequences of Schrödinger operators

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Exponential convergence of the first eigenvalue divided by the dimension, for certain sequences of Schrödinger operators

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0. Introduction

In **[HS]** we introduced a class of semi-classical Schrödinger operators of the form $-\frac{1}{2}h^2\Delta + V^{(m)}$ on $\mathbb{R}^m$ for $m = 1, 2, \ldots$, where $V^{(m)}$ satisfy various assumptions, implying in particular convexity. If $\mu(m;h)$ denotes the first eigenvalue, we showed among other things that $\mu(m;h)/m$ tends to a limit $\mu(\infty;h)$ when $m \to \infty$ and that :

$$\mu(m;h)/m - \mu(\infty;h) = \mathcal{O}(h/m) \ . \tag{0.1}$$

We also proved (by adapting the methods of **[S1, 2]**) that $\mu(\infty;h)$ has an asymptotic expansion $\sim h(\mu_0 + \mu_1 h + \ldots)$, when $h \to 0$. One element of the proof was the use of certain WKB-expansions, more precisely, we showed that if $h(\mu_0(m) + \mu_1(m)h + \ldots)$ is the formal asymptotic expansion of $\mu(m;h)$, then $\mu_k(m)/m \to \mu_k$ when $m \to \infty$ with an exponential rate of convergence. A natural question is then wether (0.1) can be improved to :

$$\mu(m;h)/m - \mu(\infty;h) = \mathcal{O}(e^{-\kappa m}) \tag{0.2}$$

for some suitable $\kappa > 0$.

In this work, we establish estimates of the form (0.2) for certain sequences of $V^{(m)}$. A general result of this type is given in Theorem 3.1, and in Theorem 4.1 we obtain a better rate of exponential convergence for a somewhat more restricted class of potentials. In particular, we study in section 5 the same sequence of potentials related to statistical mechanics as in **[HS]**, and show that we get exponential convergence with a rate which seems to be optimal.

In **[HS]** we obtained exponential convergence at the level of WKB-eigenvalues by introducing exponential weights in the study of certain Hessians of the logarithm of certain WKB approximations to the first eigenfunction. These estimates were obtained by adapting the WKB-constructions in the complex domain of [**S1, 2**], and by introducing certain exponential weights in these estimates. In the present work, we also establish exponentially weighted estimates of certain Hessians of the logarithm of the first eigenfunction, but this time we work with the exact first eigenfunctions, and inspired by the appendix b in **[SiWYY]**, we use systematically the maximum principle in order to obtain these estimates. In particular, we never use any small h expansions, and our results are uniform in h.

The plan of the paper is the following : In section 1, we make some estimates for the log. of the first eigenfunction near $|x| = \infty$, in the case when the potential is a compactly supported perturbation of $\frac{1}{2}x^2$. These estimates, which are not necessarily uniform with respect to the dimension, form a preparation for the more refined estimates that we obtain in section 2. In section 3 we get a first result about the validity of (0.2).

In section 4, we start by examining a sequence of simple quadratic potentials, and we see that Theorem 3.1 does not give the optimal κ in this case. Then after some further exponential estimates in the style of section 2, we obtain the sharper Theorem 4.1, which is valid under somewhat different assumptions. In section 5, we apply this result to the model problem from statistical mechanics already studied in **[HS]**, and establish (0.2) with a set of κ which seems to be optimal.

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1. Some estimates for the exterior Dirichlet problem for the harmonic oscillator

Let B be an open a ball in $\mathbb{R}^n$ centered at 0. Then the Dirichlet realization P of $-\Delta+x^2$ in $\mathbb{R}^n\setminus B$ has discrete spectrum. Choose $\mu\in\mathbb{R}$ such that $x^2-\mu>0$ in $\mathbb{R}^n\setminus B$. Then μ is also below the infimum of the spectrum of the operator P just defined, and we let $K: C^\infty(\partial B)\to C^\infty(\mathbb{R}^n\setminus B)$ be the operator such that $u=Kv$ belongs to the domain of P outside a compact set and solves the problem:

$$(1.1)\qquad (-\Delta+x^2-\mu)u=0\ ,\quad u|_{\partial B}=v\ .$$

Using weighted L^2 estimates we see that $\partial^\alpha Kv(x)\to 0$, $|x|\to\infty$, for every α. Using the maximum principle we then have that $v\geq 0\Rightarrow Kv\geq 0$. This implies that if $v_1\leq v_2$ then $Kv_1\leq Kv_2$, and also $Kv\leq\sup v$, if $\sup v\geq 0$, $Kv\geq\inf v$ if $\inf v\leq 0$. Of particular interest is $K(1)$ which is a radial function $u_0=u_0(|x|)$, with:

$$(1.2)\qquad (-\partial_r^2-((n-1)/r)\partial_r+r^2-\mu)u_0(r)=0\ ,\ u_0(1)=1\ .$$

Here and in the following we assume (without loss of generality) that B is the unit ball. Writing $u_0=r^{-(n-1)/2}f(r)$, we know that f is in $L^2([1,\infty[,dr)$ and satisfies the Schrödinger equation:

$$(1.3)\qquad (-\partial_r^2+r^2+(n-1)(n-3)/4r^2-\mu)f=0\ ,\quad f(1)=1\ .$$

We can construct $\varphi(r)$ with

$$(1.4)\qquad \varphi'(r)\sim r+a_{-1}r^{-1}+a_{-3}r^{-3}+\ldots,\ r\to+\infty\ ,$$

such that

$$(1.5)\qquad (-\partial_r^2+r^2+(n-1)(n-3)/4r^2-\mu)(e^{-\varphi(r)})=e^{-\varphi(r)}\widetilde{R}(r)\ ,$$

where $\widetilde{R}$ is rapidly decreasing with all its derivatives when $r\to+\infty$. Actually we solve asymptotically the equation $(\varphi')^2-\varphi''=r^2+(n-1)(n-3)/4r^2-\mu$, and it is a routine procedure to verify that $f=e^{-(\varphi+R)}$, with $\partial^\alpha R=\mathcal{O}(r^{-\infty})$ for every $\alpha>0$. Replacing φ by $\varphi+R$, we still have (1.4). With $g(r)=\varphi(r)+((n-1)/2)\log r$, we get:

$$(1.6)\qquad u_0=e^{-g(|x|)}\ .$$

Here we note that $\partial_{x_\nu}g(|x|)=g'(|x|)x_\nu/|x|=x_\nu+\mathcal{O}(1/|x|)$,

$$(1.7)\qquad \partial_{x_\mu}\partial_{x_\nu}g=\delta_{\nu,\mu}+\mathcal{O}(|x|^{-2})\ .$$

Let now $v \in C^\infty(\mathbb{S}^{n-1})$ be strictly positive everywhere and let $u = Kv$. If $0 < v_{\min} < v_{\max}$ denote the infimum and the supremum of v, then we have :

$$v_{\min} u_0 \le u \le v_{\max} u_0 \ , \tag{1.8}$$

and hence :

$$u = e^{-g(|x|)+k(x)} \ , \tag{1.9}$$

where k is a bounded function. If the vectorfield ν is an infinitesimal generator of a rotation of $\mathbb{S}^{n-1}$, and if we extend the definition of ν to $\mathbb{R}^n$ by means of polar coordinates, (r,θ), $x = r\theta$, then $\nu \circ K = K \circ \nu$. Since v is C^∞, it follows that $\partial_\theta^\alpha u = \mathcal{O}(1)e^{-\psi(r)}$ for every α. We conclude that

$$\partial_\theta^\alpha k = \mathcal{O}(1) \text{ for every } \alpha \ . \tag{1.10}$$

We also need to control some radial derivatives of k. Writing

$$\Big(-\partial_r^2 - ((n-1)/r)\partial_r + r^2 - \mu - r^{-2}\Delta_\theta\Big)(u_0(r)e^k) = 0 \ ,$$

and using (1.2), we get :

$$\Big(\partial_r^2 + (2(\partial_r u_0)/u_0 + (n-1)/r)\partial_r\Big)(e^k) = -r^{-2}\Delta_\theta e^k \ . \tag{1.11}$$

Here $\partial_\theta^\alpha(r^{-2}\Delta_\theta(e^k)) = \mathcal{O}(r^{-2})$, and we have $2(\partial_r u_0)/u_0 = -2\partial_r g$, so (1.11), (1.5) imply that

$$(\partial_r - f(r))\partial_r(e^k) = -r^{-2}\Delta_\theta(e^k) = \mathcal{O}(r^{-2}) \ , \tag{1.12}$$

where $f(r) = 2r + \mathcal{O}(1/r)$, $f'(r) = 2 + \mathcal{O}(1/r^2)$ etc. Let $F(r) = \displaystyle\int_1^r f(t)\,dt$. Then

$$\partial_r e^k = -\int_r^{+\infty} e^{F(r)-F(s)}\mathcal{O}(s^{-2})\,ds + Ce^{F(r)} \ . \tag{1.13}$$

The first term is $\mathcal{O}(r^{-3})$ since $F(r) - F(s) \sim r^2 - s^2 \le 2r(r-s)$, for $s \ge r$, and since we know that $\partial_r e^k$ cannot tend to $+\infty$ or $-\infty$, when $r \to \infty$, we conclude that $C = 0$ in (1.13), and hence :

$$\partial_r e^k = \mathcal{O}(r^{-3}) \ . \tag{1.14}$$

More generally,

$$\partial_r \partial_\theta^\alpha e^k = \mathcal{O}(r^{-3}) \ . \tag{1.15}$$

Differentiating (1.12) and using (1.15), we get :

$$(1.16)\qquad (\partial_r - f(r))\partial_r^2(e^k) = \mathcal{O}(r^{-3}) \ ,$$

and similarly for the $\theta-$ derivatives.

The same argument then shows that :

$$(1.17)\qquad \partial_r^2 \partial_\theta^\alpha e^k = \mathcal{O}(r^{-4}) \ .$$

Continuing this way, we get by induction

$$(1.18)\qquad \partial_r^\nu \partial_\theta^\alpha e^k = \mathcal{O}(r^{-2-\nu}) \ , \quad \nu = 1, 2, \ldots$$

and remembering that k is bounded, we deduce (by differentiating the identity $k = \log e^k$) that

$$(1.19)\qquad \partial_r^\nu \partial_\theta^\alpha k = \mathcal{O}(r^{-2-\nu}) \ , \quad \nu = 1, 2, \ldots$$

Going back to the $x-$ coordinates, we get :

$$(1.20)\qquad \partial_x^\alpha k = \mathcal{O}(|x|^{-|\alpha|}) \ , \text{ for every } \alpha \neq 0 \ .$$

Using also the properties of g we get $-\log u = \frac{1}{2}x^2 + \psi(x)$, where ψ satisfies the estimates (1.20).

Let us finally remark that everything works equally well for the operator $-h^2\Delta + V$, when V satisfies the assumptions above. We then obtain $-h\log u = \frac{1}{2}x^2 + \psi(x)$, with ψ satisfying (1.20), not necessarily uniformly with respect to h.

2. Estimates on the logarithm of the first eigenfunction

Let $V : \mathbb{R}^m \to \mathbb{R}$ be a smooth potential which is equal to $x^2/2$ outside some bounded set. Let $u = e^{-\varphi(x)/h}$ be the first normalized eigenfunction of $-\frac{1}{2}h^2\Delta + V$. (Here φ also depends on h.) Let μ be the corresponding eigenvalue, and let $\mathbf{0}$ be an open ball centered at 0 with the property that $V = x^2/2 > \mu$ in the exterior of $\mathbf{0}$. If K is the exterior Poisson operator associated to $-\frac{1}{2}h^2\Delta + \frac{1}{2}x^2 - \mu$, then in the exterior of $\mathbf{0}$, we have $u = K(u|_{\partial\mathbf{0}})$, and after a scaling we are in the situation of section 1. We then know that $\varphi(x) = x^2/2 + \psi(x)$, where $\psi^{(\alpha)}(x) \to 0$, when $|x| \to \infty$, for $\alpha \neq 0$. Here, we have apriori no uniformity with respect to m or h, however, we shall use the maximum principle in a way inspired from the appendix B of **[SiWYY]**, to get some uniform estimates on the Hessian and on the third order derivatives of φ.

Proposition 2.1. *Let B be the space $\mathbb{R}^m$ equipped with some norm $\|\cdot\|_B$, and assume that for some fixed θ :*

$$\|V''(x) - I\|_{\mathcal{L}(B,B)} \leq \theta < 1 \text{ for every } x \in \mathbb{R}^m . \tag{2.1}$$

Then for every $x \in \mathbb{R}^m$:

$$\|\varphi''(x) - I\|_{\mathcal{L}(B,B)} \leq \widetilde{\theta} , \tag{2.2}$$

where $\widetilde{\theta} = \theta/(1 + (1-\theta)^{\frac{1}{2}})$.

PROOF : Write $\mu = hE$ and recall that

$$\frac{1}{2}(\varphi')^2 = V + \frac{1}{2}h\Delta\varphi - hE . \tag{2.3}$$

Taking the Hessian of this relation, we get (as in **[SiWYY]**) :

$$\varphi' \cdot \partial_x(\varphi'') + \varphi''^2 = V'' + \frac{1}{2}h\Delta(\varphi'') . \tag{2.4}$$

Write $\varphi'' = 1 + \psi''$, $V'' = 1 + W''$:

$$\varphi' \cdot \partial_x(\psi'') + 2\psi'' + \psi''^2 = W'' + \frac{1}{2}h\Delta(\psi'') . \tag{2.5}$$

In section 1 we showed that $\|\psi''(x)\|_{\mathcal{L}(B,B)} \to 0$, $|x| \to \infty$, so there is a point x_0, where $\|\psi''(x)\|_{\mathcal{L}(B,B)}$ is maximal, and we let M denote the maximal value. Let $\nu \in B$ be a normalized vector such that $\|\psi''(x_0)\nu\|_B = M$, and let $\mu \in B^*$ be a normalized vector such that $\langle\psi''(x_0)\nu, \mu\rangle = M$. Then $x \mapsto \langle\psi''(x)\nu, \mu\rangle$ reaches its maximum value (M) at the point x_0. We apply the terms in (2.5) to ν and take the scalar product with μ. Then with $x = x_0$, we get :

$$2\langle\psi''(x_0)\nu, \mu\rangle + \langle\psi''(x_0)^2\nu, \mu\rangle \leq \langle W''(x_0)\nu, \mu\rangle , \tag{2.6}$$

and hence

$$2M - M^2 \leq \theta , \tag{2.7}$$

or equivalently :

$$\text{Either } M \leq \theta/\left(1 + (1-\theta)^{\frac{1}{2}}\right) \text{ or } M \geq 1 + (1-\theta)^{\frac{1}{2}} . \tag{2.8}$$

The last possibility can be excluded by a deformation argument : Putting $V_t = x^2/2 + tW$, we see that $M_t = \sup_x \|\psi''(x)\|_{\mathcal{L}(B,B)}$ depends continuously on t. □

We also need to estimate the third derivatives of φ. In order to do so we assume that the assumptions of Proposition 2.1 are fulfilled also in the case $B = \ell^\infty$:

$$\begin{aligned} &\|V''(x) - I\|_{\mathcal{L}(B,B)} \text{ and } \|V''(x) - I\|_{\mathcal{L}(\ell^\infty,\ell^\infty)} \\ &\text{are } \leq \theta \text{ for all } x \in \mathbb{R}^m. \end{aligned} \tag{2.9}$$

Here it is assumed that $0 \leq \theta < 1$.

We can rewrite (2.4) as :

$$\left\langle \varphi^{(3)}, \varphi' \otimes t \otimes s \right\rangle + \langle \varphi'' t, \varphi'' s \rangle = \langle V'', t \otimes s \rangle + \frac{1}{2} h\Delta \langle \varphi'', t \otimes s \rangle \tag{2.10}$$

for all $t, s \in \mathbb{R}^N$, and if we take the derivative of this relation in the constant direction r, we get

$$\begin{aligned} &\left\langle \varphi' \cdot \partial_x(\psi^{(3)}) + 3\psi^{(3)}, r \otimes s \otimes t \right\rangle + \left\langle \psi^{(3)}, \psi''(r) \otimes s \otimes t \right\rangle + \\ &\qquad \left\langle \psi^{(3)}, r \otimes \psi''(s) \otimes t \right\rangle + \left\langle \psi^{(3)}, r \otimes s \otimes \psi''(t) \right\rangle = \\ &\qquad\qquad \left\langle V^{(3)}, r \otimes s \otimes t \right\rangle + \frac{1}{2} h\Delta \left\langle \psi^{(3)}, r \otimes s \otimes t \right\rangle . \end{aligned} \tag{2.11}$$

In section 1 we established that $\psi^{(3)}(x) \to 0$ when $x \to \infty$, and hence there is a point x_0 where $\left\|\psi^{(3)}(x)\right\|_{(B\otimes B^*\otimes \ell^\infty)^*}$ reaches its supremum that we shall denote by $M^{(3)}(\psi)$. Here we identify the dual space of a tensorproduct of normed spaces with the normed space of multilinear forms on the corresponding Cartesian product. Let $r \in B$, $s \in B^*$, $t \in \ell^\infty$ be normalized vectors such that $\langle \psi^{(3)}(x_0), r \otimes s \otimes t \rangle = M^{(3)}(\psi)$. The same argument as before gives :

$$3M^{(3)}(\psi) - 3M^{(3)}(\psi)\widetilde{\theta} \leq \left\langle V^{(3)}(x_0), r \otimes s \otimes t \right\rangle \leq M^{(3)}(V) , \tag{2.12}$$

where $M^{(3)}(V)$ is defined as $\sup_x \left\| V^{(3)}(x) \right\|_{(B\otimes B^*\otimes \ell^\infty)^*}$. We then get :

$$\sup_x \left\|\psi^{(3)}(x)\right\|_{(B\otimes B^*\otimes \ell^\infty)^*} \leq (3(1-\widetilde{\theta}))^{-1} \sup_x \left\|V^{(3)}(x)\right\|_{(B\otimes B^*\otimes \ell^\infty)^*} . \tag{2.13}$$

We shall now take two potentials V_0 and V_1, which satisfy the assumptions above and in particular the assumption (2.9). We shall estimate $\varphi_1' - \varphi_0'$

and $\varphi_1'' - \varphi_0''$, where φ_j denotes the phase associated to V_j, so that

$$\frac{1}{2}(\varphi_j')^2 - \frac{1}{2}h\Delta\varphi_j + hE_j = V_j \ , \ j = 0,1 \ . \tag{2.14}$$

Taking the difference of these two equations, we get:

$$\frac{1}{2}(\varphi_1' + \varphi_0') \cdot \partial_x(\varphi_1 - \varphi_0) + h(E_1 - E_0) = V_1 - V_0 + \frac{1}{2}h\Delta(\varphi_1 - \varphi_0), \tag{2.15}$$

and taking the gradient of this relation gives:

$$\frac{1}{2}(\varphi_1' + \varphi_0') \cdot \partial_x(\varphi_1' - \varphi_0') + \frac{1}{2}(\varphi_1'' + \varphi_0'')(\varphi_1' - \varphi_0') = V_1' - V_0' + \frac{1}{2}h\Delta(\varphi_1' - \varphi_0') \ . \tag{2.16}$$

From section 1 it follows that $\varphi_1'(x) - \varphi_0'(x) \to 0$ when $x \to \infty$, so $\sup\limits_x \|\varphi_1'(x) - \varphi_2'(x)\|_B \underset{\text{def}}{=} m$ is reached at some point x_0. Let $\nu \in B^*$ be a normalized vector such that $\langle \varphi_1'(x_0) - \varphi_2'(x_0), \nu\rangle = m$. Then applying (2.16) to ν and putting $x = x_0$, we get:

$$\left\langle \frac{1}{2}(\varphi_1''(x_0) + \varphi_0''(x_0))(\varphi_1'(x_0) - \varphi_0'(x_0)), \nu \right\rangle \le \langle (V_1' - V_0')(x_0), \nu\rangle \ . \tag{2.17}$$

Here we use that $\varphi_j''(x) = 1 + \psi_j''(x)$ with $\left\|\psi_j''(x)\right\|_{\mathcal{L}(B,B)} \le \widetilde{\theta}$, and obtain: $m - \widetilde{\theta}m \le \|(V_1' - V_0')(x_0)\|_B$.

We have then proved:

$$\sup_x \|\varphi_1'(x) - \varphi_0'(x)\|_B \le (1 - \widetilde{\theta})^{-1} \sup_x \|V_1'(x) - V_0'(x)\|_B \ . \tag{2.18}$$

We shall also estimate $\varphi_1'' - \varphi_0''$ in $\mathcal{L}(\ell^\infty, B)$. We first apply (2.16) to a constant vector ν:

$$\left\langle \varphi_1'' - \varphi_0'', \frac{1}{2}(\varphi_1' + \varphi_0') \otimes \nu \right\rangle + \left\langle \frac{1}{2}(\varphi_1'' + \varphi_0''), (\varphi_1' - \varphi_0') \otimes \nu \right\rangle = \langle V_1' - V_0', \nu\rangle + \frac{1}{2}h\Delta(\langle \varphi_1' - \varphi_0', \nu\rangle) \ , \tag{2.19}$$

and differentiate in the constant direction μ:

$$\begin{aligned} &\left\langle \varphi_1''' - \varphi_0''', \frac{1}{2}(\varphi_1' + \varphi_0') \otimes \nu \otimes \mu \right\rangle + \\ &\left\langle \varphi_1'' - \varphi_0'', \frac{1}{2}(\varphi_1'' + \varphi_0'')(\mu) \otimes \nu \right\rangle + \left\langle \frac{1}{2}(\varphi_1''' + \varphi_0'''), (\varphi_1' - \varphi_0') \otimes \nu \otimes \mu \right\rangle + \\ &\left\langle \frac{1}{2}(\varphi_1'' + \varphi_0''), (\varphi_1'' - \varphi_0'')(\mu) \otimes \nu \right\rangle = \\ &\langle V_1'' - V_0'', \nu \otimes \mu\rangle + \frac{1}{2}h\Delta\left(\langle \varphi_1'' - \varphi_0'', \nu \otimes \mu\rangle\right) \ , \end{aligned} \tag{2.20}$$

which can be rewritten as:

$$
\begin{aligned}
(2.21)\quad & \frac{1}{2}(\varphi_1' + \varphi_0') \cdot \partial_x \langle(\varphi_1'' - \varphi_0''), \nu \otimes \mu\rangle + 2\langle \varphi_1'' - \varphi_0'', \nu \otimes \mu\rangle + \\
& \left\langle \varphi_1'' - \varphi_0'', \frac{1}{2}(\psi_1'' + \psi_0'')(\mu) \otimes \nu \right\rangle + \left\langle \varphi_1'' - \varphi_0'', \mu \otimes \frac{1}{2}(\psi_1'' + \psi_0'')(\nu) \right\rangle + \\
& \left\langle \frac{1}{2}(\psi_1''' + \psi_0'''), (\varphi_1' - \varphi_0') \otimes \nu \otimes \mu \right\rangle = \langle V_1'' - V_0'', \nu \otimes \mu\rangle + \\
& \frac{1}{2} h\Delta(\langle \varphi_1'' - \varphi_0'', \nu \otimes \mu\rangle) .
\end{aligned}
$$

We know that $\sup_x \|\varphi_1'' - \varphi_0''\|_{\mathcal{L}(\ell^\infty, B)} \underset{\text{def}}{=} M$ is attained at some point x_0. Let $\nu \in \ell^\infty$, $\mu \in B^*$ be normalized vectors with $\langle \varphi_1''(x_0) - \varphi_0''(x_0), \nu \otimes \mu\rangle = M$. Taking these vectors in (2.21) and $x = x_0$ gives:

$$
\begin{aligned}
(2.22)\quad & 2M + \left\langle \varphi_1'' - \varphi_0'', \frac{1}{2}(\psi_1'' + \psi_0'')(\mu) \otimes \nu \right\rangle + \\
& \left\langle \varphi_1'' - \varphi_0'', \mu \otimes \frac{1}{2}(\psi_1'' + \psi_0'')(\nu) \right\rangle + \\
& \left\langle \frac{1}{2}(\psi_1''' + \psi_0'''), (\varphi_1' - \varphi_0') \otimes \nu \otimes \mu \right\rangle \le \langle V_1'' - V_0'', \nu \otimes \mu\rangle .
\end{aligned}
$$

Here we use that $\left\|\frac{1}{2}(\psi_1'' + \psi_0'')(\mu)\right\|_{B^*}$, $\left\|\frac{1}{2}(\psi_1'' + \psi_0'')(\nu)\right\|_{\ell^\infty} \le \widetilde{\theta}$ to bound the second and the third term of the LHS from below by $-M\widetilde{\theta}$. Using (2.13), (2.18), we can bound the fourth term from below by

$$
-\frac{1}{3}(1-\widetilde{\theta})^{-2}\left(\max_{j=0,1}\sup_x \left\|V_j'''(x)\right\|_{(B\otimes B^*\otimes \ell^\infty)^*}\right) \cdot \sup_x \|V_1'(x) - V_0'(x)\|_B
$$

and we end up with the estimate:

$$
\begin{aligned}
(2.23)\quad & \sup_x \|\varphi_1'' - \varphi_0''\|_{\mathcal{L}(\ell^\infty, B)} \le \frac{1}{2}(1-\widetilde{\theta})^{-1} \sup_x \|V_1'' - V_0''\|_{\mathcal{L}(\ell^\infty, B)} + \\
& (1/6)(1-\widetilde{\theta})^{-3}\left(\sup_{x,j}\left\|V_j'''(x)\right\|_{(B\otimes B^*\otimes \ell^\infty)^*}\right) \cdot \left(\sup_x \|V_1'(x) - V_0'(x)\|_B\right) .
\end{aligned}
$$

So far, all the estimates have been obtained under the assumption that $V - x^2/2$ and $V_j - x^2/2$ have compact support, and we shall now eliminate this assumption by means of an approximation procedure. We start by noticing that for every $\varepsilon \in]0,1]$, there exists $\chi = \chi_\varepsilon \in C_0^\infty(\mathbb{R})$ with values in $[0,1]$ such that $|\chi'(t)| \le \varepsilon/|t|$, $|\chi''(t)| \le \varepsilon/t^2$, $|\chi'''(t)| \le \varepsilon/|t|^3$, such that χ is equal to 1 on the interval $[-\varepsilon^{-1}, \varepsilon^{-1}]$. (We can take $\chi_\varepsilon(t) = f(\varepsilon \log|t|)$

for a suitable f.) Let $V = \frac{1}{2}x^2 + W(x)$ with $W \in C^\infty(\mathbb{R}^m;\mathbb{R})$ and assume that W'' and W''' are uniformly bounded as functions of x. We also assume that (2.9) is satisfied. By symmetry and interpolation we then also have $\|W''(x) - I\|_{\mathcal{L}(\ell^2,\ell^2)} \le \theta < 1$, and it follows that $V''(x) \ge 1-\theta$ in the sense of symmetric matrices. We then know that V is a strictly convex function.

We approximate W by the compactly supported functions $W_\varepsilon = \chi_\varepsilon(|x|)W$. Since $W_\varepsilon'' = \chi_\varepsilon W'' + 2\chi_\varepsilon' W' + \chi_\varepsilon'' W$, and since $\chi_\varepsilon' = \mathcal{O}(\varepsilon/|x|)$, $\chi_\varepsilon'' = \mathcal{O}(\varepsilon/|x|^2)$, $W' = \mathcal{O}(1+|x|)$, $W = \mathcal{O}((1+|x|)^2)$ (where for the moment the estimates are not necessarily uniform with respect to the dimension), we see that W_ε will satisfy (2.9) with θ replaced by $\theta_\varepsilon \to \theta$ when $\varepsilon \to 0$. Similarly we see that $\sup_x \left\|W_\varepsilon^{(3)}(x)\right\|_{(B\otimes B^*\otimes\ell^\infty)^*}$ tends to $\sup_x \left\|W^{(3)}(x)\right\|_{(B\otimes B^*\otimes\ell^\infty)^*}$ when $\varepsilon \to 0$. Let $u_\varepsilon = e^{-\varphi_\varepsilon/h}$ be the first normalized eigenfunction of $-\frac{1}{2}h^2\Delta + V_\varepsilon$, where $V_\varepsilon = \frac{1}{2}x^2 + W_\varepsilon$. Then all the estimates of this section that we obtained for a single potential of the form $\frac{1}{2}x^2 + W$ with W of compact support, apply to φ_ε when ε is small enough. Moreover it is easy to see (for instance by using exponential decay estimates) that $u_\varepsilon \to u$ in the C^∞ topology when $\varepsilon \to 0$, so $\varphi_\varepsilon \to \varphi$ in C^∞. From these remarks we see that the assumption that W have compact support can be eliminated in the estimates above, in the case of a single potential. Consider finally the case of two potentials of the form $V_j = \frac{1}{2}x^2 + W_j$ for $j = 1,2$. We assume that V_j satisfy (2.9) and that W_j'' are uniformly bounded on $\mathbb{R}^m$, and that $\sup\|V_1' - V_0'\|_B$, and $\sup\|V_1'' - V_0''\|_{\mathcal{L}(\ell^\infty,B)}$ are finite. Then we can put $V_{j,\varepsilon} = \frac{1}{2}x^2 + \chi_\varepsilon(|x|)W_j$ and perform the same approximation argument and deduce the same estimates for the difference of the phases, as we had in the case when W_j had compact support. Let us sum up our results :

Theorem 2.1.

(A) *Let $V(x) = \frac{1}{2}x^2 + W(x)$ where W is real valued and smooth on $\mathbb{R}^m$. We assume that* (2.9) *holds and that the third derivatives of V are bounded on $\mathbb{R}^m$. Let $u = e^{-\varphi/h}$ be the normalized positive eigenfunction associated to the first eigenvalue of $-\frac{1}{2}h^2\Delta + V$. Then the conclusion of Proposition* 2.1 *holds as well as the estimate* (2.13).

(B) *Let* $V_j(x) = \frac{1}{2}x^2 + W_j(x)$, $j = 1,2$ *satisfy the assumptions of* (A) *(with the same* θ *in* (2.9)*), and assume in addition that* $\sup \|V_1' - V_0'\|_B$ *, and* $\sup \|V_1'' - V_0''\|_{\mathcal{L}(\ell^\infty,B)}$ *are finite. Then if we let* $e^{-\varphi_j/h}$ *denote the first normalized eigenfunction of* $-\frac{1}{2}h^2\Delta + V_j$ *, we have the estimates* (2.18) *and* (2.23).

3. Exponential convergence

We consider a sequence of potentials $V^{(m)}(x_1,\dots,x_m)$, $m = 1,2,\dots$, and an associated sequence of functions $\rho = \rho^{(m)} : \mathbb{Z}/m\mathbb{Z} \to]0,\infty[$, with the following properties :

$$V^{(m)}(0) = 0 \ , \quad \nabla V^{(m)}(0) = 0 \ , \tag{3.1}$$

(3.2)

For $0 \le t \le 1$, $m,n \in \{1,2,\dots\}$, we have :

$$\left\| I - \nabla^2((1-t)V^{(m)} \oplus V^{(n)} + tV^{(m+n)}) \right\|_{\mathcal{L}(\ell^\infty_\rho,\ell^\infty_\rho)} \le \theta,$$

for $\rho \equiv 1$ and for $\rho = \rho^{m,n}$ given by $\rho(j) = \rho^{(m)}(j)$ when $1 \le j \le m$, $\rho(j) = \rho^{(n)}(j-m)$, $m+1 \le j \le m+n$.

$$\rho^{(m)}\left([\frac{1}{2}m]\right) \ge e^{m\kappa/2} \ , \ \rho^{(m)}(1) = \rho^{(m)}(m) = 1 \ . \tag{3.3}$$

Here $0 \le \theta < 1$, $\kappa > 0$ are fixed in the following, and we let ℓ^p_ρ denote the space $\mathbb{C}^m$ equipped with the norm : $|x|_{p,\rho} = |\rho x|_p = (\Sigma\, |\rho(j)\, x_j|^p)^{1/p}$ (with the obvious modifications when $p = \infty$). The choice of m will be clear from the context. We write :

$$V^{(m)} \oplus V^{(n)}(x_1,\dots,x_{m+n}) = V^{(m)}(x_1,\dots,x_m) + V^{(n)}(x_{m+1},\dots,x_{m+n}) \ .$$

We assume that there exists a constant C_0, such that :

$$\sup_x \left\| \nabla^3 V^{(m)}(x) \right\|_{(\ell^\infty_\rho \otimes \ell^1_{1/\rho} \otimes \ell^\infty)^*} \le C_0, \tag{3.4}$$

$$\rho = \rho^{j,k}, \ j+k = m, \ \text{and} \ \rho = \rho^{(m)}.$$

We also assume that

(3.5) $V^{(m)}$ is invariant under cyclic perturbations of the coordinates :

$$V^{(m)}(x_m, x_1, \dots, x_{m-1}) = V^{(m)}(x_1, x_2, \dots, x_m),$$

and that $V^{(m)}$ is close to $V^{(m+n)}$ in the following sense : We have

$$\sup_x \left\| \nabla (V^{(m+n)} - V^{(m)} \oplus V^{(n)}) \right\|_{\ell^\infty_\rho} \leq C_0 \ , \tag{3.6}$$

$$\sup_x \left\| \nabla^2 (V^{(m+n)} - V^{(m)} \oplus V^{(n)}) \right\|_{\mathcal{L}(\ell^\infty, \ell^\infty_\rho)} \leq C_0 \ , \tag{3.7}$$

for $\rho = \rho^{m,n}$.

We can then apply Theorem 2.1 (B) with $V_0 = V^{(m)} \oplus V^{(n)}$, $V_1 = V^{(m+n)}$, $B = \ell^\infty_\rho$, $\rho = \rho^{m,n}$ and hence :

$$\sup_{x \in \mathbb{R}^{m+n}} \left\| \nabla (\varphi^{(m+n)} - \varphi^{(m)} \oplus \varphi^{(n)}) \right\|_{\infty, \rho} \leq C_0/(1 - \widetilde{\theta}), \tag{3.8}$$

$$\sup_{x \in \mathbb{R}^{m+n}} \left\| \nabla^2 (\varphi^{(m+n)} - \varphi^{(m)} \oplus \varphi^{(n)}) \right\|_{\mathcal{L}(\ell^\infty, \ell^\infty_\rho)} \leq \\ C_0/(2(1-\widetilde{\theta})) + C_0^2/(6(1-\widetilde{\theta})^3) \ , \tag{3.9}$$

where $\widetilde{\theta}$ is defined in Proposition 2.1. Choosing $\nu = \left[\frac{1}{2} m\right]$ we get :

$$\left| \partial_{x_\nu} \varphi^{(m+n)}(0) - \partial_{x_\nu} \varphi^{(m)}(0) \right| = \mathcal{O}(1) e^{-\kappa m/2} \tag{$\widetilde{3.8}$}$$

$$\left| \partial^2_{x_\nu} \varphi^{(m+n)}(0) - \partial^2_{x_\nu} \varphi^{(m)}(0) \right| = \mathcal{O}(1) e^{-\kappa m/2} . \tag{$\widetilde{3.9}$}$$

Let $\mu(m) = \mu(m;h)$ be the lowest eigenvalue of $-\frac{1}{2} h^2 \Delta + V^{(m)}$. From (2.3) and the fact that $V^{(m)}(0) = 0$, we get :

$$\mu(m) = \frac{1}{2} h \Sigma \partial^2_{x_\nu} \varphi^{(m)}(0) - \frac{1}{2} \Sigma (\partial_{x_\nu} \varphi^{(m)}(0))^2 \ ,$$

with $-\varphi^{(m)}/h$ being the logarithm of the first eigenfunction. From (3.5), we deduce that $\varphi^{(m)}$ is invariant under cyclic permutations of the coordinates, and hence the terms in each of the sums are independent of ν. For an arbitrary ν in $\{1, 2, \ldots, m\}$, we then get :

$$\mu(m)/m = \frac{1}{2} h \partial^2_{x_\nu} \varphi^{(m)}(0) - \frac{1}{2} (\partial_{x_\nu} \varphi^{(m)}(0))^2 \ . \tag{3.10}$$

Choosing ν so that $(\widetilde{3.8})$, $(\widetilde{3.9})$ hold, and noticing that $\partial_{x_\nu} \varphi^{(m)}(0) = \mathcal{O}(h^{\frac{1}{2}})$ by (2.3), we get :

$$|\mu(m+n)/(m+n) - \mu(m)/m| = \mathcal{O}(h^{\frac{1}{2}} + h) e^{-\kappa m/2} \ . \tag{3.11}$$

This implies that $\lim\limits_{m \to \infty} \mu(m)/m$ exists (as we already know from **[HS]**). If we denote the limit by $\mu(\infty)$, then (3.11) implies :

$$|\mu(m)/m - \mu(\infty)| = \mathcal{O}(h^{\frac{1}{2}} + h) e^{-\kappa m/2} \ . \tag{3.12}$$

Summing up, we have proved:

Theorem 3.1. *Let $V^{(m)}(x_1,\dots,x_m)$ satisfy* (3.1)-(3.7) *and let $\mu(m)$ be the lowest eigenvalue of $-\frac{1}{2}h^2\Delta+V^{(m)}$ on $\mathbb{R}^m$. Let $\mu(\infty)=\lim_{m\to\infty}\mu(m)/m$ (which exists according to* **[HS]***). Then uniformly with respect to h we have* (3.12).

REMARK. If $V^{(m)}$ are even, then $\varphi^{(m)}$ are even, and the second term of the RHS of (3.10) vanishes. Then we can replace $\mathcal{O}(h^{\frac{1}{2}}+h)$ in (3.12) by $\mathcal{O}(h)$.

4. Improved bounds on the speed of convergence

We first study the speed of convergence for the family of quadratic potentials, $V^{(m)}=\frac{1}{2}\Sigma_1^m x_j^2-\frac{1}{2}\alpha\Sigma_1^m x_jx_{j+1}$ (with the convention that subscripts are in $\mathbb{Z}/m\mathbb{Z}$). A similar discussion was given in **[HS]**. Here α is fixed in $[0,1[$. If we view $\nabla^2V^{(m)}$ as a map from $\mathbb{C}^m$ to itself and identify $\mathbb{C}^m$ with $\ell^2(\mathbb{Z}/m\mathbb{Z})$, we have:

$$\nabla^2V^{(m)}=1-\alpha\frac{1}{2}(\tau_1+\tau_{-1})\ , \tag{4.1}$$

where $(\tau_kx)_j=x_{j-k}$. The eigenvectors $e_k=(x_0,x_1,\dots,x_{m-1})$ of $\nabla^2V^{(m)}$ are given by $x_j=\exp(2\pi ikj/m)$, $0\le k<m$, and the corresponding eigenvalues are $1-\alpha\cos(2\pi k/m)$. The lowest eigenvalue $\mu(m)$ of $P^{(m)}=-\frac{1}{2}\Delta+V^{(m)}$ therefore satisfies:

$$\mu(m)/m=(2m)^{-1}\Sigma_0^{m-1}(1-\alpha\cos(2\pi k/m))^{\frac{1}{2}}\,, \tag{4.2}$$

and this is a Riemann sum corresponding to the integral:

$$(4\pi)^{-1}\int_0^{2\pi}(1-\alpha\cos x)^{\frac{1}{2}}\,dx\ . \tag{4.3}$$

Let $v(x)=(1-\alpha\cos x)^{\frac{1}{2}}$. Then the right hand side of (4.2) can be rewritten:

$$\frac{1}{2}\int_0^{2\pi}v(x)u_m(x)dx,\ \text{ with } u_m(x)=\sum_{k\in\mathbb{Z}}m^{-1}\delta(x-2\pi k/m). \tag{4.4}$$

The Fourier coefficients of u_m are given by:

$$\hat{u}_m(j)=1/2\pi \text{ if } e^{-ij2\pi/m}=1 \tag{4.5}$$
(i.e. if j is a multiple of m) and $\hat{u}_m(j)=0$ otherwise.

Rewriting (4.4) with Plancherel's formula, we get :

$$(4.6)\quad \mu(m)/m=\frac{1}{2}\sum_{\nu\in\mathbb{Z}}\widehat{v}(\nu m)=(4\pi)^{-1}\int_0^{2\pi}(1-\alpha\cos x)^{\frac{1}{2}}\,dx+\frac{1}{2}\sum_{\nu\neq 0}\widehat{v}(\nu m).$$

Here,

$$(4.7)\qquad v(\nu m)=(2\pi)^{-1}\int_0^{2\pi}(1-\alpha\cos x)^{\frac{1}{2}}\,e^{-i\nu m x}\,dx\ ,$$

and depending on the sign of ν, we wish to deform the integration contour into the upper or the lower half plane. The amount of deformation is limited by the singularities of the function $x\mapsto(1-\alpha\cos x)^{\frac{1}{2}}$, i.e. by the points x such that $1-\alpha\cos x=0$. These are the points of the form $iy+2\pi k$, with $ch\,y=1/\alpha$. The deformation argument then shows that

$$|\widehat{v}(\nu m)|\le C_\varepsilon\exp[-(1-\varepsilon)\,|\nu|\,m\,ch^{-1}(1/\alpha)]\ \text{ for every }\varepsilon>0,$$

and (4.6) then gives :

$$(4.8)\qquad |\mu(m)/m-\mu(\infty)|\le\widetilde{C}_\varepsilon\exp[-(1-\varepsilon)m\,ch^{-1}(1/\alpha)]\ ,$$

for every $\varepsilon>0$. Pushing the same method a little further would probably give an asympotic expansion of $(\mu(m)/m-\mu(\infty))\exp[m\,ch^{-1}(1/\alpha)]$ in decreasing powers of m.

Let us interpret the exponent in (4.8) in terms of exponential weights. If $\rho:\mathbb{Z}/m\mathbb{Z}\to]0,+\infty[$, then the norm of $\frac{1}{2}\alpha(\tau_1+\tau_{-1}):\ell^p_\rho\to\ell^p_\rho$, or equivalently the norm of $\rho\circ\frac{1}{2}\alpha(\tau_1+\tau_{-1})\circ\rho^{-1}:\ell^p\to\ell^p$ can be bounded by

$$\alpha\max\Big[\sup_j\frac{1}{2}\Big(\rho(j)/\rho(j-1)+\rho(j)/\rho(j+1)\Big),\ \sup_k\frac{1}{2}\Big(\rho(k-1)/\rho(k)+\rho(k+1)/\rho(k)\Big)\Big]\ .$$

Put $\nu(j)=\rho(j+1)/\rho(j)$ and assume that $e^{-\delta}\le\nu(j+1)/\nu(j)\le e^{\delta}$ for some small δ. Then the quantity above can be estimated by $\alpha e^{\delta}\sup_k\frac{1}{2}(\nu(k)+1/\nu(k))$, and we are then naturally led to the assumption that $\alpha e^{\delta}\sup_k\frac{1}{2}(\nu(k)+\nu(k)^{-1})\le\theta<1$, or equivalently : $|\log(\rho(k+1)/\rho(k))|\le ch^{-1}(e^{-\delta}\theta/\alpha)$. Choosing ρ conveniently and approaching the limiting case $\theta=1$, $\delta=0$, we see that the estimate of section 3 gives :

$$(4.9)\qquad |\mu(m)/m-\mu(\infty)|\le\widetilde{C}_\varepsilon\exp[-(1-\varepsilon)\frac{1}{2}m\,ch^{-1}(1/\alpha)],$$

which is not as good as (4.8).

In the remainder of this section we shall establish improved bounds of the form (4.8) for sequences of potentials which are not necessarily quadratic. As a preparation we need bounds on the fourth order derivatives of the phase. Let $V : \mathbb{R}^m \to \mathbb{R}$ satisfy the assumptions of Proposition 2.1, for some B and also for $B = \ell^\infty$, and let $u = e^{-\varphi/h}$ be the positive normalized eigenfunction associated to the first eigenvalue of $-\frac{1}{2}h^2\Delta + V$. We then have (2.2) and (2.13) (where $\varphi'' = 1 + \psi''$, so that $\varphi^{(3)} = \psi^{(3)}$).

Rewrite (2.4) as:

$$(4.10)\quad \left\langle \varphi^{(3)}, \varphi' \otimes t \otimes s \right\rangle + \langle \langle \varphi'', t\rangle, \langle \varphi'', s\rangle\rangle = \langle V'', t \otimes s\rangle + \frac{1}{2} h \langle \Delta\varphi'', t \otimes s\rangle ,$$

where we use the following notation: if A is a symmetric $k-$tensor and B a $\ell-$tensor with $\ell \le k$, then $\langle A, B\rangle$ is the symmetric $k - \ell$ tensor C with $\langle C, t\rangle = \langle A, B \otimes t\rangle$. We differentiate (4.10) in the constant direction r:

$$\begin{aligned} &\left\langle \varphi^{(4)}, \varphi' \otimes r \otimes s \otimes t \right\rangle + \left\langle \varphi^{(3)}, \langle \varphi'', r\rangle \otimes s \otimes t \right\rangle + \\ &\qquad \left\langle \left\langle \varphi^{(3)}, r \otimes t \right\rangle, \langle \varphi'', s\rangle \right\rangle + \left\langle \langle \varphi'', t\rangle, \left\langle \varphi^{(3)}, r \otimes s \right\rangle \right\rangle = \\ &\qquad\qquad \left\langle V^{(3)}, r \otimes s \otimes t \right\rangle + \frac{1}{2} h\Delta \left\langle \varphi^{(3)}, r \otimes s \otimes t \right\rangle \ , \end{aligned}$$

which can be rewritten as:

$$\begin{aligned} (4.11)\quad &\left\langle \varphi^{(4)}, \varphi' \otimes r \otimes s \otimes t \right\rangle + \\ &\qquad \left\langle \varphi^{(3)}, \langle \varphi'', r\rangle \otimes s \otimes t + r \otimes \langle \varphi'', s\rangle \otimes t + r \otimes s \otimes \langle \varphi'', t\rangle \right\rangle = \\ &\qquad\qquad \left\langle V^{(3)}, r \otimes s \otimes t \right\rangle + \frac{1}{2} h\Delta \left\langle \varphi^{(3)}, r \otimes s \otimes t \right\rangle \ . \end{aligned}$$

We differentiate this in the constant direction u and get:

$$\begin{aligned} (4.12)\quad &\varphi' \cdot \partial_x \Big(\left\langle \varphi^{(4)}, u \otimes r \otimes s \otimes r \right\rangle \Big) + 4 \left\langle \varphi^{(4)}, u \otimes r \otimes s \otimes t \right\rangle + \\ &\qquad \Big\langle \varphi^{(4)}, \langle \psi'', u\rangle \otimes r \otimes s \otimes t + u \otimes \langle \psi'', r\rangle \otimes s \otimes t + \\ &\qquad\quad u \otimes r \otimes \langle \psi'', s\rangle \otimes t + u \otimes r \otimes s \otimes \langle \psi'', t\rangle \Big\rangle = \\ &\qquad \left\langle V^{(4)}, u \otimes r \otimes s \otimes t \right\rangle + \frac{1}{2} h\Delta \left\langle \varphi^{(4)}, u \otimes r \otimes s \otimes t \right\rangle - \\ &\Big[\left\langle \left\langle \varphi^{(3)}, s \otimes t \right\rangle, \left\langle \varphi^{(3)}, u \otimes r \right\rangle \right\rangle + \left\langle \left\langle \varphi^{(3)}, u \otimes s \right\rangle, \left\langle \varphi^{(3)}, r \otimes t \right\rangle \right\rangle + \\ &\qquad\qquad \left\langle \left\langle \varphi^{(3)}, r \otimes s \right\rangle, \left\langle \varphi^{(3)}, u \otimes t \right\rangle \right\rangle \Big] \ . \end{aligned}$$

Let $M_B^3(\varphi) = M_B^3(\psi)$ be defined as in (2.12) and recall (2.13) :

$$M_B^3(\varphi) \leq (3(1-\widetilde{\theta}))^{-1} M_B^3(V) \ . \tag{4.13}$$

Since everything also works in the case when $B = \ell^\infty$, we have :

$$M_{\ell^\infty}^3(\varphi) \leq (3(1-\widetilde{\theta}))^{-1} M_{\ell^\infty}^3(V) \ . \tag{4.14}$$

Put $M_B^4(\varphi) = \sup\limits_x \left\| \varphi^{(4)}(x) \right\|_{(B\otimes B^*\otimes \ell^\infty \otimes \ell^\infty)^*}$, where the norm is the one for multilinear forms on $B \times B^* \times \ell^\infty \times \ell^\infty$. Let x_0 be a point where the supremum is attained and let $u \in B$, $r \in B^*$, $s, t \in \ell^\infty$ be corresponding normalized vectors. Then

$$\begin{aligned}
&\left|\left\langle \varphi^{(3)}, s \otimes t \right\rangle\right|_\infty \leq M_{\ell^\infty}^3(\varphi), && \left|\left\langle \varphi^{(3)}, u \otimes r \right\rangle\right|_1 \leq M_B^3(\varphi), \\
&\left|\left\langle \varphi^{(3)}, u \otimes s \right\rangle\right|_B \leq M_B^3(\varphi), && \left|\left\langle \varphi^{(3)}, r \otimes t \right\rangle\right|_{B^*} \leq M_B^3(\varphi), \\
&\left|\left\langle \varphi^{(3)}, r \otimes s \right\rangle\right|_{B^*} \leq M_B^3(\varphi), && \left|\left\langle \varphi^{(3)}, u \otimes t \right\rangle\right|_B \leq M_B^3(\varphi).
\end{aligned}$$

Hence the last term in (4.12) can be bounded by

$$M_{\ell^\infty}^3(\varphi) \cdot M_B^3(\varphi) + 2(M_B^3(\varphi))^2 \ .$$

The usual argument gives :

$$\begin{aligned}
4(1-\widetilde{\theta}) M_B^4(\varphi) &\leq M_B^4(V) + M_{\ell^\infty}^3(\varphi) M_B^3(\varphi) + 2 M_B^3(\varphi)^2 \leq \\
&M_B^4(V) + (9(1-\widetilde{\theta})^2)^{-1} [M_{\ell^\infty}^3(V) M_B^3(V) + 2 M_B^3(V)^2].
\end{aligned} \tag{4.15}$$

Here we used (4.13), (4.14) in order to get the last inequality. Hence

$$\begin{aligned}
M_B^4(\varphi) \leq{}& (4(1-\widetilde{\theta}))^{-1} M_B^4(V) + \\
&(36(1-\widetilde{\theta})^3)^{-1} [M_{\ell^\infty}^3(V) M_B^3(V) + 2 M_B^3(V)^2].
\end{aligned} \tag{4.16}$$

Everything works the same way with $B = \ell^\infty$ and we get :

$$M_{\ell^\infty}^4(\varphi) \leq (4(1-\widetilde{\theta}))^{-1} M_{\ell^\infty}^4(V) + (12(1-\widetilde{\theta})^3)^{-1} M_{\ell^\infty}^3(V)^2 . \tag{4.17}$$

As before, these estimates extend to the case of potentials of the form $\frac{1}{2}x^2 + W(x)$, where W need not have compact support, but with (2.9) fulfilled and with $\nabla^3 V(x)$, $\nabla^4 V(x)$ bounded as functions of x.

Let $V^{(m)}$, $m = 1, 2, \ldots$ be a sequence of strictly convex smooth potentials on $\mathbb{R}^m$ with $V^{(m)}(x) \to +\infty$ when $|x| \to \infty$. More assumptions will be made later, for the moment, we only assume that for m sufficiently large and for some fixed $k \geq 2$:

$$V^{(km)}(x, x, \dots, x) = kV^m(x), \ x \in \mathbb{R}^m \ , \tag{4.18}$$

$$V^{(m)}(x_m, x_1, \dots, x_{m-1}) = V^{(m)}(x_1, \dots, x_m) \ . \tag{4.19}$$

Let $u^{(m)} = e^{-\varphi^{(m)}/h}$ be the positive normalized eigenfunction associated to the first eigenvalue, $hE_m(h)$ of $-\frac{1}{2}h^2\Delta + V^{(m)}$. Our goal is to estimate $(E^{(km)}/km) - E^{(m)}/m$, when m tends to infinity, and in order to do so, we shall show that $k^{-1}\varphi^{(km)}(x, x, \dots, x)$ is close to $\varphi^{(m)}(x)$ when m is large.

If $f(x) = \varphi^{(km)}(x, x, \dots, x)$, $x \in \mathbb{R}^m$, then :

$$\begin{aligned}
\Delta f = \sum_{1 \leq \nu \leq m} \Big((\partial_{x_\nu} + \partial_{x_{\nu+m}} + \dots + \partial_{x_{\nu+(k-1)m}})^2 \varphi^{(km)} \Big)(x, x, \dots, x) = \\
\sum_{1 \leq \nu \leq m} \ \sum_{0 \leq \alpha \leq k-1} \ \sum_{0 \leq \beta \leq k-1} \Big(\partial_{x_{\nu+\alpha m}} \partial_{x_{\nu+\beta m}} \varphi^{(km)} \Big)(x, x, \dots, x) = \\
\sum_{1 \leq \nu \leq m} \ \sum_{0 \leq \alpha \leq k-1} \ \sum_{0 \leq \gamma \leq k-1} \Big(\partial_{x_{\nu+\alpha m}} \partial_{x_{\nu+(\alpha+\gamma)m}} \varphi^{(km)} \Big)(x, x, \dots, x) = \\
\sum_{1 \leq \mu \leq km} \ \sum_{0 \leq \gamma \leq k-1} \Big(\partial_{x_\mu} \partial_{x_{\mu+\gamma m}} \varphi^{(km)} \Big)(x, \dots, x).
\end{aligned}$$

(Here we use the cyclic convention : $x_{j+km} = x_j$.) Hence :

$$\begin{aligned}
\Delta f(x) = (\Delta\varphi^{(km)})(x, x, \dots, x) + \\
\sum_{1 \leq \mu \leq km} \ \sum_{1 \leq \gamma \leq k-1} \Big(\partial_{x_\mu} \partial_{x_{\mu+\gamma m}} \varphi^{(km)} \Big)(x, \dots, x).
\end{aligned} \tag{4.20}$$

Similarly, since $(\partial_{x_{\nu+m}} \varphi^{(km)})(x, \dots, x) = (\partial_{x_\nu} \varphi^{(km)})(x, \dots, x)$ (by (4.19) with m replaced by km) :

$$\begin{aligned}
(\nabla f)^2 = \sum_{1 \leq \nu \leq m} \Big((\partial_{x_\nu}\varphi)(x, \dots, x) + \\
(\partial_{x_{\nu+m}}\varphi)(x, \dots, x) + \dots + (\partial_{x_{\nu+(k-1)m}}\varphi)(x, \dots, x) \Big)^2 = \\
k^2 \sum_{1 \leq \nu \leq m} \Big((\partial_{x_\nu}\varphi)(x, \dots, x) \Big)^2 = k \sum_{1 \leq \nu \leq km} \Big((\partial_{x_\nu} \varphi^{(km)})(x, \dots, x) \Big)^2 .
\end{aligned} \tag{4.21}$$

Still with k fixed, we put $\widetilde{\varphi}^{(m)} = k^{-1}\varphi^{(km)}(x,\dots,x)$, $\widetilde{E}^{(m)} = k^{-1}E^{(km)}$. Then :

$$V^{(m)}(x) - \frac{1}{2}(\nabla\widetilde{\varphi}^{(m)})^2 + \frac{1}{2}h\Delta\widetilde{\varphi}^{(m)} - h\widetilde{E}^{(m)} = -\frac{1}{2}hk^{-1}\sum_{1\le\mu\le km}\ \sum_{1\le\gamma\le k-1}\left(\partial_{x_\mu}\partial_{x_{\mu+\gamma m}}\varphi^{(km)}\right)(x,\dots,x). \tag{4.22}$$

We now add one more assumption. We assume that for sufficiently large m :

(4.23) $V = V^{(m)}$ satisfies the assumption (2.9) with $B = \ell^\infty_\rho$, for some family $\rho^{(m)}$ with the properties (4.24), and that with the same ρ :

$$\sup_x \left\|\nabla^3 V^{(m)}\right\|_{(\ell^\infty_\rho\otimes\ell^1_{1/\rho}\otimes\ell^\infty)^*},$$
$$\sup_x \left\|\nabla^3 V^{(m)}\right\|_{(\ell^\infty\otimes\ell^1\otimes\ell^\infty)^*}$$
$$\sup_x \left\|\nabla^4 V^{(m)}\right\|_{(\ell^\infty_\rho\otimes\ell^1_{1/\rho}\otimes\ell^\infty\otimes\ell^\infty)^*},$$
$$\sup_x \left\|\nabla^4 V^{(m)}\right\|_{(\ell^\infty\otimes\ell^1\otimes\ell^\infty\otimes\ell^\infty)^*}$$

are all finite and bounded by some constant which is independent of m.

Here the property of ρ should be :

(4.24) For $j \in \mathbb{Z}/m\mathbb{Z}$ we have : $e^{-\kappa} \le \rho(j+1)/\rho(j) \le e^{\kappa}$. Moreover $\rho(0) = 1$ and we have $\rho(j+1)/\rho(j) = e^{\kappa}$ for $C \le j \le \frac{1}{2}m - C$, $\rho(j+1)/\rho(j) = e^{-\kappa}$ for $-(\frac{1}{2}m - C) \le j \le -C$, with $\kappa > 0$ and C independent of m.

It follows from our earlier estimates that

(4.25) $M^j_{\ell^\infty_\rho}(\varphi)$, $M^j_{\ell^\infty}(\varphi)$ for $j = 3,4$ are bounded by a constant independent of m (when m is sufficiently large),

are bounded by a constant independent of m (when m is sufficiently large), and using this fact for $\varphi^{(km)}$ (with k fixed) we shall estimate the right hand side, F of (4.22). To shorten the formulas, we take $k = 2$, but everything works the same way for any fixed $k \geq 2$. Then we have:

$$F = -\frac{1}{2}h \sum_{1\leq\mu\leq m} \left(\partial_{x_\mu}\partial_{x_{\mu+m}}\varphi^{(2m)}\right)(x,x) \ . \tag{4.26}$$

From (2.2), it follows that

$$(\partial_{x_1}\partial_{x_{1+m}}\varphi^{(2m)})(x,x) = \mathcal{O}(1)e^{-\kappa m} \ , \tag{4.27}$$

uniformly in x and in m. Using (4.25), we also get:

$$\left|\nabla\left((\partial_{x_1}\partial_{x_{1+m}}\varphi^{(2m)})(x,x)\right)\right|_1 = \mathcal{O}(1)e^{-\kappa m} \ , \tag{4.28}$$

$$\left\|\nabla^2\left((\partial_{x_1}\partial_{x_{1+m}}\varphi^{(2m)})(x,x)\right)\right\|_{(\ell^\infty\otimes\ell^\infty)^*} = \mathcal{O}(1)e^{-\kappa m} \ . \tag{4.29}$$

For instance, the last estimate follows from:

$$\left\langle\nabla^2\left((\partial_{x_1}\partial_{x_{1+m}}\varphi^{(2m)})(x,x)\right), \nu\otimes\mu\right\rangle =$$
$$\left\langle(\nabla^4\varphi^{(2m)})(x,x), e_1\otimes e_{1+m}\otimes(\nu_1\otimes\mu_1+\nu_1\otimes\mu_2+\nu_2\otimes\mu_1+\nu_2\otimes\mu_2)\right\rangle \ ,$$

where $\nu_1 = (\nu,0)$, $\nu_2 = (0,\nu)$ etc., and the fact that $\|e_1\|_{\infty,\rho} = \mathcal{O}(1)$, $\|e_{1+m}\|_{1,1/\rho} = \mathcal{O}(e^{-\kappa m})$. Since $\varphi^{(2m)}$ is invariant under cyclic permutation of the coordinates (cf. (4.19)), we have (4.27)-(4.29) also in the case when $\partial_{x_1}\partial_{x_{1+m}}$ is replaced by $\partial_{x_\mu}\partial_{x_{\mu+m}}$, so by (4.26):

$$F(x),\ |\nabla F(x)|_1\ ,\ \|\nabla^2 F(x)\|_{(\ell^\infty\otimes\ell^\infty)^*} = \mathcal{O}(1)mhe^{-\kappa m}. \tag{4.30}$$

We now compare (4.22):

$$V^{(m)}(x) - \frac{1}{2}(\nabla\widetilde{\varphi}^{(m)})^2 + \frac{1}{2}h\Delta\widetilde{\varphi}^{(m)} - h\widetilde{E}^{(m)} = F$$

and

$$V^{(m)}(x) - \frac{1}{2}(\nabla\varphi^{(m)})^2 + \frac{1}{2}h\Delta\varphi^{(m)} - hE^{(m)} = 0 \tag{4.31}$$

as in section 2. Taking the gradient of the difference gives:

$$\begin{aligned}\frac{1}{2}(\nabla\widetilde{\varphi}^{(m)} + \nabla\varphi^{(m)})\cdot\partial_x(\nabla\widetilde{\varphi}^{(m)} - \nabla\varphi^{(m)}) &+ \\ \frac{1}{2}(\nabla^2\widetilde{\varphi}^{(m)} + \nabla^2\varphi^{(m)})(\nabla\widetilde{\varphi}^{(m)} - \nabla\varphi^{(m)}) &= \\ -\nabla F + \frac{1}{2}h\Delta(\nabla\widetilde{\varphi}^{(m)} - \nabla\varphi^{(m)}).&\end{aligned} \tag{4.32}$$

Here we recall that $\nabla^2\varphi^{(m)} = 1 + \nabla^2\psi^{(m)}$ with $\|\nabla^2\psi^{(m)}\|_{(\ell^\infty\otimes\ell^1)^*} \le \widetilde{\theta}$. Using this with m replaced by $2m$, we get :

$$\left\langle \nabla^2\widetilde{\varphi}^{(m)}(x), \nu\otimes\mu \right\rangle = \frac{1}{2}\left\langle (\nabla^2\varphi^{(2m)})(x,x), (\nu,\nu)\otimes(\mu,\mu) \right\rangle = \langle \nu,\mu\rangle + \frac{1}{2}\left\langle (\nabla^2\psi^{(2m)})(x,x), (\nu,\nu)\otimes(\mu,\mu) \right\rangle .$$

The absolute value of the last term is $\le \frac{1}{2}\widetilde{\theta}\,|\nu|_\infty\, 2\,|\mu|_1 = \widetilde{\theta}\,|\nu|_\infty\,|\mu|_1$, so $\nabla^2\widetilde{\varphi}^{(m)} = 1 + \nabla^2\widetilde{\psi}^{(m)}$ with

$$\left\|\nabla^2\widetilde{\psi}^{(m)}\right\|_{(\ell^\infty\otimes\ell^1)^*} \le \widetilde{\theta}\ . \tag{4.33}$$

The same argument as in section 2 then gives :

$$\left|\nabla(\widetilde{\varphi}^{(m)} - \varphi^{(m)})\right|_1 \le (1-\widetilde{\theta})^{-1}\sup_x |\nabla F(x)|_1 = \mathcal{O}(1)mhe^{-\kappa m}. \tag{4.34}$$

Taking the scalar product of (4.32) with the constant vector t and differentiating in the constant direction s, we get as in section 2 :

$$\begin{aligned}(4.35)\quad &\frac{1}{2}(\nabla\widetilde{\varphi}^{(m)} + \nabla\varphi^{(m)})\cdot\partial_x\left\langle \nabla^2(\widetilde{\varphi}^{(m)} - \varphi^{(m)}), s\otimes t\right\rangle + \\ &2\left\langle \nabla^2(\widetilde{\varphi}^{(m)} - \varphi^{(m)}), s\otimes t\right\rangle + \Big\langle \nabla^2(\widetilde{\varphi}^{(m)} - \nabla\varphi^{(m)}), \\ &\frac{1}{2}(\nabla^2\widetilde{\psi}^{(m)} + \nabla^2\psi^{(m)})(s)\otimes t + s\otimes\frac{1}{2}(\nabla^2\widetilde{\psi}^{(m)} + \nabla^2\psi^{(m)})(t)\Big\rangle + \\ &\left\langle \frac{1}{2}\nabla^3(\widetilde{\varphi}^{(m)} + \varphi^{(m)}), (\nabla\widetilde{\varphi}^{(m)} - \nabla\varphi^{(m)})\otimes s\otimes t\right\rangle = \\ &-\left\langle \nabla^2 F, s\otimes t\right\rangle + \frac{1}{2}h\Delta\left\langle \nabla^2(\widetilde{\varphi}^{(m)} - \varphi^{(m)}), s\otimes t\right\rangle .\end{aligned}$$

As in section 2 we conclude that :

$$\left\|\nabla^2(\widetilde{\varphi}^{(m)} - \varphi^{(m)})\right\|_{(\ell^\infty\otimes\ell^\infty)^*} = \mathcal{O}(1)mhe^{-\kappa m}. \tag{4.36}$$

Combining (4.22), (4.31), we get :

$$\begin{aligned}(4.37)\quad & m^{-1}(h\widetilde{E}^{(m)} - hE^{(m)}) = \\ & -m^{-1}F - (2m)^{-1}(\nabla\widetilde{\varphi}^{(m)} + \nabla\varphi^{(m)})\cdot(\nabla\widetilde{\varphi}^{(m)} - \nabla\varphi^{(m)}) + \\ & (h/2m)\Delta(\widetilde{\varphi}^{(m)} - \varphi^{(m)})\ ,\end{aligned}$$

and choosing x such that $\nabla\widetilde{\varphi}^{(m)} + \nabla\varphi^{(m)} = 0$ at x, we get from (4.30), (4.36), (4.37) and Lemma 1.2 of **[S1]** :

$$m^{-1}(h\widetilde{E}^{(m)} - hE^{(m)}) = \mathcal{O}(h+h^2)e^{-\kappa m}\ . \tag{4.38}$$

Summing up, we have proved :

Theorem 4.1. *Let $V^{(m)} = V^{(m)}(x_1, x_2, \dots, x_m)$, $m = 1, 2, \dots$ be a sequence of potentials with $V^{(m)}(0) = 0$, $\nabla V^{(m)}(0) = 0$, which for m large enough satisfy the assumptions* (4.18) *(with a fixed $k \geq 2$),* (4.19), (4.23). *Let $\mu(m)$ be the smallest eigenvalue of $-\frac{1}{2}h^2\Delta + V^{(m)}$. Then for sufficiently large m (uniformly in h):*

$$(km)^{-1}\mu(km) - m^{-1}\mu(m) = \mathcal{O}(h + h^2)e^{-\kappa m} . \tag{4.39}$$

If $\lim_{m\to\infty} \mu(m)/m \underset{\text{def}}{=} \mu(\infty)$ exists (as we know under certain assumptions, cf. section 3 and [**HS**]*), then* (4.39) *gives:*

$$m^{-1}\mu(m) - \mu(\infty) = \mathcal{O}(h + h^2)e^{-\kappa m} . \tag{4.40}$$

5. Application to a model related to statistical mechanics

In [**HS**] we studied the following model operator (inspired by [**K**]):

$$P_m = -h^2\Delta + V^{(m)}(x) \tag{5.1}$$

on $\mathbb{R}^m$, where:

$$V^{(m)}(x) = \frac{1}{4}\Sigma x_j^2 - \Sigma \log ch\Big(\sqrt{\frac{\nu}{2}}(x_j + x_{j+1})\Big) \quad \text{with } j \in \mathbb{Z}/m\mathbb{Z} \tag{5.2}$$

and assumed that ν is fixed in $\left]0, \frac{1}{4}\right[$. We keep the same assumption on ν and we then know ([**HS**]) that $V^{(m)}$ is strictly convex and vanishes to the second order at 0. If $f(t) = \log ch t$, then $f'(t) = sh t / ch t$, $f''(t) = (ch t)^{-2}$, and hence (as we saw in [**HS**]):

$$\partial_{x_j}^2 V^{(m)}(x) = \frac{1}{2} - \frac{1}{2}\nu\Big(\big(ch\sqrt{\frac{\nu}{2}}(x_{j-1}+x_j)\big)^{-2} + \big(ch\sqrt{\frac{\nu}{2}}(x_j+x_{j+1})\big)^{-2}\Big), \tag{5.3}$$

$$\partial_{x_j}\partial_{x_{j+1}} V^{(m)}(x) = -\frac{1}{2}\nu\big(ch\sqrt{\frac{\nu}{2}}(x_j + x_{j+1})\big)^{-2}, \tag{5.4}$$

$$\partial_{x_j}\partial_{x_k} V^{(m)}(x) = 0 \text{ if } j - k \not\equiv -1, 0, 1 \mod (m). \tag{5.5}$$

We can then write:

$$\nabla^2 V^{(m)}(x) = \frac{1}{2}(I + A(x)) , \tag{5.6}$$

$$A(x) = \begin{pmatrix} d_1(x) & c_1(x) & 0\dots & 0 & c_m(x) \\ c_1(x) & d_2(x) & c_2(x) & & 0 \\ 0 & & & & 0 \\ \cdot & & & \cdot & \\ 0 & & c_{m-2}(x) & d_{m-1}(x) & c_{m-1}(x) \\ c_m(x) & 0\dots & \dots & c_{m-1}(x) & d_m(x) \end{pmatrix} \tag{5.7}$$

where

$$|d_j(x)| \leq 2\nu \ , \quad |c_j(x)| \leq \nu \ . \tag{5.8}$$

We may also notice that $d_j(0) = -2\nu$, $c_j(0) = -\nu$.

Let $\rho : \mathbb{Z}/m\mathbb{Z} \to]0, \infty[$ satisfy :

$$e^{-\delta} \leq \mu(j+1)/\mu(j) \leq e^{\delta} \ , \tag{5.9}$$

where $\mu(j) = \rho(j+1)/\rho(j)$. Then the argument after (4.8) shows that

$$\|A(x)\|_{\mathcal{L}(\ell^p_\rho, \ell^p_\rho)} \leq 2\nu(1 + e^{\delta} \sup_{1\leq k \leq m} \frac{1}{2}(\mu(k) + \mu(k)^{-1})). \tag{5.10}$$

Let $\kappa > 0$ satisfy

$$2\nu(1 + ch\,\kappa) < 1 \ , \quad \text{i.e. } \kappa < ch^{-1}((1-2\nu)/2\nu) \ . \tag{5.11}$$

Then, if we choose $\delta > 0$ sufficiently small, it follows that :

$$\|A(x)\|_{\mathcal{L}(\ell^p_\rho, \ell^p_\rho)} \leq \theta < 1 \ , \tag{5.12}$$

for some fixed θ, provided that ρ satisfies (5.9) and :

$$e^{-\kappa} \leq \rho(j+1)/\rho(j) \leq e^{\kappa} \ . \tag{5.13}$$

We can clearly find such a ρ which also satisfies (4.24).

A part from the factor $\frac{1}{2}$ in (5.6) and the fact that there is no " $\frac{1}{2}$ " in (5.1) (which is not essential, as can be seen by a scaling in h), we have then verified the part of (4.23) which concerns the Hessian of $V^{(m)}$. The remaining parts of (4.23) (concerning the higher order Hessians of $V^{(m)}$ are easy to check, and it is also clear that we have (4.18), (4.19), so we can apply Theorem 4.1 and get :

Theorem 5.1. *Let $\mu(m;h)$ be the lowest eigenvalue of the operator* (5.1), (5.2), *and assume that* $0 \leq \nu < \frac{1}{4}$. *If* $\kappa > 0$ *satisfies* (5.11), *then for* ν , κ *fixed we have uniformly with respect to* h :

$$\mu(\infty, h) - \mu(m;h)/m = \mathcal{O}(h + h^2)e^{-\kappa m} \ , \quad m \to \infty \ . \tag{5.14}$$

Here $\mu(\infty;h)$ *denotes the limit of* $\mu(m;h)/m$ *as* m *tends to infinity. (The existence of the limit was established in* **[HS]** *and also follows from Theorem 3.1.)*

REMARK 5.2. In analogy with (4.1) we can write

$$\nabla^2 V^{(m)}(0) = \Big(\frac{1}{2} - \nu\Big)(I - (2\nu/(1-2\nu))\frac{1}{2}(\tau_{-1} + \tau_1)) \ , \tag{5.15}$$

so if we compare (4.8) and (5.11), we see that Theorem 5.1 produces a decay rate which is equal to the (probably optimal) one that we get for the quadratic approximations of $V^{(m)}$, by applying (4.8). We have therefore every reason to believe that the set of exponents in Theorem (5.14) is optimal, and by applying the WKB results of **[HS, S1S2,]**, it seems quite possible to prove that so is the case, if we require uniformity in h, as in (5.14).

References

[HS] B. HELFFER, J. SJÖSTRAND, *Semiclassical expansions of the thermodynamical limit for a Schrödinger equation, I. The one well case.* Preprint (1991).

[K] M. KAC, *Mathematical mechanisms of phase transitions.* Brandeis Lectures, Gordon and Breach, New York, (1966).

[K2] M. KAC, *Statistical mechanics of some one dimensional systems.* Studies in Math. An. and Rel. Top. : essays in hon. of G. Polya, Stanford Univ. Press, Stanford, California, 165-169, (1962).

[SiWYY] I.M. SINGER, B. WONG, S.T. YAU, S.T. YAU, *An estimate for the gap of the first two eigenvalues of the Schrödinger operator.* Ann. di Sc. Norm. Sup. di Pisa, Ser. IV, 319-333, 12 (1985).

[S1] J. SJÖSTRAND, *Potential wells in high dimensions.* Preprint (1991).

[S2] J. SJÖSTRAND, *Potential wells in high dimensions II. More about the one well case.* Preprint (1991).

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SCATTERING OF WAVES IN A MEDIUM DEPENDING PERIODICALLY ON TIME

B. R. VAINBERG

I. INTRODUCTION

We obtain the asymptotic behaviour as $t \to \infty, |x| \leq a < \infty$ of solutions of exterior mixed problems for hyperbolic equations and systems when the boundary of a domain and coefficients of the equations depend periodically on time. Our method can be regarded as an alternative one to the Lax-Phillips scattering theory. Using the Lax-Phillips method we have to construct at first waves operators and a scattering matrix. Then we study some analytic properties of the scattering matrix and some properties of a special Lax-Phillips semigroup $Z(t)$ and then we derive asymptotic behavior of solutions of the exterior mixed problem as $t \to \infty$. In our direct method at first we find the asymptotic behavior of the solution of the exterior mixed problem. Unlike Lax-Phillips we do it without using any abstract result on spectral representation, outgoing and ingoing subspaces and so on. Then we obtain existence of the wave operators and the scattering operator. In fact, it is not a difficult problem if you know asymptotic behavior of the solutions.

Both of these methods were constructed earlier in the stationary case, when the domain and coefficients of the equations did not depend on time (there are references in [6]). Recently a few papers by J. Cooper and W. Strauss appeared which contain some results of Lax-Phillips theory for scattering of waves by a body moving periodically in t ([1],[2],[3]). Another method of research of this problem is based on the theorem of RAGE type and is suggested by V. Petkov [4]. These authors proved the existence of a scattering operator for wave equation in exterior of a body which depends periodically on t if $n \geq 3$ and obtained asymptotic behavior of solutions of this problem for odd n. They also studied hyperbolic systems of first order when dimension n is odd. Our method gives the possibility to study general time periodic systems of any order and moreover the dimension of the space can be arbitrary and the energy of solution can be unbounded with respect to time. Some of the proofs given below are very concise. The omitted details can be reconstructed with the help of [7], [8], [9].

II. ASYMPTOTIC BEHAVIOR OF SOLUTIONS

Let $x \in I\!R^n$, $\partial_t = \partial/\partial_t$, $\partial_x = (\partial/\partial x_1, \cdots, \partial/\partial x_n)$, $\Omega \in I\!R^{n+1}_{(t,x)}$ be the exterior of the cylinder with a curvelinear boundary which depends periodically on t. Let $u = (u^{(1)}, ..., u^{(\ell)})$,
$L = L(t, x, \partial_t, \partial_x) = \{L_{i,j}\}$ be a hyperbolic $\ell \times \ell$ matrix. We consider the exterior mixed problem

$$(1) \qquad \begin{cases} Lu = 0, \quad (t,x) \in \Omega, \quad t > \tau; \qquad Bu|_{\partial\Omega} = 0, \quad t > \tau; \\ \partial_t^j u|_{t=\tau} = f_j, \quad 0 \le j \le m-1, \quad x \in \Omega_\tau = \Omega \bigcap \{t = \tau\}. \end{cases}$$

Here $B = B(t, x, \partial_x)$ is a boundary operator of general type, $m = \max_{i,j}$ ord $L_{i,j}$.

The main problem of this part of the article is the following. Let $f = (f_0, ..., f_{m-1})$ be a function with a compact support. The asymptotic behavior of solution u is to be found when $t \to \infty$ and x is bounded, that is the initial data are localized in space and the solution at large t is of interest only in the limited part of the space.

We fix an arbitrary constant a for which $\partial\Omega \subset \{(t,x) : |x| < a-1\}$, condition H_1 is satisfied and $f = 0$ when $|x| > a$.

Conditions.

H_1. The medium is homogeneous in the neighborhood of infinity, that is $L = L_0(\partial_t, \partial_x)$ when $|x| > a$, where L_0 is a homogeneous matrix with constant coefficients.

H_2. The problem (1) is time periodic, that is $\Omega_{t+T} = \Omega_t$ and coefficients of the operators L and B are periodic functions with respect to t with the same period T.

H_3. The problem (1) is correct and Duhamel principle is valid.

Let $C_a^\infty(\bar\Omega_\tau), C_a^\infty(\bar\Omega)$ be spaces of infinitely smooth functions in $\bar\Omega_\tau$ or $\bar\Omega$ which are equal to zero when $|x| > a$; $H^s(D)$ be a Sobolev space of functions in domain D, $H^s_{loc}(\bar D)$ be a space of functions in the domain D belonging to $H^s(V)$ for any bounded domain $V \subset D$;

$\psi \in H^{s,A}$ if $\exp(At)\psi \in H^s(\Omega)$;
$\psi \in H^{s,A}_{a,0}$ if $\psi \in H^{s,A}$ and $\psi = 0$ when $|x| \geq a$ *or* $t < 0$.

If $\nu \Rightarrow (\nu_0, ..., \nu_{m-1})$, then we denote $H^\nu(\Omega_\tau) = \sum_{0 \leq j \leq m-1} H^{\nu_j}(\Omega_\tau)$. Let $f = (f_0, \ldots, f_{m-1}) \in F_\tau$ if $f_j \in C^\infty_a(\bar{\Omega}_\tau)$ and compatibility conditions are satisfied, that is there exists $w \in H^m_{loc}(\bar{\Omega})$ for which boundary and initial data of problem (1) are valid.

We shall use the same notation for the space of functions and vector-functions if the latter is a direct product of n copies of the space of functions. At last let H(ν) be the closure of the space F_τ with respect to the norm of the space $H^\nu(\Omega_\tau)$.

The correctness of the problem (1) means that it has the unique solution $u \in H^m_{loc}(\bar{\Omega} \bigcap \{t \geq \tau\})$ for any $f \in F_\tau$ and there are $\nu_j, q \in I\!R$ such that the operator

$$U_\tau : f \to \begin{cases} u, & t > \tau \\ 0, & t < \tau, \end{cases} \quad f \in F_\tau$$

has the following continuous extension: $U_\tau : H(\nu) \to H^q_{loc}(\bar{\Omega})$.

According to Duhamel principle there exist $A_0(s)$ such that the problem

$$Lw = g, \quad (t, x) \in \Omega; \quad Bw|_{\partial\Omega} = 0; \quad w = 0 \quad \text{when} \quad t < 0$$

is uniquely solvable in the space $H^{s,A}$ for any $g \in H^{s,A}_{a,0}$ if $s \geq m, A \geq A_0(s)$. Besides the operator

$$(2) \qquad V : H^{s,A}_{a,0} \to H^{s,A}, \quad Vg = w, \quad s \geq m, \quad A \geq A_0(s)$$

is bounded and

$$w(t, x) = \int_0^t u(t, \tau, x)\, d\tau\,.$$

Here u is the solution of the problem (1) with $f = Pg(\tau, \cdot)$, where $Pg = (0, ..., 0, g(\tau, x))$. It is implied that $Pg \in H(\nu)$ if $g \in H^{m,A}_{a,0}$.

The condition H_3 means that the boundary of the body must not move too quickly. For example, for the wave equation the velocity of the moving boundary must be lower than the velocity of propagation of waves in the medium. In this case the condition H_3 is satisfied for all the basic problems for wave equation.

In the case of general hyperbolic equations and systems we change the variables $(t, x) \to (t, y)$, $y = y(t, x)$ so that Ω could take the form of the straight cylinder. The velocity of the moving boundary must be such that the system in the new variables remains hyperbolic at t. Then the condition H_3 is satisfied if boundary operators satisfy uniform Shapiro-Lopatinsky condition.

H_4. Non-trapping condition. It means the following.

Let $E = E(t, \tau, x, x^0)$ be the Schwartz kernel of the operator U_τ, that is E is Green matrix of the problem (1). It is supposed that there exists such a function $T(\rho)$, that E is infinitely smooth when $|x|, |x^0| < \rho, \quad t - \tau > T(\rho)$. This condition is equivalent to the following: all the bicharacteristics are outgoing to infinity when t tends to infinity.

H_5. The operator L_0 has no waves with zero propagation velocity, that is $det L_0(0, \sigma) \neq 0$ when $\sigma \neq 0$. One can give up this condition in the same way as it was done in the stationary case in |5|.

Let (1^0) denote the problem (1), when $\tau = 0$.

THEOREM 1. *Let the conditions $H_1 - H_5$ be satisfied, $f \in H(\nu)$. Then there exists a sequence of complex points k_j which are called the scattering frequencies and integers p, q, p_j and periodic on t functions $u_0(t,x), u_{j,l}(t,x) \in C^\infty$ with period T such that*

1) $-\pi/\mathrm{T} \leq \mathrm{Re} k_j < \pi/\mathrm{T}, \quad \mathrm{Im} k_{j+1} \leq \mathrm{Im}\, k_j, \quad \mathrm{Im}\, k_j \to -\infty \quad as \quad j \to \infty$

2) *If n is odd then the solution of the problem (1^0) has the following expansion*

$$u = \sum_{j=1}^{N} \sum_{t=0}^{p_j} C_{j,l} u_{j,l}(t,x) t^l \exp(-ik_j t) + u_N, \tag{3}$$

where there exist λ and $C = C(a, N, j, \alpha)$ such that

$$|\partial_t^j \partial_x^\alpha u_N| \leq C t^\lambda \exp(\mathrm{Im} k_{N+1} t) \|f\|_{H(\nu)}, \quad |x| \leq a, \quad t \to \infty. \tag{4}$$

3) If *n is even then*

$$u = \sum_{\mathrm{Im} k_j \geq 0} \sum_{l=0}^{p_j} C_{j,l} u_{j,l}(t,x) t^l \exp(-ik_j t) + C_0 u_0(t,x) t^p ln^q t + w, \tag{5}$$

where $C_{j,l} = C_{j,l}(f), C_0 = C_0(f)$ and

$$|\partial_t^j \partial_x^\alpha w| \leq C |\partial_t^j (t^p ln^{q-1} t)| \, \|f\|_{H(\nu)}, \quad |x| \leq a, \quad t \to \infty. \tag{6}$$

Remark. The scattering frequencies k_j belonging to the upper half plane correspond to the exponentially growing terms. They are finite in number. The scattering frequencies k_j belonging to the real axis correspond to the terms, which are the product of the oscillating exponent with periodic function $u_{j,l}$. Such points are finite in number too. The points on the lower half-plane correspond to the exponentially decreasing terms. The less $\operatorname{Im} k_j$ are, the faster they decrease.

PROOF. We change the variables $(t,x) \to (t,y)$, $y = y(t,x)$ so that Ω takes the form of a straight cylinder and $y = x$ when $|x| > a$. The condition that L is a hyperbolic operator isn't used in the proof of the theorem, and the condition that L_0 is a hyperbolic operator is used only in the proof of lemma 6. The matrix L_0, conditions $H_1 - H_5$ and the assertions of the theorem don't change when the variables are changed. We'll use the same notations (t,x) for new variables. Thus we can suppose that there exists a domain $\omega \subset \mathbb{R}^n$ such that $\Omega = \mathbb{R} \times \omega \subset \mathbb{R}^{n+1}_{(t,x)}$.

A special parametrix W_τ of the problem (1) plays an important role in the proof of the theorem. Let us construct this parametrix. We can choose the function $T = T(\rho)$ defined in the condition H_4 in such a way that $T \subset C^\infty(\mathbb{R})$ and $T(\rho) = T(a)$ if $\rho \leq a$. Let $T_1 \in C^\infty(\mathbb{R})$, $T_1(\rho) > T(\rho)$ for any $\rho \geq 0$. Let $\zeta = \zeta(t-\tau, x)$ be such a function, that $\zeta \in C^\infty(\mathbb{R}^{n+1})$, $\zeta = 1$ when $t - \tau < T(|x|)$, $\zeta = 0$ when $t - \tau > T_1(x)$. Let $\psi \in C^\infty(\mathbb{R}^n_x)$, $\psi = 1$ when $|x| > a - 1$, $\psi = 0$ when $|x| < a - 2/3$. We define:

$$W_\tau = \zeta U_\tau - \psi N_\tau, \qquad N_\tau = V^0 \psi [L, \zeta] U_\tau$$

Here $[L,\zeta]$ is a commutator of L and the multiplication operator on the function ζ; V^0 is the operator (2) for case $L = L_0$, $\Omega = \mathbb{R}^{n+1}$; the function $\psi[L,\zeta]U_\tau$ is not defined in the domain $\mathbb{R}^{n+1} \backslash \Omega$ and we continue it by zero in this domain (here $\psi = 0$).

It is easy to see that for any $f \in F_\tau$

$$\begin{cases} LW_\tau f = G\tau f, & t > \tau, \quad x \in \omega; \\ BW_\tau f|_{\partial\Omega} = 0, & t > \tau; \quad \partial_t^j W_\tau f|_{t=\tau} = f_j, \quad 0 \leq j \leq m-1. \end{cases} \tag{7}$$

where

$$G_\tau = (1 - \psi^2)[L,\zeta]U_\tau - [L_0, \psi] V^0 \psi [L,\zeta] U_\tau. \tag{8}$$

Let P be the operator defined in condition $H_3, l_t h = h(t,\cdot)$ for any $h = h(t,x)$, $G(t,\tau) = l_t G_\tau$.

LEMMA 1. A. *The Schwartz kernel* $g = g(t,\tau,x,x^0)$ *of the operator* G_τ *has* *the following properties when* $|x^0| \le a$:

$$g \in C^\infty,$$
$$g = 0 \quad \text{if} \quad |x| \ge a \quad \textit{or} \quad t - \tau \le T(a),$$
$$g(t+T, \tau+T, x, x^0) = g(t, \tau, x, x^0).$$

B. *The equation*

$$\phi(t,\cdot) + \int_0^t G(t,\tau)P\phi(\tau,\cdot)d\tau = -G(t,0)f, \quad \phi \in I\!R^l, \tag{9}$$

is uniquely solvable in the space $C_a^\infty(\bar{\Omega})$ *for any* $f \in F_\tau$. *Also* $\phi = 0$ *when* $t < 0$.

C. *If* $f \in F_\tau$ *then the solution* $u = U_0 f$ *of problem* (1^0) *is equal to*

$$u = W_0 f + \int_0^t W_\tau P\phi(\tau,\cdot)d\tau, \tag{10}$$

where ϕ *is the solution of equation (9).*

PROOF. Assertion A follows from (8) and conditions $H_1 - H_4$. Assertion B is the consequence of assertion A and the fact that equation (9) is the equation of Volterra type. Assertion C follows from (7).

Formula (8) when $t - \tau > T_1(a)$ can be transformed in the following way. Since $(1-\psi^2)[L,\zeta] = 0$ for $t - \tau > T_1(a)$ we have

$$G_\tau = -[L_0,\psi]V^0\psi[L,\zeta]U_\tau, \quad t - \tau > T_1(a).$$

Since $LU_\tau f = \delta(t-\tau)f$ where δ is the delta function, we have

$$G_\tau f = -[L_0,\psi]V^0\psi L\zeta U_\tau f + [L_0,\psi]V^0\psi(\delta(t-\tau)f), \quad t - \tau > T_1(a).$$

We transform the first summand with the help of the relations:

$$\psi L = \psi L_0 = -[L_0,\psi] + L_0\psi, \quad V^0 L_0 \psi\zeta U_\tau = \psi\zeta U_\tau.$$

Since $[L_0,\psi]\psi\zeta = 0$ for $t - \tau > T_1(a)$, we have

$$G_\tau f = [L_0,\psi]V^0 Qf + [L_0,\psi]V^0\psi(\delta(t-\tau)f), \quad t - \tau > T_1(a) \tag{11}$$

where $Qf = [L_0,\psi]\zeta U_\tau f$ is zero when $|x| \ge a$ or $t - \tau > T_1(a)$. From (11) it follows that asymptotic behaviors of the functions $G(t,\tau)f$ and $V^0(\delta(t-\tau)f)$ as $t - \tau \to \infty$ are alike. From this and assertion A of lemma 1 the following lemma can be received.

LEMMA 2. 1) *For any* s *there exists* $A_0(s)$ *such that the operators*

$$\begin{aligned} &G : H_{a,0}^{s,A} \to H_{a,0}^{s+1,A}, \quad (G\phi)(t) = \textstyle\int_0^t G(t,\tau)P\phi(\tau)d\tau, \\ &G_0 : H(\nu) \to H_{a,0}^{s,A}, \quad (G_0 f)(t) = G(t,0)f \end{aligned} \tag{12}$$

are bounded.

2) *The solution of equation* (9) *belongs to the space* $H^{s,A}_{a,0}$, *for any* s *and* $A \geq A_0(s)$.

We research equation (9) with the help of the transformation

$F' = \exp(i\theta t/T)F$, where F is the transformation of Fourier-Bloch-Gelfand:

$$\phi(t) \to (F\phi)(\theta,t) = \sum_{k=-\infty}^{\infty} \phi(kT+t)\exp(ik\theta).$$

Let $C^\infty_{a,per} = \{\phi : \phi \in C^\infty_a(\bar\Omega), \quad \phi(t+T,x) = \phi(t,x)\}$, where T is defined in condition H_2. Let $H^s_{a,per}$ be the closure of the space $C^\infty_{a,per}$ with respect to the norm of the space $H^s(\Omega \cap \{0 < t < T\})$. The next lemma easily follows from the definition of the operator F'.

LEMMA 3. 1) *The operator* $F' : H^{s,A}_{a,0} \to H^s_{a,per}$ *is bounded and analytically depends on* θ *when* $\operatorname{Im}\theta > AT$.

2) If $\phi \in H^{s,A}_{a,0}$ then

$$(13) \qquad \begin{aligned} (F\phi)(\theta+2\pi,t) &= (F\phi)(\theta,t), \quad \operatorname{Im}\theta > AT, \\ (F'\phi)(\theta+2\pi,t) &= (F'\phi)(\theta,t), \quad \operatorname{Im}\theta > AT, \end{aligned}$$

$$(14) \qquad \phi(t) = \tfrac{1}{2\pi}\textstyle\int_{d_\alpha} (F\phi)(\theta,t)d\theta, \quad d_\alpha = [\alpha i - \pi, \alpha i + \pi], \quad \alpha > AT.$$

Let us fix s and $A > A_0(s)$. Let us apply the transformation F' with $\operatorname{Im}\theta > AT$ to the equation (9). Since $G(t,\tau) = 0$ when $t < \tau$ and $\phi(\tau) = 0$ when $\tau < 0$, we can replace the interval of integration in (12) by $\mathbb{R}$. Then the operators G and F become commutative. Therefore $F'G\phi = G(\theta)F'\phi$ where for any $h \in H^s_{a,per}$ we have

$$\begin{aligned} G(\theta)h &= \textstyle\int_\infty^\infty G(t,\tau)\exp(i\theta(t-\tau)/T)Ph(\tau)d\tau = \\ &= \textstyle\sum_{k=-\infty}^\infty \int_{-kT}^{(-k+1)T} G(t,\tau)\exp(i\theta(t-\tau)/T)Ph(\tau)d\tau = \\ &= \textstyle\int_0^T (F'G)(\theta,t,\tau)\exp(-i\theta\tau/T)Ph(\tau)d\tau. \end{aligned}$$

So the function $\psi = F'\phi$ is a solution of the equation

$$(15) \qquad \psi + G(\theta)\psi = -G_0(\theta)f, \qquad (G_o(\theta)f)(t) = F'G(t,0)f,$$

where $\operatorname{Im}\theta > AT$ and the operators

$$G(\theta) : H^s_{a,per} \to H^s_{a,per}, \qquad G_0(\theta) : H(\nu) \to H^s_{a,per}$$

are compact and analytically depend on θ when $\operatorname{Im}\theta > AT$.

The important property of the parametrix W_τ is the existence of a meromorphic extension of the operators $G(\theta)$, $G_0(\theta)$ in the domain $\operatorname{Im}\theta < AT$.

Let H be a Hilbert space. A family of the operators $A(\theta) : H \to H$ is called finitely-meromorphic if 1) the operators $A(\theta)$ depend meromorphically on the parameter θ, 2) for any pole $\theta = \theta_0$ of the family $A(\theta)$ the coefficients of negative powers of $(\theta - \theta_0)$ in the Laurent-series expansions of $A(\theta)$ are finite-dimensional operators (i.e. they take the whole space H into a finite-dimensional subspace of H). We denote by $\mathbb{C}'$ the complex θ-plane $\mathbb{C}$ with cuts:

$$l_k = \{\theta : \theta = 2k\pi - i\rho, \rho > 0\}, k = 0, \pm 1, \pm 2, \cdots$$

We'll say that $A(\theta)$ possesses property $S(S')$ if either n is odd and $A(\theta), \theta \in \mathbb{C}$, is a finitely-meromorphic family or n is even, $A(\theta), \theta \in \mathbb{C}'$, is a finitely-meromorphic family and $A(\theta)$ has the following asymptotic behavior as $\theta \to 0$

a) for property S:

$$A(\theta) = B(\theta)\ln\theta + \sum_{0 \le j \le m} B_j \theta^{-j} + C(\theta), \quad m < \infty,$$

where the operators $B(\theta), C(\theta)$ analytically depend on θ when $|\theta| << 1$, and operators $B_j, \partial_\theta^j B|_{\theta=0}, j \ge 0$, are finite-dimensional

b) for property S':

$$A(\theta) = A_0(\theta) + \theta^{-m} \sum_{j \ge 0} \left(\frac{\theta}{P(\ln \theta)} \right)^j P_j(\ln \theta), \tag{16}$$

where $A_0(\theta)$ analytically depends on θ when $|\theta| << 1$, P is a polynomial with constant coefficients, P_j are polynomials of orders less or equal to jl, constants $m, l \ge 0$ are integers, coefficients of P_j are finite-dimensional operators.

LEMMA 4. ([6]). *If a family of compact operators $G(\theta) : H \to H$ possesses property* S *and there exists $\theta = \theta_0$ such that the operator $1 + G(\theta_0)$ is reversible then the family of operators $(1 + G(\theta))^{-1}$ possesses property S'.*

LEMMA 5. *Let $Q : H^{s,A}_{a,0} \to H^{s,A}_{a,0}$ be a bounded operator and its kernel $q(t, \tau, x, x^0)$ possesses the following properties*

$$q(t + T, \tau + T, x, x^0) = q(t, \tau, x, x^0),$$
$$q(t, \tau, x, x^0) = 0 \quad if \quad 0 \le t - \tau \le T_0 < \infty.$$

Then there exists an analytical operator-valued function $Q(\theta) : H^s_{a,per} \to H^s_{a,per}$, $\theta \in \mathbb{C}$, such that $F'Q = Q(\theta)F'$.

Let $\chi \in C^\infty(\mathbb{R}^n_x)$, $\chi = 1$ when $|x| < a - 1$, $\chi = 0$ when $|x| > a$. Let $\alpha \in C^\infty(\mathbb{R})$, $\alpha(t) = 1$ when $t > 1$, $\alpha(t) = 0$ when $t < 0$. Let $V^{0,\alpha}$ be the operator with the kernel equal to $\alpha(t-t_0)E^0(t-\tau, x-x^0)$, where E^0 is kernel of the operator V^0.

LEMMA 6. *There exist such t_0 and such a family of compact operators $P(\theta)$: $H^s_{a,per} \to H^s_{a,per}$, that $P(\theta)$ possesses property S and $F'\chi V^{0,\alpha} = P(\theta)F'$.*

Lemma 5 is rather simple, lemma 6 is a consequence of Herglotz-Petrovskii formulas. From Lemmas 5,6 and formula (11) we obtain the following lemma.

LEMMA 7. *The operators $G(\theta)$ and $G_0(\theta)$ admit meromorphic extensions, which possesses property S.*

From this, (15) and lemma 4 it follows that

(17) $\quad F'\phi = L(\theta)f \quad$ where $\quad L(\theta) = -(1+G(\theta))^{-1}G_0(\theta) : H(\nu) \to H^s_{a,per}$

is an operator which possesses property S'. The operator $L(\theta)$ has no poles when $\operatorname{Im}\theta > AT$ since $F'\phi$ exists for any f if $\operatorname{Im}\theta > AT$. From (17) and (10) it follows that there exist t_0 and an operator-function $R(\theta) : H(\nu) \to H^s_{a,per}$, such that $R(\theta)$ possesses property S' and has no poles when $\operatorname{Im}\theta > AT$ and

$$F'(\chi\alpha(t-t_0)u) = R(\theta)f \tag{18}$$

We denote by θ_j the poles of the operator $R(\theta)$ lying in the stripe $-\pi \leq \operatorname{Re}\theta < \pi$. We number them so that $\operatorname{Im}\theta_{j+1} \leq \operatorname{Im}\theta_j$. Let $k_j = \theta_j/T$. From (14) and (18) it follows that

$$\chi u = (2\pi)^{-1}) \int_{d_\alpha} R(\theta) f \exp(-i\theta t/T) d\theta, \qquad t > t_0 + 1. \tag{19}$$

Let n be odd. From (19), (13) and lemma 7 it follows that

(20)

$$\chi u = i \sum_{\operatorname{Im}\theta_j \geq \operatorname{Im}\theta_{N+1}} res_{\theta=\theta_j} R(\theta) f \exp(-i\theta t/T) + \frac{1}{2\pi} \int_{d_\beta} R(\theta) f \exp(-i\theta t/T) d\theta,$$

where $t > t_0 + 1$ and $\beta = \operatorname{Im}\theta_{N+1} - \epsilon, 0 < \epsilon << 1$. The estimate (4) is true for the second term in right side of (20). Thus (3), (4) follow from (20). Let n be even. Then

$$\chi u = i \sum_{\operatorname{Im}\theta_j \geq \theta} res_{\theta=\theta_j} R(\theta) f \exp(-i\theta t/T) + \frac{1}{2\pi} \int_d R(\theta) f \exp(-i\theta t/T) d\theta, \tag{21}$$

where $t > t_0 + 1$ and $d = d_+ \cup \lambda_\epsilon \cup d_-$, $\quad d_\pm = d_{-\epsilon} \cap \{\pm\operatorname{Re}\theta > 0\}, 0 < \epsilon << 1, \lambda_\epsilon$ is the circle $|\theta| = \epsilon$ with the beginning in the point $-i\epsilon - 0$ and the end in the point $-i\epsilon + 0$. The integral along $d_{-\epsilon}$ can be estimated. The asymptotic behavior of the integral along λ_ϵ at $t \to \infty$ can be found with the help of expansion (16) for R(θ). So if n is even the assertion of the theorem 1 follows from (21). The theorem 1 is proved.

III. SYSTEMS WITH BOUNDED ENERGY, SCATTERING OPERATOR

In this part of the article we consider only systems of the first order ($m = 1$) for the sake of simplicity. In this case there are no difficulties with the description of energy space. Energy of a solution is its norm in the space $L_2(\Omega_t)$. We suppose that the following additional condition is satisfied:

H_6. There exists such constant $M < \infty$ that the norm of operator

$$U(t,\tau): \quad L_2(\Omega_\tau) \to L_2(\Omega_t)$$

is not greater than M if $t \geq \tau$. Here $U(t,\tau) = l_t U_\tau$, where U_τ was defined in condition H_3, l_t is the operator of restriction on hyperplane $t = const$.

Let us denote the monodromy operator $U(T,0)$ of the problem (1^0) by M and its eigenvalues belonging to the unit circle S^1 by $\exp(i\lambda_j T)$, $\lambda_j \in [0, 2\pi/T]$. Let $L_{2,b}$ be the space of functions belonging to $L_2(\Omega_0)$ and equal to zero when $|x| > b$.

THEOREM 2. *Let conditions* $H_1 - H_6$ *be satisfied. Then the operator M does not have more than the finite number of the eigenvalues* $\exp(i\lambda_j T), 1 \leq j \leq N$ *(taking their multiplicity into account) belonging to the unit circle* S^1. *Let* f_j, $1 \leq j \leq N$, *be the corresponding system of linearly independent eigenfunctions.*

There exist such eigenfunctions h_j *of the operator* M^* *with the eigenvalues* $\exp(-i\lambda_j T)$, $1 \leq j \leq N$ *that the solutions* $u = U(t,0)f$ *of the problem* (1^0) *with* $f \in L_{2,a}$ *have the following asymptotic behavior as* $t \to \infty$

$$u = \sum_{j=1}^{M} C_j U(t,0) f_j + w, \qquad C_j = (f, h_j), \tag{22}$$

where the following estimates are valid:

1) if n is odd then there exists $\epsilon > 0$ *such that for arbitrary* $j, \alpha = (\alpha_1, \cdots, \alpha_n)$ *and some* $C = C(j,\alpha,a)$ *we have*

$$|\partial_t^j \partial_x^\alpha w| \leq C \exp(-\epsilon t) ||f||_{L_{2,a}}, \quad t \to \infty, \quad |x| \leq a; \tag{23}$$

2) if n is even then for the same j, α we have

$$(24) \qquad |\partial_t^j \partial_x^\alpha w| \le C |\partial_t^j \ln^{-1} t| \|f\|_{L_{2,a}}, \qquad t \to \infty, \quad |x| \le \alpha.$$

Remark. The functions $U(t,0)f_j$ in (22) have form $u_j(t,x)\exp(i\lambda_j t)$ where u_j are time periodic functions.

PROOF. From condition H_6 it follows that expansions (3), (5) have no terms increasing as $t \to \infty$. Thus for any $b > a$, $|x| < b$ and $f \in L_{2,b}$ these expansions can be rewritten as following

$$(25) \qquad u = \sum_{j=1}^{N} C_j u_j(t,x) \exp(i\lambda_j t) + o(1), \qquad t \to \infty, \quad |x| < b,$$

where $\mathrm{Im}\lambda_j = 0$, $u_j(t+T,x) = u_j(t,x)$, the functions u_j with the same λ_j are linearly independent and the estimates (23), (24) with b instead of a are valid for remainder $o(1)$. It follows from (1^0) and (25) that the functions u_j exp $(i\lambda_j t), 1 \le j \le N$, satisfy the equation and boundary conditions of problem (1^0).

If $u_j = 0$ when $|x| < a$ then

$$L_0(\partial_t, \partial_x) u_j \exp(i\lambda_j t) = 0, \qquad |x| < b.$$

Let $u_j = \sum a_n(x) \exp(i2\pi nt/T)$ be the Fourier-series expansion of the function u_j. Then $a_n(x) = 0$ when $|x| < a$ and

$$L_0(i(\lambda_j + 2\pi n/T), \partial_x) a_n = 0, \qquad |x| < b.$$

Thus $a_n = 0$ and $u_j = 0$ when $|x| < b$. From here it follows that the numbers λ_j, N in (25) don't depend on b and we can choose the same functions u_j for all b.

From H_6 and (1) it follows that

$$(26) \qquad \|C_j u_j\|_{L_2(\Omega_t)} \le C \|f\|_{L_{2,a}}$$

where the constant C does not depend on a. In particular $u_j(t,\cdot) \in L_2(\Omega_t)$. And as $u_j \exp(i\lambda_j t)$ satisfies the equation and the boundary condition of problem (1) the functions $u_j(0,x)$ are eigenfunctions of the monodromy operator M with the eigenvalues $\exp(i\lambda_j T)$.

Further, linear functionals $f \to C_j = C_j(f)$ are defined on the dense set S of $L_2(\Omega_0)$ (on functions with compact supports) and they are bounded according to (26). Thus by Riesz theorem there exists h_j such that

$$(27) \qquad C_j = (f, h_j), \qquad h_j \in L_2(\Omega_0).$$

If f has a compact support then Mf also has a compact support, as the propagation velocity is finite for the solutions of equation $Lu = 0$. Using successively the equality $U(t,T) = U(t-T,0)$, expansion (25), (27) for the solution of the problem (1^0) at the time $t-T$ with the initial data Mf and the periodicity of the functions u_j we obtain:

$$\begin{aligned} &U(t,T)Mf = U(t-T,0)Mf = \\ &= \textstyle\sum_{j=1}^{N} C'_j u_j(t-T,x)\exp(i\lambda_j(t-T)) + o(1) = \\ &= \textstyle\sum_{j=1}^{N} C'_j u_j(t,x)\exp(i\lambda_j(t-T)) + o(1), \quad C'_j = (Mf, h_j) \end{aligned}$$

when $t \to \infty$. On the other hand according to (25), (27)

$$U(t,0)f = \sum_{j=1}^{N} C_j u_j(t,x)\exp(i\lambda_j t) + o(1), \qquad C_j = (f, h_j).$$

Left parts of the last two equalities coincide. Thus,

$$(Mf, h_j) = (f, h_j \exp(-i\lambda_j T))$$

and h_j are eigenfunctions of M^* with the eigenvalues $\exp(-i\lambda_j T)$.

In order to complete the proof of theorem 2 it remains to prove the following assertion (A): if f is an eigenfunction of operator M with the eigenvalue $\exp(i\lambda T)$, $\lambda \in [0, 2\pi/T]$, then one or several numbers λ_j in formula (25) are equal to λ, and f is a linear combination of the corresponding functions $u_j(0,x)$.

Let us consider a sequence of functions f_ϵ with compact supports such that

$$\|f_\epsilon - f\|_{L_2(\Omega_0)} \to 0 \quad \text{when} \quad \epsilon \to 0. \tag{28}$$

If u_ϵ is the solution of problem (1^0) with initial data f_ϵ then by virtue of (25)

$$u_\epsilon = \sum_{j=1}^{N} C_j^\epsilon u_j(t,x)\exp(i\lambda_j t) + o(1), \qquad t \to \infty. \tag{29}$$

it follows from (28) and condition H_6 that

$$\|u_\epsilon - u(t,x)\exp(i\lambda t)\|_{L_2(\Omega_0)} \to 0 \qquad \text{when} \qquad \epsilon \to 0. \tag{30}$$

The assertion (A) follows from (29), (30). Theorem 2 is proved.

Let us denote the space of functions belonging to $L_2(\Omega_0)$ and ortohogonal to h_j, $\ 1 \le j \le N$, by H. Let $U_0 = U_0(t-\tau)$ denote the opeartor $U(t,\tau)$ for case $L = L_0$, $\ \Omega = I\!R^{n+1}$.

THEOREM 3. *Let conditions $H_1 - H_6$ be satisfied. Then the wave operators*

$$W_-(U, U_0) : L_2(I\!R^n) \to H,$$
$$W_+(U_0, U) : H \to L_2(I\!R^n)$$

and scattering operator $S = W_+(U_0, U)W_-(U, U_0)$ exist and are bounded.

This theorem easily follows from the theorem 2. The only difficulty is the following: the remainder in (22) is not integrable with respect to time in the neighborhood of infinity if n is even. But we can show that the remainder can be expressed as a finite sum of an integrable summand and of summands which have the form $\alpha(t)h(t,x)$. Here $|\partial_t\alpha| \leq Ct^{-1}ln^{-2}t$ as $t \to \infty$ and function h is smooth, periodic with respect to time and equal to zero when $|x| \geq a$. Then we use the following assertion: if functions α and w have the above mentioned properties then the integral: $\int_0^t U_0(-s)\alpha(s)h(s,x)ds$ converges in the space $L_2(I\!R^n)$ when $t \to \infty$.

REFERENCES

[1] Cooper, J. and Strauss, W. Scattering of waves by periodically moving bodies. J. Funct. Anal., 1982, v.47; p. 180-229.

[2] Cooper, J. and Strauss, W. Abstract scattering theory for time periodic system with applications to the electromagnetism. Indiana Univ. Math., 1987, v.34, p. 33-83.

[3] Cooper, J. and Strauss, W. Time periodic scattering of symmetric hyperbolic systems. J. Math. Anal. A., 1987, v.122, p. 444-452.

[4] Petkov, V. Scattering theory for hyperbolic operator. Amsterdam: North-Holland, 1989.

[5] Rauch, J. Asymptotic behavior of solution of hyperbolic partial differential equations with zero speeds. Comm. Pure Appl. Math., 1978, v.31, No. 1, p. 431-480.

[6] Vainberg, B. Asymptotic methods in equations of mathematical physics. Publ. Moscow Univ., 1982; English translation: Gordon and Breach Publ., 1989.

[7] Vainberg, B. Asymptotic behavior as $t \to \infty$ of exterior mixed problems periodic with respect to t. Math. Notes, 1990, v.47, No. 4, p. 315-322.

[8] Vainberg, B. Scattering by periodically moving obstacles. Mat. Sbornic, 1991, v. 182, No. 6, p. 911-927 ; English translation:Math USSR Sbornik, 1992, v.73, No 1, p.289-304.

[9] Vainberg, B. On local energy of solutions of exterior mixed problems periodic with respect to t. Proc. Moscow Math. Soc., 1991, v.54 (in Russian).

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Long Range Scattering and the Stark Effect

Denis A.W. White

1 Introduction.

In this Article we discuss long range quantum mechanical scattering in the presence of a constant electric field. The electric field is assumed to be of unit strength in the $\mathbf{e}_1 = (1, 0, \ldots, 0)$ direction of n-dimensional space, $\mathbf{R}^n$. The corresponding Hamiltonian for a quantum particle of unit mass is $H_0 = -(1/2)\Delta - x_1$, with $\Delta = \sum_{j=1}^{n} \partial^2/\partial x_j^2$. ($H_0$ is essentially self adjoint (as an operator on $L^2(\mathbf{R}^n)$) on the Schwartz space of rapidly decreasing smooth functions.) A second Hamiltonian $H = H_0 + V$ is regarded as a perturbation of H_0 by a potential V. The potential $V = V_S + V_L$ consists of a "short range" term V_S and a "long range" term V_L. More precisely,

SR Hypothesis. *V_S is a symmetric operator, $V_S(H_0 + i)^{-1}$ is a compact operator and*

$$\int_1^\infty \|F(x_1 > r^2)V_S(H_0 + i)^{-1}\|\, dr \;<\; \infty$$

where $F(\cdot)$ is multiplication by the characteristic function of the indicated set.

LR Hypothesis. *$V_L(x)$ is real valued on $\mathbf{R}^n$, infinitely differentiable and for some $\epsilon > 0$ and for every multi-index α*

$$\begin{aligned} |D^\alpha V_L(x)| \;&<\; C_\alpha \langle x_1 \rangle^{-|\alpha|/2-\epsilon} \\ |D^\alpha V_L(x)| \;&<\; o(1) \quad \textit{as } |x| \to \infty. \end{aligned}$$

Here $\langle x_1 \rangle^2 = 1 + x_1^2$ and $D = -i\nabla$.

Example. If V_S is multiplication by a real valued function

$$V_S(x) = \{\chi(x_1)(1 + x_1^2)^{-\sigma/2} + \chi(-x_1)(1 + x_1^2)^{1/2}\}\tilde{V}_S(x)$$

where $\sigma > 1/2$ and $\tilde{V}_S = o(1)$ as $|x| \to \infty$ and $\tilde{V}_S$ is bounded and measurable and where

$$\chi(x_1) = \begin{cases} 1 & \text{if } x_1 > 1 \\ 0 & \text{if } x_1 < -1 \end{cases} \tag{1.1}$$

then V_S verifies the above short range hypothesis. (See Yajima [16]; local singularities may also be allowed.) The long range assumption is satisfied if, for some $0 \leq \alpha, \beta \leq 1/2$ and some real b_1 and b_2,

$$V_L(x) = \langle x \rangle^{-\epsilon} \cos(b_1 |x_1|^{\alpha}) \cos(b_2 |x|^{\beta}).$$

In general these assumptions assure that $V(H_0 + i)^{-1}$ is compact so that H is self adjoint on the domain of H_0. (Perry's book [14] is a good general reference.)

Introduce now the wave operators. Dollard's [3] *modified* wave operators W_D^- and W_D^+ are defined by

$$W_D^{\pm} = \text{s-}\lim_{t \to \pm\infty} e^{itH} e^{-itH_0} e^{-iX_D(t)} \tag{1.2}$$

where "s-lim" indicates that the limit is taken in the strong operator topology. The "modifier" $e^{-iX_D(t)}$ was first introduced by J.D. Dollard [3] in the case of no electric field ($H_0 = -\Delta/2$) to extend the usual scattering theory which was based on the *Møller* wave operators,

$$W^{\pm} = \text{s-}\lim_{t \to \mp\infty} e^{itH} e^{-itH_0}, \tag{1.3}$$

to the case $V = V_L$ was the Coulomb potential ($V_L(x) = C/|x|$, for C a constant). An alternative choice of wave operators, are the *two Hilbert space* wave operators

$$W^{\pm}(J^{\pm}) = \text{s-}\lim_{t \to \mp\infty} e^{itH} J^{\pm} e^{-itH_0} \tag{1.4}$$

where $J^{\pm}$ are bounded operators conveniently chosen (as in §2 below.) The application of these operators to study long range scattering is due to Isozaki-Kitada [8] (who called $J^{\pm}$ "time independent modifiers") and Kitada-Yajima [12] who considered the case of no electric field. The two Hilbert space wave operators have certain technical advantages over the modified wave operators but the latter are the historical vehicle for studying long range scattering and are important for proving the non-existence of $W^{\pm}$; see Theorem 3.1 below. Each of the wave operators (for example W_D^+) is said to be (strongly asymptotically) *complete* if its range is the *subspace* $L^2(\mathbf{R}^n)_c$ *of continuity* of H. ($L^2(\mathbf{R}^n)_c$ is the orthogonal complement of all the eigenvectors of H.) Each wave operator (W_D^+, to be specific) is said to *intertwine* H and H_0 if

$$e^{-itH} W_D^+ = W_D^+ e^{-itH_0}.$$

To state our results we must introduce the "modifiers." For the two Hilbert space wave operators we choose [8]

$$J^{\pm} u(x) = \int e^{ix \cdot \xi + i\theta^{\pm}(x,\xi)} \hat{u}(\xi) d\xi \tag{1.5}$$

where $\hat{u}$ denotes the Fourier transform of u and $\theta^{\pm}$ are smooth real valued functions to be specified in §2 below. ($J^{\pm}$ are not unique.) Here and below integrals are understood to be over all of $\mathbf{R}^n$ unless otherwise indicated and $đ\xi = (2\pi)^{-n/2}\,d\xi$.

Theorem 1.1 *Hypotheses LR and SR imply that the two Hilbert space wave operators $W^{\pm}(J^{\pm})$ exist and are complete and are isometries that intertwine H and H_0. Moreover H has no singularly continuous spectrum and its eigenvalues are discrete and of finite multiplicity.*

Dollard's time dependent modifier can be defined as follows: Let $X_D(t)$ be Fourier equivalent to multiplication by a real valued function, X where

$$X(\xi_2,\ldots,\xi_n,t) = \int_0^{\pm t} V_L(\tau Y(\xi_2,\ldots,\xi_n,\tau) + (\tau^2/2)\mathbf{e}_1)\,d\tau \qquad (1.6)$$

for $\pm t > 0$ and where Y is some smooth function of $n-1$ momentum variables plus time (t) taking values in $\mathbf{R}^n$ such that the first component $Y_1(\xi_2,\ldots,\xi_n,t) \equiv 0$ and

$$\begin{aligned} |D^{\beta}_{\xi_\perp}(Y(\xi_2,\ldots,\xi_n,t) - \xi_\perp)| &= O(|t|^{-\epsilon}); \\ |\frac{d}{dt}Y(\xi_2,\ldots,\xi_n,t)| &= O(|t|^{-1-\epsilon}) \end{aligned}$$

for all multi-indices β, locally uniformly in $\xi_\perp = (0,\xi_2,\ldots,\xi_n)$. (In particular in the one-dimensional case $Y \equiv 0$. In §3, Y is explicitly constructed.) Thus $X_D(t) = X(D_2,\ldots,D_n,t)$.

Theorem 1.2 *Assume Hypotheses LR and SR. Then the modified wave operators $W_D^{\pm}$ exist and are complete and are isometries which intertwine H and H_0. Moreover the Møller wave operators $W^{\pm}$ exist if and only if $e^{iX(\xi_2,\ldots,\xi_n,t)}$ converges in measure as $t \to \pm\infty$ on every compact subset of $\mathbf{R}^n$. Whenever $W^{\pm}$ exist, they are complete.*

Example. This continues the preceding example. Suppose for simplicity that b_1 and b_2 are nonzero and $\alpha \neq \beta$. Then the Møller wave operators (1.3) exist if and only if $\max\{\alpha,\beta\} + \epsilon > 1/2$ by Theorem 1.2. Ozawa [13] and Jensen-Ozawa [9] have already established a non-existence results for the Møller wave operators for a related class of potentials but by different methods.

Remark. In the case $n = 1$ the modifier depends only on time so that $e^{iX_D(t)} = e^{iX(t)}$ commutes with all operators. In particular, for any $u \in L^2(\mathbf{R}^n)$

$$|e^{-itH_0 - iX(t)}u(x)|^2 = |e^{-itH_0}u(x)|^2$$

which says that the position probability density of any free state is the same whether one uses the modified evolution or the usual free evolution. The same is true for the momentum probability density or any other observable in place of position or momentum. Therefore although the Møller wave operators $W^\pm$ do not exist the modified and free evolutions are indistinguishable by any quantum mechanical observable. It is therefore not surprising that in classical mechanics the usual wave operators exist as was observed by Jensen and Ozawa [9]. In general, for $n > 1$ the modifier is nontrivial. If however one further assumes

$$D^\alpha V_L(x) = O((1 + |x|)^{-\alpha-\epsilon} \quad \text{for } |\alpha| \le 1 \tag{1.7}$$

($\epsilon > 0$) then again one can replace $X(\xi, t)$ by a different modifier depending only on time (see Theorem 3.1 below) and which therefore cannot be observed. This last result is due to G.M. Graf [6] who assumed simply (1.7). Thus he requires less smoothness but more decay than here. He remarks that from the perspective of the Heisenberg picture of quantum mechanics there is no difference between quantum and classical mechanics in this setting. Graf uses Mourre's method.

In the remaining two Sections we outline the construction of $\theta^\pm$ for the proof of Theorem 1.1 (in §2). In §3 the proof of completeness in Theorem 1.2 is given; the remaining conclusions of Theorem 1.2 are standard and their proofs are only outlined.

2 Completeness of $W_D^\pm$.

In this Section we outline the construction of the operators $J^\pm$ of (1.5) or, more precisely, the phase terms $\theta^\pm$ as required for the proof of Theorem 1.1. In the process we indicate some key steps of the proof of Theorem 1.1 but our primary goal is to establish the properties of $\theta^\pm$ required for the proof of Theorem 1.2 in §3. A detailed proof of Theorem 1.1 is given in [15].

The construction of $\theta^\pm$ is as follows. It suffices to consider θ^+; the construction of θ^- is similar and in fact $\theta^-(x,\xi) = -\theta^+(x, -\xi)$. Choose $\chi_1 \in C^\infty(\mathbf{R})$ so that

$$\chi_1(x_1) = \begin{cases} 1 & \text{if } x_1 > 3 \\ 0 & \text{if } x_1 < 1 \end{cases} \tag{2.1}$$

The proof of Theorem 1.1 is based on the Enss method [4] in a two Hilbert space setting. One begins therefore with Cook's argument and so the key is to prove that the operator norm of $(d/dt)e^{itH} J^+ e^{-itH_0}\chi_1(D_1)$ is an integrable function of $t > 1$, where $D_1 = -i\partial/\partial x_1$ so that $\chi_1(D_1)$ maps onto "outgoing states." The free evolution on outgoing states $e^{-itH_0}\chi_1(D_1)$ can be estimated as in the short range case [14] so that the crucial estimate to be established is: for arbitrary compact real interval I there is some integer $N \geq 0$, so that

$$\int_1^\infty \|E(I)(HJ^\pm - J^\pm H_0)\chi_1(\pm D_1/r)\chi_1(x_1/r^2)(H_0+i)^{-N}\|dr \; < \; \infty. \quad (2.2)$$

where E denotes the spectral measure of H. We consider this estimate in the case $V_S = 0$; the general case requires an auxiliary argument. To verify (2.2) we compute, for $\hat{u} \in C_0^\infty(\mathbf{R}^n)$,

$$[(H_0 + V_L)J^+ - J^+H_0]u\,(x) = \int e^{ix\cdot\xi + i\theta^+(x,\xi)} p^+(x,\xi)\hat{u}(\xi)d\xi \quad \text{where}$$

$$\begin{aligned} p^+(x,\xi) \;&=\; \xi\cdot\nabla_x\theta^+(x,\xi) \;+\; \frac{\partial}{\partial\xi_1}\theta^+(x,\xi) \;+\; \tfrac{1}{2}|\nabla_x\theta^+(x,\xi)|^2 \\ &\quad -\; \tfrac{i}{2}\Delta_x\theta^+(x,\xi) \;+\; V_L(x). \end{aligned} \quad (2.3)$$

Intuitively θ^+ should be chosen so that p^+ is roughly short range. More precisely (2.2) is verified if

$$D_x^\alpha D_\xi^\beta p^+(x,\xi) = O(\langle x_1\rangle^{-1/2-\epsilon}) \text{ for } x_1 > 0 \text{ and } \xi_1 > 0. \quad (2.4)$$

One tries to construct θ^+ as a solution of the equation $p^+(x,\xi) = 0$ but in fact it suffices to ignore the term $\frac{i}{2}\Delta_x\theta^+(x,\xi)$ in (2.3) intuitively because the second order derivatives of θ^+ should be better behaved than the lower order derivatives simply because V_L has this property. This leads to us to solving the transport equations,

$$\xi\cdot\nabla_x\theta_k + \partial\theta_k/\partial\xi_1 + b_k = 0 \quad (2.5)$$

where $b_0(x) = V_L(x)$ and for $k \geq 1$

$$b_k(x,\xi) = \frac{1}{2}\left(\left|\sum_{0\leq j\leq k-1}\nabla_x\theta_j(x,\xi)\right|^2 - \left|\sum_{0\leq j\leq k-2}\nabla_x\theta_j(x,\xi)\right|^2\right).$$

The transport equations are first order linear and there are many solutions but the solutions of interest are those that vanish as rapidly as possible as $x_1 \to \infty$. To enhance this decay we in fact settle for a solution of the transport equations with b_k replaced by $\tilde{b}_k$ where $\tilde{b}_k(x,\xi) = \chi(x_1)\chi(\xi_1)b_k(x,\xi)$. An appropriate solution is

$$\theta_k(x,\xi) = \int_0^\infty \tilde{b}_k(x + t\xi + (t^2/2)\mathrm{e}_1, \xi + t\mathrm{e}_1) - \tilde{b}_k(t\xi_\perp + (t^2/2)\mathrm{e}_1, \xi_\perp + t\mathrm{e}_1)\,dt$$

where $\xi_\perp = (0, \xi_2, \ldots, \xi_n)$. (The second term in the above integrand is needed to assure that the integral exists.) One finds that

$$D_x^\alpha D_\xi^\beta\theta_k(x,\xi) = O(\langle x_1\rangle^{(1-|\alpha|)/2-(k+1)\epsilon} \text{ for } |\alpha| > 1.$$

and for $x_1 > 0$ and $\xi_1 > 0$ and all β. The improved decay for increased k is due to the squaring in b_k.) Then (2.4) is verified provided k is chosen so that $(k+2)\epsilon > 1/2$. This completes the construction of θ^+.

We pause now to record the properties of $\theta^\pm$, needed in §3 for the proof of Theorem 1.2. There we will need estimates on $\theta^\pm(x + (t^2/2)e_1, \xi + te_1)$ which are locally uniform in ξ (that is ξ is restricted to a compact set) as $t \to \infty$. Not surprisingly $\theta^\pm$ is larger in the direction opposite to the electric field, $x_1 < 0$.

For $\epsilon > 0$ as in Hypothesis LR, choose $\hat\epsilon$, $0 < \hat\epsilon < min\{1, \epsilon\}$. Then, for $\pm t > 1$

$$D_\xi^\beta \theta^\pm(x + \tfrac{t^2}{2}e_1, \xi + te_1) = \begin{cases} O((|x| + |t|)(\langle x_1\rangle^{(|\beta|-1-\hat\epsilon)/2} + t^{-\hat\epsilon/2})) & \text{if } x_1 < -\frac{t^2}{4}; \\ O((|x| + |t|)t^{-\epsilon}) & \text{if } x_1 > -\frac{t^2}{4}; \end{cases} \tag{2.6}$$

$$|D_\xi^\beta \frac{\partial}{\partial \xi_1}\theta^\pm(x + (t^2/2)e_1, \xi + te_1)| = \begin{cases} O(\langle x_1\rangle^{-\hat\epsilon/2}) & \text{if } x_1 < -t^2/4; \\ O(t^{-\epsilon}) & \text{if } x_1 > -t^2/4, \end{cases} \tag{2.7}$$

locally uniformly in ξ and for all multi-indices β. If $x_1 > -t^2/4$ then

$$|D_x^\alpha D_\xi^\beta \frac{\partial}{\partial x_1}\theta^\pm(x + (t^2/2)e_1, \xi + te_1)| = O(|t|^{-1-|\alpha|-\epsilon}); \tag{2.8}$$

$$|D_x^\alpha D_\xi^\beta \frac{\partial}{\partial \xi_1}\theta^\pm(x + \tfrac{t^2}{2}e_1, \xi + te_1)| + |D_x^\alpha D_\xi^\beta \frac{\partial}{\partial x_j}\theta^\pm(x + \tfrac{t^2}{2}e_1, \xi + te_1)| = O(|t|^{-|\alpha|-\epsilon}), \tag{2.9}$$

again locally uniformly in ξ and for each j, $1 \le j \le n$ and all α and β and $\pm t > 1$. These estimates follow from the construction of $\theta^\pm$. For the estimates (2.6; 2.7) observe that

$$\int_t^\infty \tau^k \langle y + \tau^2/2\rangle^{-(k+1+\epsilon)/2}\, d\tau = \begin{cases} O(\langle y\rangle^{(k-\hat\epsilon)/2}) & \text{if } y < -t^2/4; \\ O(t^{-\epsilon}) & \text{if } y > -t^2/4, \end{cases} \tag{2.10}$$

for each nonnegative integer k. The same reasoning shows that, for $\pm t > 1$

$$D_\xi^\beta p^\pm(x + (t^2/2)e_1, \xi + te_1) = \begin{cases} O(\langle x_1\rangle^{-\hat\epsilon/2}) & \text{if } x_1 < -t^2/4; \\ O(|t|^{-1-\epsilon}) & \text{if } x_1 > -t^2/4. \end{cases} \tag{2.11}$$

3 Proof of Theorem 1.2.

In this Section we outline the proof of Theorem 1.2 emphasizing the proof of completeness of the modified wave operators $W_D^\pm$. Let us begin by noting that the conclusion about the non-existence of the Møller wave operators is a direct consequence of a result formulated by Hörmander [7, Theorem 3.1]:

Theorem 3.1 *Assume that the limits (1.2) exist with* $X_D(t) = X(D,t)$ *as well as the the corresponding limits* $\tilde{W}_D^{\pm}$ *when* $X(D,t)$ *is replaced by* $\tilde{X}(D,t)$*. Then* $W_D^{\pm}$ *has the same range as* $\tilde{W}_D^{\pm}$ *(same sign) if and only if* $\exp i(X(\xi,t) - \tilde{X}(\xi,t))$ *converges in measure as* $t \to \pm\infty$ *to functions* $F^{\pm}$*. In this case* $\tilde{W}_D^{\pm} = W_D^{\pm}F^{\pm}(D)$.

Applying this result with $\tilde{X} = 0$, we derive non-existence of the Møller wave operators from the completeness of the modified wave operators. (The ranges of $W_D^{\pm}$ are, in general, contained in $L^2(\mathbf{R}^n)_c$; see [14, p. 48].)

The existence of the modified wave operators can be established by an argument very similar to that given by Hörmander [7] for the case of no electric field. The reason similar arguments apply is the Avron-Herbst formula [1]:

$$e^{-itH_0} = e^{-it^3/6}e^{itx_1}e^{-iD_1t^2/2}e^{-i(-\Delta)t/2}. \tag{3.1}$$

Therefore, up to an inconsequential phase factor $e^{-it^3/6}$, e^{-itH_0} is the evolution $e^{-i(-\Delta)t/2}$, free of the electric field, followed by a translation $e^{-iD_1t^2/2}$ of $t^2/2$ units in the $\mathbf{e}_1$ direction of configuration space followed by a translation e^{itx_1} of t units in the $\mathbf{e}_1$ direction in momentum space. With this formula, existence follows by the argument of [7] based on stationary phase and constructing a solution of a Hamilton-Jacobi equation.

The proof of the intertwining principle is well known (see Hörmander [7, p. 75], for example).

With these brief remarks about the other conclusions of Theorem 1.2 we proceed to the proof of completeness. This proof is entirely independent of the existence proof because, as we shall show, the wave operators $W_D^{\pm}$ exist at least on some subspace of $L^2(\mathbf{R}^n)$ and both have range the subspace $L^2(\mathbf{R}^n)_c$ of continuity of H. It is not necessary that the modifier be the same in both proofs, by Theorem 3.1.

To establish completeness it suffices by Theorem 1.1 to show that $W_D^{\pm}$ has the same range as $W^{\pm}(J^{\pm})$. To do so, we introduce the auxiliary operators

$$\tilde{W}_D^{\pm} \equiv \operatorname*{s-lim}_{t\to\pm\infty} e^{itH}e^{-itH_0}e^{i\tilde{X}(D,t)}u$$

where $\tilde{X}(\xi,t)$ is some function chosen suitably for a stationary phase argument. Significantly $\tilde{X}$ may depend on all n of the ξ-variables whereas X of Theorem 1.1 depends only on (the last) $n-1$ variables. We show that $\tilde{W}_D^{\pm}$ has the same range as do $W^{\pm}(J^{\pm})$; this is the bulk of the work. We further show, with the help of Theorem 3.1, that $W_D^{\pm} = \tilde{W}_D^{\pm}F^{\pm}$ for some unitary operators $F^{\pm}$. This will establish the completeness of $W_D^{\pm}$. The intermediary operators $\tilde{W}_D^{\pm}$ are a convenience and not of independent interest because they do not intertwine H and H_0.

The operators $\tilde{W}_D^\pm$ and $W^\pm(J^\pm)$ have the same range if, for every $u \in L^2(\mathbf{R}^n)$ there exists $v \in L^2(\mathbf{R}^n)$ so that

$$e^{itH} J^\pm e^{-itH_0} u - e^{itH} e^{-itH_0} e^{-i\tilde{X}(D,t)} v$$

converges to 0 as $t \to \pm\infty$ or, equivalently, if the operators

$$\Omega^\pm \equiv \text{s-}\lim_{t\to\pm\infty} e^{i\tilde{X}(D,t)} e^{itH_0} J^\pm e^{-itH_0} \tag{3.2}$$

exist. We therefore prove the Proposition below.

Proposition 3.2 *Assuming the hypotheses of Theorem 1.1 the operators $\Omega^\pm$ of (3.2) exist on all of $L^2(\mathbf{R}^n)$ when $\tilde{X}$ is defined by*

$$\tilde{X}(\xi, t) = \int_0^t V_L(\tau \tilde{Y}(\xi, \tau) + \tau^2/2 \mathrm{e}_1)\, d\tau \tag{3.3}$$

where $\mathrm{e}_1 = (1, 0, \ldots, 0) \in \mathbf{R}^n$ and $\tilde{Y}$ is a smooth, real valued function such that

$$\begin{aligned} |D_\xi^\beta(\tilde{Y}(\xi,t) - \xi)| &= O(|t|^{-\epsilon}) & (3.4)\\ |\frac{d\tilde{Y}}{dt}(\xi,t)| + |D_\xi^\beta \frac{\partial}{\partial \xi_1}(\tilde{Y}(\xi,t) - \xi)| &= O(|t|^{-1-\epsilon}) & (3.5) \end{aligned}$$

for all β, locally uniformly in ξ. In particular the operators $\tilde{W}_D^\pm$ of (1.2) are complete.

Before proving this Proposition, let us see how it implies completeness in Theorem 1.2. Define Y there componentwise: $Y_1 = 0$ and for $2 \le j \le n$

$$Y_j(\xi_2, \ldots, \xi_n, t) = \tilde{Y}_j(0, \xi_2, \ldots, \xi_n, t).$$

Completeness will follow from Theorem 3.1 if

$$e^{i\tilde{X}(\xi,t) - iX(\xi_\perp, t)}$$

converges locally in measure (or locally uniformly) as $t \to \pm\infty$. This follows from the mean value theorem and the estimates for $\tilde{Y}$. The only troublesome term is

$$\int_0^t \int_0^1 \tau \frac{\partial}{\partial x_1} V_L(\tau(s\tilde{Y}(\xi,\tau) + (1-s)Y(\xi_\perp,\tau)) + \frac{\tau^2}{2}\mathrm{e}_1)\, ds\, \tilde{Y}_1(\xi,\tau)\, d\tau. \tag{3.6}$$

Its convergence can be checked by integration by parts in the τ variable.

Proof of Proposition 3.2. We consider only the case of Ω^+ ($t > 0$). To prove the strong convergence in (3.2), it suffices to prove convergence on a subset of $L^2(\mathbf{R}^n)$ whose linear span is dense. This subset will consist of all u so that $\hat{u}$ is in $C_0^\infty(\mathbf{R}^n)$ and supported in a ball of radius $\eta/2$ centered at $\xi^0 \in \mathbf{R}^n$ where ξ^0 is arbitrary and $\eta > 0$ will be specified below. Apply Cook's method (differentiate and integrate in (3.2)): $\Omega^+ u$ exists if the L^2-norm of

$$X_t(D,t)e^{itH_0}J^+e^{-itH_0}u + e^{itH_0}[H_0J^+ - J^+H_0]e^{-itH_0}u$$

is an integrable function of t on an interval $[t_0, \infty)$, for some $t_0 > 1$. We add and subtract $e^{itH_0}V_LJ^+e^{-itH_0}u$ and apply the Avron-Herbst formula (3.1). It suffices to show that the L^2-norms $\|A(\cdot,t)\|$ and $\|C(\cdot,t)\|$ are integrable functions of $t > t_0$ where A and C are defined by

$$\begin{aligned} A(x,t) &= [X_t(D,t) - V_L(x + (t^2/2)\mathrm{e}_1)]B(x,t) \quad \text{where} \\ B(x,t) &= \int e^{ix\cdot\xi - it|\xi|^2/2 + i\theta^+(x+(t^2/2)\mathrm{e}_1, \xi + t\mathrm{e}_1)}\hat{u}(\xi)d\!\!^{-}\xi; \\ C(x,t) &= e^{iD_1t^2/2}e^{-itx_1}[(H_0 + V_L)J^+ - J^+H_0]e^{-itH_0}u(x) \\ &= \int e^{ix\cdot\xi - it|\xi|^2/2 + i\theta^+(x+(t^2/2)\mathrm{e}_1, \xi+t\mathrm{e}_1)}p^+(x + (t^2/2)\mathrm{e}_1, \xi + t\mathrm{e}_1)\hat{u}(\xi)d\!\!^{-}\xi \end{aligned}$$

where p^+ was defined by (2.3).

We start by estimating $\|A(\cdot,t)\|$. As is typical in stationary phase arguments we estimate first the integral $B(x,t)$ far from the critical point of the phase function

$$\phi(\xi,x,t) = x\cdot\xi - t|\xi|^2/2 + \theta^+(x + (t^2/2)\mathrm{e}_1, \xi + t\mathrm{e}_1).$$

Choose therefore $\chi_0 \in C_0^\infty(\mathbf{R}^n)$ so that

$$\chi_0(x) = \begin{cases} 1 & \text{if } |x| < \eta \\ 0 & \text{if } |x| > 2\eta \end{cases} \tag{3.7}$$

Then

$$(1 - \chi_0\left(\frac{x - \xi^0 t}{1+t}\right))B(x,t) = O((1 + |x| + t)^{-N}). \tag{3.8}$$

because $|\nabla_\xi \phi| > c(1 + |x| + t)$, for some $c > 0$, on the relevant region; see Fedoryuk [5] or Hörmander [7, Lemma A.1]. (The proof is essentially integration by parts.)

Therefore to check the integrability of $\|A(\cdot,t)\|$ in $t > t_0$ it suffices to check that of the $L^2(d\zeta)$-norm of

$$\int \chi_0\left(\frac{x - \xi^0 t}{1+t}\right)\int e^{-ix\cdot\zeta + i\phi(\xi,x,t)}[(\tilde{X}_t(\zeta,t) - V_L(x + t^2/2\mathrm{e}_1)]\hat{u}(\xi)d\!\!^{-}\xi d\!\!^{-}x. \tag{3.9}$$

It is again possible to estimate the $L^2(d\zeta)$ norm of the expression (3.9) away from the critical point of the phase function $-x\cdot\zeta + \phi(\xi,x,t)$, regarded as a function of x. Therefore multiply by $1 - \chi_0(\zeta - \xi^0)$ in (3.9). Then there is no critical point for the phase: Indeed $|\zeta - \nabla_x\phi(\xi, x, t)| > c(1 + |\zeta|)$ for some $c > 0$, in the relevant region. Since

$$|D_x^\alpha \nabla_x \phi(\xi, x, t)| + |D_x^\alpha\{\chi_0\left(\frac{x - \xi^0 t}{1+t}\right)[\tilde{X}_t(t, \zeta) - V_L(x + \frac{t^2}{2})]\}| = O(t^{-|\alpha|-\epsilon}),$$

it follows that the expression (3.9) times $1 - \chi_0(\zeta - \xi^0)$ is $O((1 + |\zeta|)^{-N} t^{-N-\epsilon})$ for any integer N and so its $L^2(d\zeta)$ is integrable in $t > t_0$. (See the references after equation (3.8).)

It remains to estimate the expression (3.9) times $\chi_0(\zeta - \xi^0)$. This is not quite the "usual" stationary phase estimate near the critical point because $X_t(\zeta, t)$ depends on ζ, not ξ. To remedy this we expand $X_t(\zeta, t)$ in a Taylor series, not around ξ but around the critical point for the phase, $\zeta = \nabla_x\phi(\xi, x, t)$. The expression (3.9) times $\chi_0(\zeta - \xi^0)$ is, for some positive integer k

$$\chi_0(\zeta - \xi^0)\hat{A}_0(\zeta, t) + \chi_0(\zeta - \xi^0) \sum_{1 \le |\alpha| \le k} \frac{i^{|\alpha|}}{\alpha!} A_\alpha(\zeta, t) + \sum_{|\alpha| = k+1} \frac{i^{k+1}}{\alpha!} R_\alpha(\zeta, t)$$

where

$$\begin{aligned}
A_0(x,t) &= \chi_0\left(\frac{x - \xi^0 t}{1+t}\right) \times \\
&\qquad \int e^{i\phi(\xi,x,t)}[(\tilde{X}_t(\nabla_x\phi(\xi, x, t), t) - V_L(x + (t^2/2)\mathrm{e}_1)]\hat{u}(\xi) d\xi; \\
A_\alpha(\zeta, t) &= \int \chi_0\left(\frac{x - \xi^0 t}{1+t}\right) \int e^{-i\zeta\cdot x + i\phi(\xi,x,t)}(\zeta - \nabla_x\phi(\xi, x, t))^\alpha \times \\
&\qquad (D_\xi^\alpha \tilde{X}_t)(\nabla_x\phi(\xi, x, t), t)\hat{u}(\xi) d\xi dx; \\
R_\alpha(\zeta, t) &= \sum_{|\alpha|=k+1} \frac{1}{\alpha!}\chi_0(\zeta - \xi^0) \int \chi_0\left(\frac{x - \xi^0 t}{1+t}\right) \int e^{-i\zeta\cdot x + i\phi(\xi,x,t)} \times \\
&\qquad (\zeta - \nabla_x\phi(\xi, x, t))^\alpha \times \\
&\qquad \int_0^1 (1-s)^k (D_\xi^\alpha \tilde{X}_t)(s\zeta + (1-s)\nabla_x\phi(\xi, x, t), t)\, ds\, \hat{u}(\xi) d\xi dx
\end{aligned}$$

and $\hat{A}_0$ is the Fourier transform of $A_0(\cdot, t)$. We shall show that the $L^2(d\zeta)$ norms of each term is an integable function of $t > t_0$. (The factor $\chi_0(\zeta - \xi^0)$ only plays a role in the consideration of R_α.)

The $A_0(x, t)$ term is the most interesting because the choice of $\tilde{X}$ is critical here. First we change variables, $x = ty$: The $L^2(dx)$ norm of $A_0(x, t)$ equals the $L^2(dy)$ norm of $t^{n/2} A_0(ty, t)$. Optimally $\tilde{X}$ will satisfy

$$\tilde{X}_t((\nabla_x\phi)(\xi, ty, t), t) = V_L(ty + t^2/2\mathrm{e}_1)$$

at the critical point of the phase, that is where $\nabla_\xi \phi(\xi, ty, t) = 0$. In order to specify $\tilde{X}$ we begin by defining $y(\xi, t)$ by the equation for the critical point:

$$y(\xi,t) - \xi + t^{-1}\nabla_\xi \theta(ty(\xi,t) + t^2/2\mathrm{e}_1, \xi + t\mathrm{e}_1) = 0. \tag{3.10}$$

The implicit function theorem guarantees $y(\xi, t)$ is well defined for $(\xi, t) \in U_1 \times [t_1, \infty)$ where U_1 is any bounded open set and $t_1 > 1$ is suitably large; y is smooth and

$$\begin{aligned} |D_\xi^\beta(y(\xi,t) - \xi)| &= O(t^{-\epsilon}); \\ |\frac{dy}{dt}(\xi,t)| + |D_\xi^\beta \frac{\partial}{\partial \xi_1}(y(\xi,t) - \xi)| &= O(t^{-1-\epsilon}), \end{aligned}$$

for all β, by estimates (2.8, 2.9). Since U_1 is arbitrary, it is possible to extend $y(\xi, t)$ smoothly, by a partition of unity argument, to all of $\mathbf{R}^n \times [0, \infty)$ so that whenever ξ is restricted to a compact set the above bounds are valid and (3.10) holds for t large enough and $y(\xi, t) = \xi$ for small t.

The definition of $\tilde{X}$ further requires defining $\Xi(\cdot, t)$ to be the inverse of the mapping $\xi \mapsto (\nabla_x \phi)(\xi, ty(\xi, t), t)$. Provided ξ is restricted to a bounded open set and t is large then $\Xi(\cdot, t)$ indeed exists and

$$\begin{aligned} |D_\zeta^\beta(\Xi(\zeta,t) - \zeta)| &= O(t^{-\epsilon}) \\ |\frac{d\Xi}{dt}(\xi,t)| + |D_\zeta^\beta \frac{\partial}{\partial \zeta_1}(\Xi(\zeta,t) - \zeta)| &= O(t^{-1-\epsilon}) \end{aligned}$$

by (2.7). Extend Ξ to $\mathbf{R}^n \times [0, \infty)$ as was done with y and so that $\Xi(\zeta, t) = \zeta$ for small t.

Define the modifier $\tilde{X}$ as

$$\tilde{X}(\xi,t) = \int_0^t V_L(\tau \tilde{Y}(\xi,\tau) + (\tau^2/2)\mathrm{e}_1)\, d\tau \quad \text{where} \quad \tilde{Y}(\xi,t) = y(\Xi(\xi,t),t). \tag{3.11}$$

The estimates (3.4, 3.5) for $\tilde{Y}$ follow directly from the comparable estimates for y and Ξ.

We may now estimate the $L^2(dy)$ norm of $t^{n/2}A_0(ty, t)$ by a well known stationary phase argument [7, Lemma A.4]. Since the phase function in A_0 has a non-degenerate critical point, Hörmander's Lemma A.4 [7] applies and gives an expansion for A_0 at that critical point. Our choice of $\tilde{X}$ assures that the first term of that expansion is 0 and the remaining terms times $t^{n/2}$ have $L^2(dy)$-norms which are integrable functions of $t > t_0$.

The same type of argument applies to A_α, $|\alpha| > 0$ but first it is necessary to integrate by parts in the x variables several times. Each time the factor $e^{-i\zeta\cdot x + i\phi(\xi,x,t)}(\zeta - \nabla_x\phi(\xi, x, t))$ is integrated and the process is repeated until the symbol no longer contains the variable ζ (which is at most $|\alpha|$ times).

Then the outer integral over x is simply a Fourier transform so that we may estimate the L^2-norm of the inverse Fourier transform of $A_\alpha(\cdot,t)$. For example, the inverse Fourier transform of $A_\alpha(\cdot,t)$ in the special case $|\alpha|=1$, say $\alpha=\mathbf{e}_j$ for some $j, 1\le j\le n$, is

$$-i\int e^{i\phi(\xi,x,t)}\frac{\partial}{\partial x_j}\{\chi\left(\frac{x-\xi^0 t}{1+t}\right)(D_\xi^{\mathbf{e}_j}\tilde{X}_t)(\nabla_x\phi(\xi,x,t),t)\}\hat{u}(\xi)d\xi$$

We now argue as for A_0. We change variables $x=ty$ and apply Hörmander's Lemma [7, Lemma A.4]. Since, by (2.9), the x derivatives of θ and hence ϕ decay rapidly in t on the support of the above integrand, Hörmander's Lemma implies that $\|A_\alpha(\cdot,t)\|$ is an integrable function of $t>t_0$.

Next we estimate R_α when $|\alpha|=k+1$ and k is large. As above we integrate by parts repeatedly in x until all factors of $(\zeta-\nabla_x\phi(\xi,x,t))$ have been integrated (or differentiated) out. Here however the integral over x is not simply a Fourier transform but again the integrand will decay rapidly in t and in fact if k is large enough the integral may be estimated directly: $\|R_\alpha(\cdot.t)\|$ is an integrable function of $t>t_0$; there is no need for Hörmander's Lemma here.

The proof that $\|C(\cdot,t)\|$ is an integrable function of t follows arguments already given. The initial argument estimating B far from the critical point applies to C as it did to B and so it suffices to consider the $L^2(dx)$-norm of $\chi((x-\xi^0 t)/(1+t))C(x,t)$. (See (2.11).) Changing variables $x=ty$ it suffices to show that the $L^2(dy)$-norm of $t^{n/2}\chi((y-\xi^0)/(1+t^{-1}))C(ty,t)$ is an integrable function of t. This follows again from Hörmander's Lemma A.4 [7] and the estimate (2.11). This proves the Proposition. □

References

[1] J.E. Avron and I.W. Herbst, *Spectral and scattering theory for Schrödinger operators related to the Stark effect,* Commun. Math. Phys. **52**(1977), 239-254.

[2] A. P. Calderón and R. Vaillancourt, *A class of bounded pseudo-differential operators,* Proc. Nat. Acad. Sci. U.S.A. **69**(1972), 1185-1187.

[3] J.D. Dollard, *Asymptotic convergence and the Coulomb interaction,* J. Math. Phys. **5**(1964), 729-738.

[4] V. Enss, *Asymptotic completeness for quantum mechanical potential scattering, I. Short range potentials,* Commun. Math. Phys. **61**(1978), 285-291.

[5] M.V. Fedoryuk, *The stationary phase method and pseudodifferential operators,* Russian Math. Surveys **26**(1971), 65-115.

[6] G.M. Graf, *A remark on long-range Stark scattering,* Helv. Phys. Acta **64**(1991). 1167-1174.

[7] L. Hörmander, *The existence of wave operators in scattering theory,* Math Z. **146**(1976), 69-91.

[8] H. Isozaki and H. Kitada, *Modified wave operators with time-independent modifiers,* J. Fac. Sci. Univ. Tokyo Sect. IA **32**(1985), 77-104.

[9] A. Jensen and T. Ozawa, *Classical and quantum scattering for Stark Hamiltonians with slowly decaying potentials,* Ann. Inst. Henri Poincaré, Phys. Théor., **54**(1991), 229-243.

[10] A. Jensen and K. Yajima, *On the long range scattering for Stark Hamiltonians,* J. reine angew. Math. **420**(1991), 179-193.

[11] H. Kitada, *A relation between the modified wave operators* $W_J^{\pm}$ *and* $W_D^{\pm}$*,* Sci. Pap. Coll. Arts Sci. Univ. Tokyo **36**(1987), 91-105.

[12] H. Kitada and K. Yajima, *A scattering theory for time-independent long-range potentials,* Duke Math. J. **49**(1982), 341-376.

[13] T. Ozawa, *Non-existence of wave operators for Stark effect Hamiltonians,* Math Z. **207**(1991), 335-339.

[14] P.A. Perry, *Scattering theory by the Enss Method,* Mathematical Reports, No.1, Harwood, New York, 1983.

[15] D.A.W. White, *The Stark effect and long range scattering in two Hilbert spaces,* Indiana Univ. Math. J. **39**(1990), 517-546.

[16] K. Yajima, *Spectral and scattering theory for Schrödinger operators with Stark-effect,* J. Fac. Sci. Univ. Tokyo, Sec IA, **26**(1979), 377-390.

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RADIATION CONDITIONS AND SCATTERING THEORY FOR THREE-PARTICLE HAMILTONIANS

D.Yafaev

1. INTRODUCTION

One of the main problems of scattering theory is a description of asymptotic behaviour of N interacting quantum particles for large times. The complete classification of all possible asymptotics (channels of scattering) is called asymptotic completeness. The final result can easily be formulated in physics terms. Two particles can either form a bound state or are asymptotically free. In case $N \geq 3$ a system of N particles can also be decomposed asymptotically into its subsystems (clusters). Particles of the same cluster form a bound state and different clusters do not interact with each other.

There are two essentially different approaches to a proof of asymptotic completeness for multiparticle ($N \geq 3$) quantum systems. The first of them, started by L. D. Faddeev [1], relies on the detailed study of a set of equations derived by him for the resolvent of the corresponding Hamiltonian. This approach was developped in [1] for the case of three particles and was further elaborated in [2, 3]. The attempts [4, 5] towards a straightforward generalization of Faddeev's method to an arbitrary number of particles meet with numerous difficulties. However, the results of [6] for weak interactions are quite elementary.

Another approach relies on the commutator method [7] of T. Kato. In the theory of N-particle scattering it was introduced by R. Lavine [8, 9] for repulsive potentials. A proof of asymptotic completeness in the general case is much more complicated and is due to I. Sigal and A. Soffer [10]. In the recent paper [11] G. M. Graf gave an accurate proof of asymptotic completeness in the time-dependent framework. The distinguishing feature of [11] is that all intermediary results are also purely time-dependent and most of them have a direct classical interpretation. Papers [10, 11] were to a large extent inspired by V. Enss (see e.g. [12]) who was the first to apply a time-dependent technique for the proof of asymptotic completeness.

The aim of the present paper is to give an elementary proof of asymptotic completeness (for the precise statement, see section 2) for three-particle Hamiltonians with short-range potentials which fits into the theory of smooth perturbations [7, 13]. Our approach admits a straightforward generalization to an arbitrary number of particles. This will be discussed elsewhere. Our proof of asymptotic completeness relies on new estimates which establish some kind of radiation conditions for three-particle systems. Compared to the limiting absorption principle (see below) radiation conditions-estimates give us an additional information on the asymptotic behaviour of a quantum system for large distances or large times. Limiting absorption principle suffices for a proof of asymptotic completeness in case of two-particle Hamiltonians with short-range potentials. However, radiation conditions-estimates are crucial in scattering for long-range potentials (see e.g. [14]), in scattering by unbounded obstacles [15, 16] and in scattering for anisotropically decreasing potentials [17]. In the latter paper the role of radiation conditions was also advocated for three-particle Hamiltonians. Our proof of radiation conditions-estimates hinges on the commutator method rather than the integration-by-parts machinery used in the two-particle case (see e.g. [14]).

Our interpretation of radiation conditions is, of course, different from the two-particle case. Before discussing their precise form let us introduce the generalized three-particle Hamiltonians. We consider the self-adjoint Schrödinger operator $H = -\Delta + V(x)$ in the Hilbert space $\mathcal{H} = L_2(\mathbb{R}^d)$. Suppose that some finite number α_0 of subspaces X^α of $X := \mathbb{R}^d$ is given and let x^α, x_α be the orthogonal projections of $x \in X$ on X^α and $X_\alpha = X \ominus X^\alpha$, respectively. We assume that

$$V(x) = \sum_{\alpha=1}^{\alpha_0} V^\alpha(x^\alpha), \tag{1.1}$$

where V^α are decreasing real functions of variables x^α. We prove asymptotic completeness under the assumption that V^α are short-range functions of x^α but many intermediary results (in particular, radiation conditions-estimates) are as well true for long-range potentials. Clearly, $V^\alpha(x^\alpha)$ tends to zero as $|x| \to \infty$ outside of any conical neighbourhood of X_α and $V^\alpha(x^\alpha)$ is constant on planes parallel to X_α. Due to this property the structure of the spectrum of H is much more complicated than in the two-particle case. Operators H considered here were introduced in [18] and are natural generalizations of N-particle Hamiltonians. We further assume that

$$X_\alpha \cap X_\beta = \{0\}, \quad \alpha \neq \beta, \tag{1.2}$$

so that regions where different V^α "live" have compact intersection (for potentials of compact support). For the Schrödinger operator this is true only for the case of three particles. Thus the assumption (1.2) distinguishes the three-particle problem.

Our proof of asymptotic completeness requires only the "angular part" of radiation conditions. Let $\langle \cdot, \cdot \rangle$ be the scalar product in the space $\mathbb{C}^d$ and let $\nabla^{(s)}$,

$$\nabla^{(s)}u(x) = \nabla u(x) - |x|^{-2}\langle \nabla u(x), x\rangle x, \tag{1.3}$$

be the projection of the gradient ∇ on the plane, orthogonal to x. Denote by χ_0 the characteristic function of any closed cone Γ_0 such that $\Gamma_0 \cap X_\alpha = \{0\}$ for all α. We prove that the operator

$$G_0 = \chi_0(|x| + 1)^{-1/2}\nabla^{(s)} \tag{1.4}$$

is locally (away from thresholds and eigenvalues of H) H-smooth (in the sense of T. Kato – see e.g. [19]). In neighbourhoods of X_α we have only a weaker result. Namely, let ∇_{x_α} be the gradient in the variable x_α (i.e. $\nabla_{x_\alpha}u$ is the orthogonal projection of ∇u on X_α),

$$\nabla^{(s)}_{x_\alpha}u(x) = \nabla_{x_\alpha}u(x) - |x_\alpha|^{-2}\langle \nabla_{x_\alpha}u(x), x_\alpha\rangle x_\alpha \tag{1.5}$$

and let χ_α be the characteristic function of such a closed cone Γ_α that $\Gamma_\alpha \cap X_\beta = \{0\}$ for all $\beta \neq \alpha$. Then the operator

$$G_\alpha = \chi_\alpha(|x| + 1)^{-1/2}\, \nabla^{(s)}_{x_\alpha} \tag{1.6}$$

is locally H-smooth. A definition of H-smoothness of the operators G_0 and G_α can be given either in terms of the resolvent of the operator H or of its unitary group $U(t) = \exp(-iHt)$. In both versions results are formulated as certain estimates which we call radiation conditions-estimates.

Our proof in section 3 of H-smoothness of the operators G_0 and G_α is based on consideration of the commutator $[H, M] := HM - MH$, where M is a self-adjoint first-order differential operator with *bounded* coefficients. We find an operator M such that $i[H, M]$ is essentially bounded from below by $G_0^*G_0$ and $G_\alpha^*G_\alpha$. Here we take into account that certain terms, those vanishing as $O(|x|^{-\rho}), \rho > 1$, at infinity, are negligible. This is a consequence of local H-smoothness of the operator $(|x|+1)^{-r}, r > 1/2$, (limiting absorption principle) which, in turn, is ensured by the Mourre estimate [20, 21, 22]. We emphasize that all our considerations are localized in energy.

The H-smoothness of the operators G_0 and G_α suffices for the proof in section 4 of existence of suitable wave operators (both "direct" and "inverse") with non-trivial identifications which are first-order differential operators. The sum of these identifications equals M, which allows us to find the asymptotics of $MU(t)f$ for large t. Since the limit $M^{\pm}$ as $t \to \pm\infty$ of the observable $U^*(t)\, M\, U(t)$ also exists, this gives the asymptotics of the function $U(t)f$ for f from the range of the operator $M^{\pm}$. Using again the Mourre estimate, we prove (also in section 4) that actually this range coincides with the whole absolutely continuous subspace of the Hamiltonian H. Finally, in section 5 we conclude our proof of asymptotic completeness.

2. BASIC NOTIONS OF SCATTERING THEORY

Let us briefly recall some basic definitions of the scattering theory. For a self-adjoint operator H in a Hilbert space $\mathcal{H}$ we introduce the following standard notation: $\mathcal{D}(H)$ is its domain; $\sigma(H)$ is its spectrum; $E(\Omega; H)$ is the spectral projection of H corresponding to a Borel set $\Omega \subset \mathbb{R}$; $\mathcal{H}^{(ac)}(H)$ is the absolutely continuous subspace of H; $P^{(ac)}(H)$ is the orthogonal projection on $\mathcal{H}^{(ac)}(H)$; $\mathcal{H}^{(p)}(H)$ is the subspace spanned by all eigenvectors of the operator H; $\sigma^{(p)}(H)$ is the spectrum of the restriction of H on $\mathcal{H}^{(p)}(H)$, i.e. $\sigma^{(p)}(H)$ is the closure of the set of all eigenvalues of H. Norms of vectors and operators in different spaces are denoted by the same symbol $\|\cdot\|$; I is always the identity operator; $\mathcal{B}$ and $\mathcal{K}_\infty$ are the classes of bounded and compact operators (in different spaces) respectively; C and c are positive constants whose precise values are of no importance; "$s - \lim$" means the strong operator limit. Note that

$$s - \lim_{|t|\to\infty} K \exp(-iHt)P^{(ac)}(H) = 0, \quad \text{if} \quad K \in \mathcal{K}_\infty. \tag{2.1}$$

Let K be H-bounded operator, acting from $\mathcal{H}$ into, possibly, another Hilbert space $\mathcal{H}'$. It is called H-smooth (in the sense of T. Kato) on a Borel set $\Omega \subset \mathbb{R}$ if for every $f = E(\Omega; H)f \in \mathcal{D}(H)$

$$\int_{-\infty}^{\infty} \|K \exp(-iHt)f\|^2 \, dt \le C\|f\|^2.$$

Obviously, BK is H-smooth on Ω if K has this property and $B \in \mathcal{B}$.

Let now H_j, $j = 1, 2$, be a couple of self-adjoint operators and let J be a bounded operator in a Hilbert space $\mathcal{H}$. The wave operator for the pair H_1, H_2 and the "identification" J is defined by the relation

$$W^{\pm}(H_2, H_1; J) = s - \lim_{t\to\pm\infty} \exp(iH_2t)J\exp(-iH_1t)P^{(ac)}(H_1) \tag{2.2}$$

under the assumption that this limit exists. We emphasize that all definitions and considerations for " + " and " − " are independent of each other. It suffices to verify existence of the limit (2.2) on some set dense in $\mathcal{H}$. If the wave operator (2.2) exists, then the intertwining property

$$E_2(\Omega)W^{\pm}(H_2, H_1; J) = W^{\pm}(H_2, H_1; J)E_1(\Omega) \tag{2.3}$$

($\Omega \subset \mathbb{R}$ is any Borel set and $E_i(\Omega) = E_i(\Omega; H_i)$) holds. It follows that the range $R(W^\pm(H_2, H_1; J))$ of the operator (2.2) is contained in $\mathcal{H}^{(ac)}(H_2)$ and its closure is an invariant subspace of H_2. Moreover, if the wave operator is isometric on some subspace $\mathcal{H}_1$, then the restrictions of H_1 and H_2 on the subspaces $\mathcal{H}_1$ and $\mathcal{H}_2 = W^\pm(H_2, H_1; J)\mathcal{H}_1$, respectively, are unitarily equivalent. This equivalence is realized by the wave operator. Clearly, for every $f_2 = W^\pm(H_2, H_1; J)f_1$

$$\exp(-iH_2t)f_2 \sim J\exp(-iH_1t)f_1, \quad t \to \pm\infty,$$

where " $\sim$ " means that the difference between left and right sides tends to zero. In case $J = I$ we omit dependence of wave operators on J. The operator $W^\pm(H_2, H_1)$ is obviously isometric on $\mathcal{H}^{(ac)}(H_1)$. The operator $W^\pm(H_2, H_1)$ is called complete if $R(W^\pm(H_2, H_1)) = \mathcal{H}^{(ac)}(H_2)$. This is equivalent to existence of the wave operator $W^\pm(H_1, H_2)$.

We note also the multiplication theorem

$$W^\pm(H_3, H_1; \tilde{J}J) = W^\pm(H_3, H_2; \tilde{J})W^\pm(H_2, H_1; J). \tag{2.4}$$

More precisely, if both wave operators in the right side exist, then the wave operator in the left side also exists and the equality (2.4) holds.

We need the following sufficient condition of existence of wave operators.

Proposition 2.1 *Let an operator $\mathcal{J}$ be H_1-bounded and let its adjoint $\mathcal{J}^*$ be H_2-bounded. Suppose that for some $N < \infty$*

$$H_2\mathcal{J} - \mathcal{J}H_1 = \sum_{n=1}^{N} K_{2,n}^* K_{1,n}$$

(in the precise sense this should be understood as an equality of sesquilinear forms on $\mathcal{D}(H_1) \times \mathcal{D}(H_2)$), where the operators $K_{j,n}$ are H_j-bounded and are H_j-smooth on some bounded interval Λ. Then the wave operators

$$W^\pm(H_2, H_1; \mathcal{J}E_1(\Lambda)), \quad W^\pm(H_1, H_2; \mathcal{J}^*E_2(\Lambda))$$

exist.

Proof for the case $\mathcal{J} = I$ can be found e.g. in [19]. For arbitrary $\mathcal{J}$ the proof is practically the same [23]. Unboundedness of $\mathcal{J}$ is inessential because real identifications $\mathcal{J}E_1(\Lambda)$ and $\mathcal{J}^*E_2(\Lambda)$ are bounded operators. We use Proposition 2.1 only in the case $\mathcal{D}(H_1) = \mathcal{D}(H_2)$ and $\mathcal{J} = \mathcal{J}^*$.

We consider an operator $H = T + V$ in the Hilbert space $\mathcal{H} = L_2(\mathbb{R}^d)$ where $T = -\Delta$ and V is multiplication by a function $V(x)$ defined by (1.1). We do not usually distinguish in notation a function and the operator of multiplication by this function. Assume that real functions V^α are sums of short-range V_s^α and long-range V_l^α terms:

$$V^\alpha = V_s^\alpha + V_l^\alpha. \tag{2.5}$$

We say that a potential V^α is short-range if $V_l^\alpha = 0$. It is convenient to split all conditions on V^α into two parts. To formulate them we need to introduce the operator $T^\alpha = -\Delta_{x^\alpha}$ in the space $\mathcal{H}^\alpha = L_2(X^\alpha)$.

Assumption 2.2 *Operators*

$$V^\alpha(T^\alpha + I)^{-1}, \quad (|x^\alpha| + 1)V_s^\alpha(T^\alpha + I)^{-1}, \quad (|x^\alpha| + 1)|\nabla V_l^\alpha|(T^\alpha + I)^{-1}$$

are compact in the space $\mathcal{H}^\alpha$.

Assumption 2.3 *For some* $\rho > 1$ *operators*

$$(|x^\alpha| + 1)^\rho V_s^\alpha(T^\alpha + I)^{-1}, \quad (|x^\alpha| + 1)^\rho|\nabla V_l^\alpha|(T^\alpha + I)^{-1}$$

are bounded in the space $\mathcal{H}^\alpha$.

Compactness of $V^\alpha(T^\alpha + I)^{-1}$ ensures that the operator H is self-adjoint on the domain $\mathcal{D}(H) = \mathcal{D}(T) =: \mathcal{D}$ and H is semi-bounded from below. Set

$$U(t) = \exp(-iHt), \quad E(\cdot) = E(\cdot; H).$$

The condition (1.2) is always assumed. Dimensions d^α of the subspaces X^α are arbitrary. In particular, we do not exclude that one of the subspaces X^α, say X^{α_0}, coincides with the whole space $X = \mathbb{R}^d$. Thus the (three-particle) potential $V^{\alpha_0}(x)$ tends to zero in all directions.

Assumption 2.2 has a preliminary nature. It is required for the Mourre estimate. Practically we use only that for $2r = \rho$ the operators

$$((x^\alpha)^2 + 1)^{r/2}|V_s^\alpha|^{1/2}(T^\alpha + I)^{-1/2} \quad \text{and} \quad ((x^\alpha)^2 + 1)^{r/2}|\nabla V_l^\alpha|^{1/2}(T^\alpha + I)^{-1/2}$$

are bounded in the space $\mathcal{H}^\alpha$. This is a consequence of Assumption 2.3 in virtue of the Heinz inequality. It follows that considered in the space $\mathcal{H}$ the operators $|V_s^\alpha|^{1/2}$ and $|\nabla V_l^\alpha|^{1/2}$ admit the representations

$$|V_s^\alpha|^{1/2} = B_s^\alpha(T + 1)^{1/2}((x^\alpha)^2 + 1)^{-r/2}, \quad B_s^\alpha \in \mathcal{B}, \tag{2.6}$$

$$|\nabla V_l^\alpha|^{1/2} = B_l^\alpha(T + 1)^{1/2}((x^\alpha)^2 + 1)^{-r/2}, \quad B_l^\alpha \in \mathcal{B}. \tag{2.7}$$

Let us introduce operators $H^\alpha = T^\alpha + V^\alpha$, $1 \le \alpha \le \alpha_1 := \alpha_0 - 1$, in the spaces $\mathcal{H}^\alpha$ playing the role of "two-particle" Hamiltonians. The point spectrum of H^α consists of eigenvalues accumulating, possibly, at the point $\lambda = 0$ only. The set of thresholds Υ_0 for H is defined as the union

$$\Upsilon_0 = \bigcup_{1\leq\alpha\leq\alpha_1} \sigma^{(p)}(H^\alpha) \cup \{0\}.$$

We need the following basic result (see [20, 21, 22]) of spectral theory of multiparticle Hamiltonians. It is formulated in terms of the auxiliary operator

$$A = \sum_{j=1}^{d} (x_j D_j + D_j x_j), \quad D_j = -i\partial_j, \quad \partial_j = \partial/\partial x_j.$$

Proposition 2.4 *Let Assumption 2.2 hold. Then eigenvalues of H may accumulate only at Υ_0 so that the "exceptional" set $\Upsilon = \Upsilon_0 \cup \sigma^{(p)}(H)$ is closed and countable. Furthermore, for every $\lambda \in \mathbb{R} \setminus \Upsilon$ there exists a small interval $\Lambda_\lambda \ni \lambda$ such that the estimate (the Mourre estimate) for the commutator holds:*

$$i([H, A]u, u) \geq c\|u\|^2, \quad c = c_\lambda > 0, \quad u \in E(\Lambda_\lambda)\mathcal{H}. \tag{2.8}$$

Remark. The quadratic form in the left side of (2.8) defined originally for $u \in \mathcal{D}(H) \cap \mathcal{D}(A)$ extends by continuity to all $u \in \mathcal{D}(H)$. Thus it is well-defined for $u \in E(\Lambda_\lambda)\mathcal{H}$.

Let Q be multiplication by $(x^2+1)^{1/2}$. *Below Λ is always an arbitrary bounded interval such that $\bar{\Lambda} \cap \Upsilon = \emptyset$*, where $\bar{\Lambda}$ is the closure of Λ. One of the main consequences of (2.8) is the following

Proposition 2.5 *Let Assumptions 2.2 and 2.3 hold. Then for any $r > 1/2$ the operator Q^{-r} is H-smooth on Λ.*

The proof of this assertion under our assumptions can be found in [17].

Corollary 2.6 *The operator H is absolutely continuous on $E(\Lambda)\mathcal{H}$. In particular, it does not have any singular continuous spectrum, i.e.*

$$\mathcal{H} = \mathcal{H}^{(p)}(H) \oplus \mathcal{H}^{(ac)}(H).$$

Note that Propositions 2.4 and 2.5 hold true also for the two-particle case. Thus the operator $(|x^\alpha| + 1)^{-r}, r > 1/2$, is H^α-smooth on any bounded positive interval separated from the point 0. According to Proposition 2.1 this implies that for short-range V^α the wave operators $W^\pm(H^\alpha, T^\alpha)$ exist and are complete.

Let us give the precise formulation of the scattering problem for three-particle Hamiltonians. We introduce auxiliary Hamiltonians $H_\alpha = T + V^\alpha$, $1 \leq \alpha \leq \alpha_1$, in the space $\mathcal{H}$ with only one pair potential each. Since $X = X_\alpha \oplus X^\alpha, \mathcal{H}$ splits into a tensor product

$$L_2(X) = L_2(X_\alpha) \otimes L_2(X^\alpha). \tag{2.9}$$

Let us introduce also the "free" operator $T_\alpha = -\Delta_{x_\alpha}$ in the space $\mathcal{H}_\alpha = L_2(X_\alpha)$. In the representation (2.9)

$$H_\alpha = T_\alpha \otimes I + I \otimes H^\alpha. \tag{2.10}$$

Denote by P^α the orthogonal projection in $\mathcal{H}^\alpha$ on the subspace $\mathcal{H}^{(p)}(H^\alpha)$ and set $P_\alpha = I \otimes P^\alpha$. Clearly, the orthogonal projection P_α commutes with H_α and its functions. Set also $V^0 = 0, H_0 = T, P_0 = I$. *Below indice a (and b) takes all values* $0, 1, ..., \alpha_1$. We use notation

$$U_a(t) = \exp(-iH_a t), \quad E_a(\cdot) = E(\cdot; H_a).$$

The basic result of the scattering theory for three-particle Hamiltonians is the following

Theorem 2.7 *Suppose that functions V^α satisfy Assumptions 2.2 and 2.3 and are short-range, i.e. $V^\alpha = V^\alpha_s$. Then the wave operators*

$$W_a^\pm = W^\pm(H, H_a; P_a) \tag{2.11}$$

exist and are isometric on $P_a\mathcal{H}$. The ranges $R(W_a^\pm)$ of $W_a^\pm$ are mutually orthogonal and the asymptotic completeness holds:

$$\sum_a \oplus R(W_a^\pm) = \mathcal{H}^{(ac)}(H). \tag{2.12}$$

Our assumptions on V^α are somewhat larger than those of I. M. Sigal and A. Soffer [10] or G .M. Graf [11] since we do not require anything about derivatives of V^α.

Scattering theory for the operator H_α containing only one pair potential reduces to that for the two-particle case. Indeed, comparing formula (2.10) and

$$H_0 = T_\alpha \otimes I + I \otimes T^\alpha,$$

we find that

$$U_\alpha(t) U_0(t) = I \otimes \exp(iH^\alpha t) \exp(-iT^\alpha t).$$

So wave operators $W^\pm(H_\alpha, H_0)$ and $W^\pm(H^\alpha, T^\alpha)$ exist at the same time and

$$W^\pm(H_\alpha, H_0) = I \otimes W^\pm(H^\alpha, T^\alpha).$$

Since wave operators $W^\pm(H^\alpha, T^\alpha)$ exist and are complete we have the following

Proposition 2.8 *In conditions of Theorem 2.7 the wave operators $W^\pm(H_\alpha, H_0)$ exist and*

$$R(W^\pm(H_\alpha, H_0)) = (I - P_\alpha)\mathcal{H}.$$

In particular, for every $f \in \mathcal{H}$ and $f_0^\pm = (W^\pm(H_\alpha, H_0))^* f$

$$U_\alpha(t) f \sim U_0(t) f_0^\pm + U_\alpha(t) P_\alpha f, \quad t \to \pm\infty. \tag{2.13}$$

We conclude this section with some standard technicalities.

Lemma 2.9 *For any $r \in [0,1]$ the operator $[H,Q^r](T+I)^{-1/2} \in \mathcal{B}$.*

Proof. – Clearly,

$$[H,Q^r] = [T,Q^r] = -2\nabla q_r \nabla - \Delta q_r, \quad q_r(x) = (x^2+1)^{r/2}.$$

Since $r \leq 1$, functions ∇q_r and Δq_r are bounded. □

Lemma 2.10 *Let $\psi \in C_0^\infty(\mathbb{R})$ and $r \in [0,1]$. Then $[\psi(H),Q^r] \in \mathcal{B}$.*

Proof. – Note that

$$[U(t),Q^r] = -i\int_0^t U(s)[H,Q^r]U(t-s)ds.$$

Thus in virtue of Lemma 2.9

$$\|[U(t),Q^r](|H|+I)^{-1/2}\| \leq C|t|. \tag{2.14}$$

For an arbitrary ψ we have that

$$[\psi(H),Q^r] = \int_{-\infty}^{\infty}[U(t),Q^r]\hat{\psi}(t)dt, \quad 2\pi\hat{\psi}(t) = \int_{-\infty}^{\infty}\exp(i\lambda t)\psi(\lambda)d\lambda.$$

By (2.14), it follows that

$$[\psi(H),Q^r](|H|+I)^{-1/2} \in \mathcal{B}, \quad \text{if} \quad \int_{-\infty}^{\infty}|t\hat{\psi}(t)|dt < \infty. \tag{2.15}$$

Finally, let $\psi_1 \in C_0^\infty(\mathbb{R})$ and $\psi_1(\lambda) = 1$ on support of ψ so that $\psi = \psi\psi_1$. Then

$$[\psi(H),Q^r] = \psi(H)[\psi_1(H),Q^r] + [\psi(H),Q^r]\psi_1(H)$$

and both terms in the right side are bounded in virtue of (2.15). □

Lemma 2.11 *For $r \in [0,1]$ and arbitrary $z \notin \sigma(H)$ the operator $Q^{-r}(T+I)(H-z)^{-1}Q^r$ is bounded.*

Proof. – Clearly,

$$(H-z)^{-1}Q^r = Q^r(H-z)^{-1} - (H-z)^{-1}[H,Q^r](H-z)^{-1}$$

and, by Lemma 2.9, $[H,Q^r](H-z)^{-1} \in \mathcal{B}$. Thus it remains to check that

$$Q^{-r}(T+I)Q^r(T+I)^{-1} \in \mathcal{B}.$$

To that end we commute T with Q^r and remark that the gradient and Laplacian of $q_r(x) = (x^2+1)^{r/2}$ are bounded. □

Quite similarly we obtain the following result.

Lemma 2.12 *Suppose that a function v obeys the estimate*

$$|v(x)| + |(\nabla v)(x)| + |(\Delta v)(x)| \leq C(|x|+1)^{-r}, \quad r \in [0,1]. \tag{2.16}$$

Then

$$(T+I)v(T+I)^{-1}Q^r \in \mathcal{B}, \quad (T+I)^{1/2}vD_j(T+I)^{-1}Q^r \in \mathcal{B}, \quad j=1,\ldots,d.$$

Combining Lemma 2.11 with Proposition 2.5 we immediately obtain

Proposition 2.13 *For every $r > 1/2$ the operator $Q^{-r}(T+I)$ is H-smooth on Λ.*

Proof. – For any $z \notin \sigma(H)$

$$Q^{-r}(T+I)U(t)f = (Q^{-r}(T+I)(H-z)^{-1}Q^r)\, Q^{-r}U(t)(H-z)f.$$

Since the first factor in the right side is bounded it suffices to apply the definition of H-smoothness to the element $(H-z)f \in E(\Lambda)\mathcal{H}$. □

In virtue of Lemma 2.12, Proposition 2.13 is more general than Proposition 2.5. Therefore we usually give references below only to Proposition 2.13. Similarly, by Lemma 2.12, Proposition 2.13 ensures H-smoothness of the operators $Q^{-r}D_j$ where $r > 1/2$ and $j = 1,\ldots,d$.

Of course, all results formulated for the operator H are as well true for H_0 and H_α.

3. POSITIVE COMMUTATORS AND RADIATION CONDITIONS

Our approach relies on consideration of the commutator of H with a first-order differential operator

$$M = \sum_{j=1}^{d}(m_jD_j + D_jm_j), \quad m_j = \partial m/\partial x_j, \tag{3.1}$$

where m is suitably chosen real function. To give an idea of this choice we note that for $m(x) = |x|$ there is the identity

$$i[H_0, M] = 4\nabla^{(s)}|x|^{-1}\nabla^{(s)}, \quad H_0 = T = -\Delta, \tag{3.2}$$

which can be deduced e.g. from the formulas (3.3) and (3.13) below. The arguments of [7] (reproduced in the proof of Theorem 3.5) show that the identity (3.2) ensures H_0-smoothness of the operator $Q^{-1/2}\nabla^{(s)}$. Furthermore, since $[V^{\alpha_0}, M] = O(|x|^{-\rho}), \rho > 1, |x| \to \infty$, using Proposition 2.5, we can prove smoothness of $Q^{-1/2}\nabla^{(s)}$ with respect to the "two-particle" Hamiltonian $H_{\alpha_0} = H_0 + V^{\alpha_0}$. However, the functions $[V^\alpha, M], 1 \leq \alpha \leq \alpha_1$, decrease only as $|x|^{-1}$ at infinity. Actually, one can not expect that the operator $Q^{-1/2}\nabla^{(s)}$ is H-smooth. To prove a weaker result about H-smoothness of the operators (1.4) and (1.6) the function $m(x)$ should be modified in such a way that $[V^\alpha, M] = O(|x|^{-\rho}), \rho > 1$ for all α. The last relation holds if $m(x)$ depends only on the variable x_α in some cone where $V^\alpha(x^\alpha)$ is concentrated. This is similar to the idea of G. M. Graf applied in [11] in the time-dependent context.

Suppose for a moment that m is an arbitrary smooth function. We start with the standard calculation of the commutator $[H_0, M]$.

Lemma 3.1 *Let an operator M be defined by (3.1). Then*

$$i[H_0, M] = 4\sum_{j,k} D_j m_{jk} D_k - (\Delta^2 m), \quad m_{jk} = \partial^2 m/\partial x_j \partial x_k. \tag{3.3}$$

Proof. – Let us consider

$$[\partial_j^2, m_k\partial_k] = \partial_j^2 m_k \partial_k - m_k\partial_k\partial_j^2. \tag{3.4}$$

Commuting ∂_j with m_k we find that the first term in the right side equals

$$\partial_j^2 m_k \partial_k = \partial_j(m_{jk} + m_k\partial_j)\partial_k.$$

Similarly, the second term

$$\begin{aligned} m_k\partial_k\partial_j^2 &= (m_k\partial_j)(\partial_k\partial_j) = (-m_{jk} + \partial_j m_k)(\partial_k\partial_j) = \\ &= -(\partial_j m_{jk} - m_{jjk})\partial_k + \partial_j m_k \partial_k \partial_j, \quad m_{jjk} = \partial^3 m/\partial x_j^2 \partial x_k. \end{aligned}$$

Inserting these expressions into (3.4) we obtain that

$$[\partial_j^2, m_k\partial_k] = 2\partial_j m_{jk}\partial_k - m_{jjk}\partial_k.$$

It follows that

$$\begin{aligned} [\partial_j^2, m_k\partial_k + \partial_k m_k] &= [\partial_j^2, m_k\partial_k] + [\partial_j^2, m_k\partial_k]^* = \\ &= 2(\partial_j m_{jk}\partial_k + \partial_k m_{jk}\partial_j) - m_{jjk}\partial_k + \partial_k m_{jjk} = \\ &= 2(\partial_j m_{jk}\partial_k + \partial_k m_{jk}\partial_j) + m_{jjkk}, \quad m_{jjkk} = \partial^4 m/\partial x_j^2 \partial x_k^2. \end{aligned}$$

Summing up these relations in j and k we arrive at (3.3). □

We choose $m(x)$ as a homogeneous function of degree 1. Such functions have singularities at $x = 0$. In virtue of Proposition 2.5 values of $m(x)$ in a bounded domain are inessential. Therefore we can get rid of singularity of $m(x)$ replacing it in a neighbourhood of $x = 0$ by an arbitrary smooth function. In such a way we obtain C^∞-function which satisfies the relation $m(sx) = sm(x)$ if $|x| \geq c > 0$ and $s \geq 1$. We say that m is homogeneous for $|x| \geq c$. A function m is constructed differently in neighbourhoods of subspaces X_α and in a "free" region, which is separated from all X_α. In order to describe necessary properties of m it is convenient to define a conical neighbourhood

$$\Gamma_\alpha(\varepsilon) = \{|x_\alpha| > (1-\varepsilon)|x|\}, \quad \varepsilon \in (0,1), \quad 1 \leq \alpha \leq \alpha_1,$$

of $X_\alpha \setminus \{0\}$. For sufficiently small ϵ and $\varepsilon \leq \epsilon$ these neighbourhoods are separated from each other, i.e. $\overline{\Gamma_\alpha(\varepsilon)} \cap \overline{\Gamma_\beta(\varepsilon)} = \{0\}$ for $\alpha \neq \beta$. This is a consequence of the assumption (1.2). Set also

$$\Gamma_0(\varepsilon) = \{(1-\varepsilon)|x| > |x_\alpha|, \ 1 \leq \alpha \leq \alpha_1\}.$$

We always assume that $\varepsilon \in (0, \epsilon)$ so that cones $\Gamma_0(\varepsilon)$ are not empty. Clearly, $\Gamma_0(\varepsilon)$ gets larger if ε decreases but never intersects with X_α. More precisely, $\Gamma_0(\varepsilon) \cap \Gamma_\alpha(\varepsilon) = \emptyset$ and

$$\overline{\Gamma_0(\varepsilon)} \cup \bigcup_{\alpha=1}^{\alpha_1} \Gamma_\alpha(\varepsilon) = X. \tag{3.5}$$

Let us subtract from $\Gamma_a(\varepsilon)$ the unit ball, that is we set

$$\overset{o}{\Gamma}_a(\varepsilon) = \Gamma_a(\varepsilon) \cap \{|x| > 1\}.$$

We submit $m(x)$ to the following requirements:

1^0 $m(x)$ is a real nonnegative C^∞-function, which is homogeneous of degree 1 for $|x| \geq 1$ and $m(x) = 0$ for $|x| \leq 1/2$.

2^0 $m(x) > 0$ if $|x| = 1$.

3^0 $m(x)$ is a (locally) convex function for $|x| \geq 1$, i.e.

$$\sum_{j,k} m_{jk}(x)\xi_j\bar{\xi}_k \geq 0, \quad \forall \xi \in \mathbb{C}^d, \ |x| \geq 1. \tag{3.6}$$

4^0 For every $\alpha = 1, \dots, \alpha_1$ there exist $\epsilon_\alpha \in (0, \epsilon)$ and $\mu_\alpha > 0$ such that $m(x) = \mu_\alpha |x_\alpha|$ if $x \in \overset{o}{\Gamma}_\alpha(\epsilon_\alpha)$. Furthermore, there exist $\epsilon_0 > \max\{\epsilon_\alpha\}$ and $\mu_0 > 0$ such that $m(x) = \mu_0|x|$ if $x \in \overset{o}{\Gamma}_0(\epsilon_0)$.

The final property is, strictly speaking, related to the family of functions satisfying $1^0 - 4^0$.

5^0 By a choice of $m(x) = m^{(\epsilon_0)}(x)$ a number ϵ_0 can be made arbitrary small (i.e. for arbitrary small neighbourhoods of X_α one can construct $m(x)$ in such a way that $m(x) = \mu_0|x|$ for $|x| \geq 1$ outside of these neighbourhoods).

Below ϵ, ϵ_0 and ϵ_α are always numbers specified here; in particular, $\epsilon > \epsilon_0 > \epsilon_\alpha, \quad \alpha = 1, \dots, \alpha_1$.

Let us give an example of a function $m(x)$ obeying all conditions $1^0 - 5^0$. First, we introduce a family of functions $m_\varepsilon(x)$ satisfying all the properties except smoothness and then average $m_\varepsilon(x)$ over ε. Set

$$m_\varepsilon(x) = \max\{|x_1|, ..., |x_{\alpha_1}|, (1-\varepsilon)|x|\}, \quad 0 < \varepsilon < \epsilon.$$

By definition, $m_\varepsilon(x)$ is a homogeneous function of degree 1. Being maximum of convex functions, $m_\varepsilon(x)$ is convex, i.e.

$$m_\varepsilon(r_1 x_1 + r_2 x_2) \le r_1 m_\varepsilon(x_1) + r_2 m_\varepsilon(x_2), \quad r_j \in [0,1], \ r_1 + r_2 = 1.$$

Clearly, $m_\varepsilon(x) = |x_\alpha|$ if $x \in \Gamma_\alpha(\varepsilon)$, and $m_\varepsilon(x) = (1-\varepsilon)|x|$ if $x \in \Gamma_0(\varepsilon)$. In other words,

$$m_\varepsilon(x) = \sum_{\alpha=1}^{\alpha_1} |x_\alpha| \theta(|x_\alpha| - (1-\varepsilon)|x|) + (1-\varepsilon)|x|(1 - \sum_{\alpha=1}^{\alpha_1} \theta(|x_\alpha| - (1-\varepsilon)|x|)), \quad (3.7)$$

where $\theta(s) = 1$ for $s \ge 0$ and $\theta(s) = 0$ for $s < 0$.

Let $\varphi(\varepsilon)$ be some smooth nonnegative function supported in a closed interval $[\epsilon_1, \epsilon_0]$, $0 < \epsilon_1 < \epsilon_0 < \epsilon$. Define

$$m(x) = \int_0^\epsilon m_\varepsilon(x) \varphi(\varepsilon) d\varepsilon. \quad (3.8)$$

Obviously, $m(x)$ is again homogeneous function of degree 1. It satisfies the property 2^0 because

$$m_\varepsilon(x) \ge 1 - \varepsilon \ge 1 - \epsilon_0 > 0, \quad |x| = 1.$$

Being an integral of convex functions, $m(x)$ is convex. Comparing (3.7) with (3.8) and denoting

$$\Phi(s) = \int_s^\epsilon \varphi(\varepsilon) d\varepsilon, \quad \tilde{\Phi}(s) = \int_s^\epsilon (1-\varepsilon)\varphi(\varepsilon) d\varepsilon,$$

we find that

$$m(x) = \sum_{\alpha=1}^{\alpha_1} |x_\alpha| \Phi(1 - |x|^{-1}|x_\alpha|) + |x|(\tilde{\Phi}(0) - \sum_{\alpha=1}^{\alpha_1} \tilde{\Phi}(1 - |x|^{-1}|x_\alpha|)). \quad (3.9)$$

Functions $\Phi(s)$ and $\tilde{\Phi}(s)$ are smooth, they equal zero if $s \ge \epsilon_0$ and they equal constants $\Phi(0)$ and $\tilde{\Phi}(0)$, respectively, if $s \le \epsilon_1$. Therefore the function (3.9) belongs to $C^\infty(\mathbb{R}^d \setminus \{0\}), m(x) = \Phi(0)|x_\alpha|$ if $x \in \Gamma_\alpha(\epsilon_1)$ and $m(x) = \tilde{\Phi}(0)|x|$ if $x \in \Gamma_0(\epsilon_0)$. Thus the property 4^0 (with $\mu_\alpha = \Phi(0), \epsilon_\alpha = \epsilon_1$ and $\mu_0 = \tilde{\Phi}(0)$) holds. Since ϵ_0 is an arbitrary small number, the property 5^0 is also fulfilled.

Finally, one can get rid of local singularity of $m(x)$ at $x = 0$ replacing it by $\tau(x)m(x)$ where $\tau \in C^\infty(\mathbb{R}^d)$, $\tau(x) = 0$ for $|x| \le 1/2$ and $\tau(x) = 1$ for $|x| \ge 1$.

Actually, the concrete construction of the function m is of no importance for us and we always use only its properties $1^0 - 5^0$ listed above. By the property 1^0 derivatives m_j of m are homogeneous functions of degree 0, m_{jk} are homogeneous of degree -1 and m_{jjkk} are homoneneous of degree -3. Therefore

$$(\Delta^2 m)(x) = O(|x|^{-3}), \quad |x| \to \infty, \tag{3.10}$$

and the main contribution to the commutator (3.3) is determined by the operator

$$L = L(m) = \sum_{j,k} D_j m_{jk} D_k. \tag{3.11}$$

To estimate it we first compute the matrix

$$\mathbf{M}(x) = \{m_{jk}(x)\} = \text{Hess } m(x)$$

in the region where $m(x) = \mu_0|x|$:

$$m_j(x) = \mu_0|x|^{-1}x_j, \quad m_{jk}(x) = \mu_0(|x|^{-1}\delta_{jk} - |x|^{-3}x_jx_k). \tag{3.12}$$

Here $\delta_{jj} = 1$ and $\delta_{jk} = 0$ if $j \neq k$. By the definition (1.3), the angular part of the gradient ∇u obeys the identity

$$|\nabla^{(s)}u|^2 = |\nabla u|^2 - |x|^{-2}|\langle \nabla u, x\rangle|^2 = \sum_j |u_j|^2 - |x|^{-2}|\sum_j u_jx_j|^2 =$$
$$= \sum_j (1 - |x|^{-2}x_j^2)|u_j|^2 - |x|^{-2}\sum_{j\neq k} x_jx_ku_j\bar{u_k}, \quad u_j = \partial u/\partial x_j.$$

According to (3.12) it follows that

$$\sum_{j,k} m_{jk}u_j\bar{u_k} = \mu_0|x|^{-1}|\nabla^{(s)}u|^2. \tag{3.13}$$

In the region where $m(x) = \mu_\alpha|x_\alpha|$ all calculations hold true if x is replaced by x_α. Thus we obtain the following

Lemma 3.2 *Let $\nabla^{(s)}u$ and $\nabla^{(s)}_{x_\alpha}u$ be defined by (1.3), (1.5) respectively and let $\overset{o}{\Gamma}_0\ (\epsilon_0), \overset{o}{\Gamma}_\alpha\ (\epsilon_\alpha)$ be the truncated cones introduced in the condition 4^0 on $m(x)$. For $x \in \overset{o}{\Gamma}_0\ (\epsilon_0)$ the identity (3.13) holds and for $x \in \overset{o}{\Gamma}_\alpha\ (\epsilon_\alpha)$*

$$\sum_{j,k} m_{jk}u_j\bar{u_k} = \mu_\alpha|x_\alpha|^{-1}|\nabla^{(s)}_{x_\alpha}u|^2, \quad \alpha = 1, ..., \alpha_1. \tag{3.14}$$

Note that in case $\dim X_\alpha = 1$ both sides of (3.14) equal zero.

By the condition (3.6) on $m(x)$

$$(Lu,u)=\sum_{j,k}\int m_{jk}u_j\bar{u}_k dx\geq\sum_{j,k}\int_\Gamma m_{jk}u_j\bar{u}_k dx-c\int_{|x|<1}|\nabla u|^2dx,$$

where Γ is any region lying outside of the unit ball. Combining this inequality with Lemma 3.2 we obtain

Proposition 3.3 *In notation of Lemma 3.2 for every* $u\in\mathcal{D}$

$$(Lu,u)\geq\mu_0\int_{\overset{o}{\Gamma}_0(\epsilon_0)}|x|^{-1}|\nabla^{(s)}u|^2dx-c\int_{|x|<1}|\nabla u|^2dx$$

and

$$(Lu,u)\geq\mu_\alpha\int_{\overset{o}{\Gamma}_\alpha(\epsilon_\alpha)}|x_\alpha|^{-1}|\nabla^{(s)}_{x_\alpha}u|^2dx-c\int_{|x|<1}|\nabla u|^2dx,\quad\alpha=1,...,\alpha_1.$$

It turns out that due to the property 4^0 the commutator $[V,M]$ is in some sense small. The precise formulation is given in the following

Proposition 3.4 *Suppose that* V^α *is defined by (2.5) where* V^α_s *and* V^α_l *satisfy Assumptions 2.2 and 2.3. Let* m *obey the property* 1^0 *and* $m(x)=m(x_\alpha)$ *if* $x\in\overset{o}{\Gamma}_\alpha(\varepsilon_\alpha)$ *for some* $\varepsilon_\alpha>0$. *Then*

$$|([V^\alpha,M]u,u)|\leq C\|Q^{-r}(T+I)u\|^2,\quad u\in\mathcal{D},\quad 2r=\rho. \tag{3.15}$$

Proof. – Suppose first that $1\leq\alpha\leq\alpha_1$. Let us introduce a smooth homogeneous (for $|x|\geq2$) function ζ_α of degree zero such that $0\leq\zeta_\alpha(x)\leq1$, $\zeta_\alpha(x)=1$ if $x\notin\overset{o}{\Gamma}_\alpha(\varepsilon_\alpha)$ and $\zeta_\alpha(x)=0$ if $x\in\Gamma_\alpha(\varepsilon)$ for some $\varepsilon\in(0,\varepsilon_\alpha)$ and $|x|\geq2$. The long-range part of V^α is differentiable so that

$$i[V^\alpha_l,M]=2[V^\alpha_l,\sum_{j=1}^d m_j\partial_j]=-2\sum_{j=1}^d m_j\partial V^\alpha_l/\partial x_j=-2\langle\nabla m(x),\nabla V^\alpha_l(x^\alpha)\rangle.$$

This scalar product equals zero for $x\in\overset{o}{\Gamma}_\alpha(\varepsilon_\alpha)$ because m depends only on x_α in this region and, consequently, $\nabla m(x)\in X_\alpha$ whereas $\nabla V^\alpha_l\in X^\alpha$. Since $|\nabla m(x)|$ is bounded, it follows that

$$|\langle\nabla m(x),\nabla V^\alpha_l(x^\alpha)\rangle|\leq C\zeta_\alpha(x)|\nabla V^\alpha_l(x^\alpha)|\zeta_\alpha(x). \tag{3.16}$$

Using the representation (2.7) we find that

$$|([V^\alpha_l,M]u,u)|\leq C\|(T+I)^{1/2}w_\alpha u\|^2,\quad w_\alpha(x)=((x^\alpha)^2+1)^{-r/2}\zeta_\alpha(x).$$

The function $w_\alpha(x)$ obeys the condition (2.16) because $\zeta_\alpha(x)=0$ if $x\in\Gamma_\alpha(\varepsilon)$ and $|x|\geq2$. Therefore, taking into account Lemma 2.12, we obtain the bound (3.15) for V^α_l.

To consider $[V_s^\alpha, M]$ we use again that the function $\zeta_\alpha(x)$ differs from 1 only if $x \in \overset{o}{\Gamma}_\alpha(\varepsilon_\alpha)$. In this region the function m does not depend on x^α. It follows that the operator

$$i\eta_\alpha M = 2\eta_\alpha(\nabla_{x_\alpha} m)\nabla_{x_\alpha} + \eta_\alpha(\Delta_{x_\alpha} m), \quad \eta_\alpha(x) = 1 - \zeta_\alpha^2(x),$$

commutes with V_s^α and hence $[V_s^\alpha, M] = [V_s^\alpha, \zeta_\alpha^2 M]$. Simple computations show that

$$[V_s^\alpha, \zeta_\alpha^2 M] = 2\sum_{j=1}^{d}(V_s^\alpha \xi_{\alpha,j} D_j - D_j V_s^\alpha \xi_{\alpha,j} - iV_s^\alpha \partial\xi_{\alpha,j}/\partial x_j), \quad \xi_{\alpha,j} = \zeta_\alpha^2 m_j. \quad (3.17)$$

Note that the functions m_j are bounded together with their derivatives and $\xi_{\alpha,j} = 0$ if $x \in \Gamma_\alpha(\varepsilon)$ and $|x| \geq 2$. In virtue of the representation (2.6) for $|V_s^\alpha|^{1/2}$ the last term in (3.17) is estimated exactly as the right side of (3.16). Similarly,

$$|(V_s^\alpha \xi_{\alpha,j} D_j u, u)| \leq C\|(T+I)^{1/2} w_\alpha D_j u\| \, \|(T+I)^{1/2} w_\alpha u\|,$$

which is estimated by the right side of (3.15) according to Lemma 2.12. In the case $\alpha = \alpha_0$ the estimates are the same but the cut-off by ζ_α is no longer necessary. □

Given Propositions 3.3 and 3.4 the proof of the main result of this section is quite standard. We formulate it only for the operator H since H_0 and H_α are its special cases.

Theorem 3.5 *Suppose that V^α are defined by (2.5) where V_s^α and V_l^α satisfy Assumptions 2.2 and 2.3. Let $\chi_a(\varepsilon;\cdot)$, $a = 0, 1, \ldots, \alpha_1$, be the characteristic function of a cone $\Gamma_a(\varepsilon)$, where $\varepsilon \in (0, \epsilon)$ is arbitrary. Then the operators*

$$G_0(\varepsilon) = \chi_0(\varepsilon) Q^{-1/2}\nabla^{(s)}, \quad G_\alpha(\varepsilon) = \chi_\alpha(\varepsilon) Q^{-1/2}\nabla_{x_\alpha}^{(s)},$$

acting from the space $L_2(\mathbb{R}^d)$ into the vector-spaces $L_2(\mathbb{R}^d)\otimes\mathbb{C}^d$ and $L_2(\mathbb{R}^d)\otimes\mathbb{C}^{d_\alpha}$, $d_\alpha = \dim X_\alpha$, respectively, are H-smooth on arbitrary bounded interval $\Lambda, \bar{\Lambda}\cap\Upsilon = \emptyset$.

Proof. – Let us consider

$$d(MU(t)f, U(t)f)/dt = i([H, M]f_t, f_t), \quad (3.18)$$

where $f_t = U(t)f$, $f \in \mathcal{D}$. By (3.3), (3.11)

$$i([H, M]f_t, f_t) = 4(Lf_t, f_t) - ((\Delta^2 m)f_t, f_t) + i([V, M]f_t, f_t).$$

Taking into account (3.10) and applying Propositions 3.3, 3.4 to elements $u = f_t$ we find that (under the assumption $\rho \leq 3$)

$$i([H, M]f_t, f_t) \geq c_1\|G_a(\epsilon_a)f_t\|^2 - c_2\|Q^{-r}(T+I)f_t\|^2, \quad 2r = \rho, \quad (3.19)$$

for any $a = 0, 1, ..., \alpha_1$. Here we have omitted $\|Q^{-r}f_t\|^2$ and the integral of $|\nabla f_t|^2$ over the unit ball because they are estimated by the last term in the right side of (3.19). Integrating (3.18), (3.19) over $t \in (t_1, t_2)$ we obtain that

$$\int_{t_1}^{t_2} \|G_a(\epsilon_a)f_t\|^2 dt \leq C(|(Mf_t, f_t)\Big|_{t_1}^{t_2}| + \int_{t_1}^{t_2} \|Q^{-r}(T+I)f_t\|^2 dt). \tag{3.20}$$

Suppose now that $f = E(\Lambda)f$. Then the first term in the right side of (3.20) is bounded by $C\|f\|^2$ because $ME(\Lambda) \in \mathcal{B}$ for bounded Λ. The second term admits the same estimate according to Proposition 2.13. It follows that the integral in the left side of (3.20) is bounded by $C\|f\|^2$ so that each of the operators $G_a(\epsilon_a)$ is H-smooth on Λ. By the property 5^0 of the function $m(x)$ a number ϵ_0 can be arbitrary small. This concludes the proof of H-smoothness of $G_0(\varepsilon)$ for arbitrary $\varepsilon > 0$. Since

$$|\nabla_{x_\alpha}^{(s)} u| \leq |\nabla^{(s)} u|, \tag{3.21}$$

H-smoothness of $G_\alpha(\varepsilon)$ for arbitrary $\varepsilon \in (0, \epsilon)$ is now a consequence of that fact for some $\varepsilon > 0$. □

Remark. Let us give for completeness a proof of (3.21). We can assume that u is real. By definitions (1.3), (1.5) the estimate (3.21) is equivalent to the bound

$$|\xi_\alpha|^2 + |x|^{-2}|\langle \xi, x\rangle|^2 \leq |\xi|^2 + |x_\alpha|^{-2}|\langle \xi_\alpha, x_\alpha\rangle|^2, \tag{3.22}$$

where ξ ($\xi = \nabla u$) is an arbitrary vector of X and ξ_α ($\xi_\alpha = \nabla_{x_\alpha} u$) is the orthogonal projection of ξ on X_α. It suffices to prove (3.22) with $|\langle \xi, x\rangle|$ replaced by $|\langle \xi_\alpha, x_\alpha\rangle| + |\xi^\alpha||x^\alpha|$. By identical transformations such an estimate can be reduced to the obvious inequality

$$2|x_\alpha|^2 |\langle \xi_\alpha, x_\alpha\rangle||\xi^\alpha||x^\alpha| \leq |\langle \xi_\alpha, x_\alpha\rangle|^2 |x^\alpha|^2 + |x_\alpha|^4 |\xi^\alpha|^2.$$

Remark. By (3.21), Theorem 3.5 gives us more information about $U(t)f$ in the "free" region Γ_0 compared to that in the regions Γ_α where potentials V^α are concentrated.

Remark. The notion of H-smoothness can be equivalently reformulated in terms of the resolvent of H. Thus radiation conditions-estimates given by Theorem 3.5 also admit a stationary formulation.

Remark. In the two-particle case (where $H = T + V^{\alpha_0}$) the result of Theorem 3.5 reduces to H-smoothness of the operator $Q^{-1/2}\nabla^{(s)}$ on any bounded positive interval separated from the point 0. This is different from the usual form of the radiation condition (see e.g. [14]). First, we consider only the angular part of $\nabla U(t)f$. Second, the estimate of [14] implies that

$$\int_{-\infty}^{\infty} \|Q^{-r}\nabla^{(s)} U(t)f\|^2 dt < \infty. \tag{3.23}$$

Here r is some number smaller than $1/2$ whereas we require that $r = 1/2$ which is less informative. On the other hand, in (3.23) f should belong to some dense (in $\mathcal{H}$) set whereas our estimate is uniform for all $f \in \mathcal{H}$.

Note, finally, that in [24] a radiation condition for N-particle case was derived in the free region Γ_0. From the viewpoint of the previous remark the result of [24] is similar to the two-particle radiation condition and thus it differs from Theorem 3.5. Results of [24] can probably be used (see the discussion at the beginning of the next section) for a proof of asymptotic completeness in the three-particle case. However, an information about $U(t)f$ in a free region only is not sufficient for the case of $N > 3$ particles.

4. MODIFIED WAVE OPERATORS

In order to explain an idea of the subsequent proof of asymptotic completeness let us recall that, as remarked by P. Deift and B. Simon [25], it is equivalent to existence of wave operators $W^{\pm}(H_a, H; J^{(a)})$, $a = 0, 1, \ldots, \alpha_1$. Here identifications $J^{(a)}$ are multiplications by smooth homogeneous functions $\eta^{(a)}$ of zero order such that $\sum \eta^{(a)}(x) = 1$. Furthermore, $\eta^{(\alpha)}(x) = 1$ in a neighbourhood Γ_α of the subspace X_α and $\eta^{(0)}(x) = 1$ if x is sufficiently far from all of them. The main contribution to the "perturbation" $HJ^{(a)} - J^{(a)}H_a$ is given by the term $\nabla\eta^{(a)}\nabla$, which equals $\nabla\eta^{(a)}\nabla^{(s)}$ because $\langle\nabla\eta^{(a)}(x), x\rangle = 0$. Remark also that $\nabla\eta^{(a)}(x)$ decays as $|x|^{-1}$ at infinity and differs from zero in a free region Γ_0 only. Therefore convergence of the integral (cf. with the last remark in section 3)

$$\int_{-\infty}^{\infty} \|\chi_0 Q^{-r}\nabla^{(s)}U(t)f\|^2 dt < \infty$$

for some $r < 1/2$ and for elements f from some set dense in $\mathcal{H}$ would have been sufficient (see [17] for more details about such a plan of the proof) for existence of the wave operators $W^{\pm}(H_a, H; J^{(a)})$.

The result of Theorem 3.5 allows us to accomodate the terms $G_a^* G_a$ which are similar to $\nabla\eta^{(a)}\nabla^{(s)}$ but are second-order differential operators. Thus we are compelled to change the identifications $J^{(a)}$. We choose new identifications as first-order differential operators $M^{(a)}$ constructed by means of functions $\eta^{(a)}m$. Coefficients of $M^{(a)}$ equal zero outside of a region Γ_a and $\sum M^{(a)} = M$. We emphasize that our proof of existence of the wave operators $W^{\pm}(H_a, H; M^{(a)}E(\Lambda))$ requires H-smoothness of all operators G_a (not only of G_0). To remove the identifications $M^{(a)}$ we introduce also the auxiliary wave operator $W^{\pm}(H, H; ME(\Lambda))$. At the end of this section we show that this operator is invertible on the subspace $E(\Lambda)\mathcal{H}$. As was explained in section 1, this is an essential step in our proof of asymptotic completeness.

Let us proceed to the formal exposition. We start with the following elementary observation.

Lemma 4.1 *Suppose that $m(x)$ is an arbitrary smooth homogeneous (for $|x| \geq 1$) function of degree 1. Let $\lambda_n(x)$ and $p_n(x)$ be eigenvalues and eigenvectors of the symmetric matrix $\mathbf{M}(x) = \{m_{jk}(x)\}$. Then vectors $p_n(x), |x| \geq 1$, corresponding to $\lambda_n(x) \neq 0$, are orthogonal to x.*

Proof. – Since $\mathbf{M}(x)$ is symmetric, it suffices to show that x is its eigenvector corresponding to the zero eigenvalue. Differentiating the identity $m(sx) = sm(x)$ in s and setting $s = 1$ we find that

$$\sum m_j(x)x_j = m(x)$$

(Euler's formula). Differentiation of this relation in x_k shows that

$$\sum_j m_{kj}(x)x_j = 0, \quad k = 1, \ldots, d.$$

Thus $\mathbf{M}(x)x = 0$. □

Let some function m satisfying conditions $1^0 - 4^0$ be given and let $\varepsilon_0 = \min \epsilon_\alpha$, $\alpha = 1, \ldots, \alpha_1$. We introduce homogeneous functions $\eta^{(\alpha)} \in C^\infty(\mathbb{R}^d \setminus \{0\})$ of degree 0, $\alpha = 1, \ldots, \alpha_1$, such that supp $\eta^{(\alpha)} \subset \overline{\Gamma_\alpha(\epsilon)}$ (and hence supports of $\eta^{(\alpha)}$ for different α intersect only at zero) and $\eta^{(\alpha)}(x) = 1$ if $x \in \Gamma_\alpha(\epsilon_\alpha)$. The function

$$\eta^{(0)}(x) = 1 - \sum_{\alpha=1}^{\alpha_1} \eta^{(\alpha)}(x) \tag{4.1}$$

equals zero if $x \notin \Gamma_0(\varepsilon_0)$ and $\eta^{(0)}(x) = 1$ if $x \in \Gamma_0(\epsilon)$. Set $m^{(a)}(x) = \eta^{(a)}(x)m(x)$, $a = 0, 1, \ldots, \alpha_1$, and

$$M^{(a)} = \sum_{j=1}^{d} (m_j^{(a)} D_j + D_j m_j^{(a)}), \quad m_j^{(a)} = \partial m^{(a)}/\partial x_j. \tag{4.2}$$

Clearly, $m^{(a)}(x)$ satisfies the properties 1^0 and 4^0 (with $\mu_a^{(a)} = \mu_a$ and $\mu_b^{(a)} = 0$ for $b \neq a$) but the properties 2^0 and 3^0 are violated.

Theorem 4.2 *Suppose that functions V^α satisfy the assumptions of Theorem 2.7 and Λ is any bounded interval such that $\bar{\Lambda} \cap \Upsilon = \emptyset$. Then the wave operators*

$$W^\pm(H, H_a; M^{(a)} E_a(\Lambda)), \quad W^\pm(H_a, H; M^{(a)} E(\Lambda)), \tag{4.3}$$

exist for all $a = 0, 1, \ldots, \alpha_1$.

Proof. – We shall show that the triple $H_a, H, M^{(a)}$ satisfies on Λ the conditions of Proposition 2.1. Let us consider

$$HM^{(a)}-M^{(a)}H_a=[T,M^{(a)}]+[V^a,M^{(a)}]+\sum_{\beta\neq a}V^\beta M^{(a)},\quad \beta=1,\ldots,\alpha_0,\ (4.4)$$

$V^0=0$. We shall verify that each term in the right side can be factored into a product of H- and H_a-smooth operators. We start with the last two terms which can be estimated with the help of Proposition 2.13 only. The commutator $[V^\alpha, M^{(\alpha)}]$ was actually already considered in Proposition 3.4. Its assumptions are fulfilled because the function $m^{(\alpha)}$ satisfies the property 1^0 and $m^{(\alpha)}(x)=\mu_\alpha|x_\alpha|$ if $x\in\overset{o}{\Gamma}_\alpha(\epsilon_\alpha)$. The estimate (3.15) is equivalent to the representation

$$[V^\alpha, M^{(\alpha)}]=(T+I)Q^{-r}B^{(\alpha)}Q^{-r}(T+I),\quad 2r=\rho,\quad B^{(\alpha)}\in\mathcal{B},$$

where $Q^{-r}(T+I)$ is H- and H_α-smooth on Λ in virtue of Proposition 2.13.

We need short-range assumption on potentials only to treat $V^\beta M^{(a)}, \beta\neq a$. Suppose first that $\beta\neq\alpha_0$. Recall that $m^{(a)}(x)=0$ if $x\in\Gamma_\beta(\epsilon_\beta)$. Therefore $m_j^{(a)}(x)=m_j^{(a)}(x)\zeta_\beta^2(x)$ and $m_{jj}^{(a)}(x)=m_{jj}^{(a)}(x)\zeta_\beta^2(x)$ for suitable $\zeta_\beta\in C^\infty(\mathbb{R}^d)$, homogeneous (for $|x|\geq 1$) of degree 0, such that $\zeta_\beta(x)=0$ if $x\in\overset{o}{\Gamma}_\beta(\varepsilon)$ for some $\varepsilon\in(0,\epsilon_\beta)$. By (2.6), (4.2) the operator $V^\beta M^{(a)}$ consists of terms

$$V^\beta m_j^{(a)}D_j=w_\beta(T+I)^{1/2}B_j^{(a,\beta)}(T+I)^{1/2}w_\beta D_j$$

and

$$V^\beta m_{jj}^{(a)}=w_\beta(T+I)^{1/2}B_{jj}^{(a,\beta)}(T+I)^{1/2}w_\beta,$$

where $j=1,\ldots,d$,

$$w_\beta(x)=((x^\beta)^2+1)^{-r/2}\zeta_\beta(x),\quad 2r=\rho,\quad B_j^{(a,\beta)}\in\mathcal{B},\quad B_{jj}^{(a,\beta)}\in\mathcal{B}.$$

The function $w_\beta(x)$ obeys the condition (2.16). Therefore, by Lemma 2.12, each of these terms equals $(T+I)Q^{-r}BQ^{-r}(T+I)$ with some bounded operator B. This proves the required factorization of $V^\beta M^{(a)}$ into a product of smooth operators. In case $\beta=\alpha_0$ the estimates are the same but the cut-off by ζ_β is no longer necessary.

Let us consider the first term in the right side of (4.4). According to Lemma 3.1 the commutator $[T,M^{(a)}]$ is defined by (3.3) with m replaced by $m^{(a)}$. Since $m^{(a)}$ is a homogeneous function of degree 1 the term $(\Delta^2 m^{(a)})(x)=O(|x|^{-3})$ as $|x|\to\infty$. Hence $\Delta^2 m^{(a)}=Q^{-3/2}B^{(a)}Q^{-3/2}$ where $B^{(a)}$ is multiplication by a bounded function and $Q^{-3/2}$ is H- and H_a-smooth by Proposition 2.5.

To estimate the operator $L^{(a)} = L(m^{(a)})$ defined by (3.11) we need Theorem 3.5. Its application relies on Lemma 4.1. Let $\lambda_n^{(a)}(x)$ and $p_n^{(a)}(x)$, $n = 1, \ldots, d$, be eigenvalues and normalized eigenvectors of the symmetric matrix $\mathbf{M}^{(a)}(x) = \{m_{jk}^{(a)}(x)\}$. Clearly, $\lambda_n^{(a)}(x)$ are homogeneous (for $|x| \geq 1$) functions of order -1 and $p_n^{(a)}(x)$ - of order 0. Diagonalizing the matrix $\mathbf{M}^{(a)}$ we find that

$$(L^{(a)}u, v) = \int_X \sum_{j,k} m_{jk}^{(a)}(x) D_k u(x) \overline{D_j v(x)} dx =$$

$$= \int_X \sum_n \lambda_n^{(a)}(x) \langle \nabla u(x), p_n^{(a)}(x) \rangle \langle p_n^{(a)}(x), \nabla v(x) \rangle dx = (K_1^{(a)} u, K_2^{(a)} v)_{\mathbf{H}},$$

where

$$(K_j^{(a)} u)(x) = \sum_n \nu_{n,j}^{(a)}(x) \langle \nabla u(x), p_n^{(a)}(x) \rangle p_n^{(a)}(x), \quad j = 1, 2, \tag{4.5}$$

$$\nu_{n,1}^{(a)}(x) = |\lambda_n^{(a)}(x)|^{1/2}, \quad \nu_{n,1}^{(a)}(x) \nu_{n,2}^{(a)}(x) = \lambda_n^{(a)}(x)$$

and $\mathbf{H} = L_2(\mathbb{R}^d) \otimes \mathbb{C}^d$. Let χ be the characteristic function of the ball $|x| \leq 1$ and $\overset{o}{\chi} = 1 - \chi$. Since

$$|(K_j^{(a)} u)(x)| \leq C |\nabla u(x)|,$$

H- and H_a-smoothness of the operators $\chi K_j^{(a)}$ is ensured by Proposition 2.13.

To treat the operators $\overset{o}{\chi}\, K_j^{(a)}$ we notice that, by the definition (1.3) and Lemma 4.1,

$$\langle \nabla u(x), p_n^{(a)}(x) \rangle = \langle \nabla^{(s)} u(x), p_n^{(a)}(x) \rangle, \quad |x| \geq 1,$$

if $\lambda_n^{(a)}(x) \neq 0$. It follows that

$$|(K_j^{(a)} u)(x)| \leq C |x|^{-1/2} |\nabla^{(s)} u(x)|, \quad |x| \geq 1, \quad C = \sup_{|x|=1} \sum_n \nu_{n,1}^{(a)}(x). \tag{4.6}$$

Set $\overset{o}{\chi}_a(\varepsilon) = \overset{o}{\chi}\, \chi_a(\varepsilon)$ where $\chi_a(\varepsilon)$ is the characteristic function of the cone $\Gamma_a(\varepsilon)$. By (4.6),

$$|(\overset{o}{\chi}_0(\varepsilon) K_j^{(a)} u)(x)| \leq C |(G_0(\varepsilon) u)(x)|$$

so that the local H- and H_a-smoothness of the operators $\overset{o}{\chi}_0(\varepsilon) K_j^{(a)}$ for arbitrary $\varepsilon > 0$ is a consequence of Theorem 3.5. Since $\mathbf{M}^{(0)}(x) = 0$ if $x \notin \Gamma_0(\varepsilon_0)$ we have that $K_j^{(0)} = \chi_0(\varepsilon_0) K_j^{(0)}$. Thus the operators $\overset{o}{\chi}\, K_j^{(0)}$ are H- and H_0-smooth. In case $a = \alpha$ we have that $\mathbf{M}^{(\alpha)}(x) = 0$ if $x \in \Gamma_\beta(\epsilon), \beta \neq \alpha$, and hence, by (3.5) ,

$$K_j^{(\alpha)} = \chi_0(\varepsilon) K_j^{(\alpha)} + \chi_\alpha(\varepsilon) K_j^{(\alpha)}, \quad \forall \varepsilon \in (0, \epsilon).$$

Consequently, in order to obtain H-and H_α-smoothness of $\overset{o}{\chi}\, K_j^{(\alpha)}$ we must additionally consider only $\overset{o}{\chi}_\alpha\, (\varepsilon)K_j^{(\alpha)}$ for any $\varepsilon > 0$. Note that $m^{(\alpha)}(x) = m(x) = \mu_\alpha |x_\alpha|$ if $x \in \overset{o}{\Gamma}_\alpha\, (\epsilon_\alpha)$. In virtue of (3.14) for such x

$$(K_j^{(\alpha)}u)(x) = \mu_\alpha^{1/2}|x_\alpha|^{-1/2}(\nabla_{x_\alpha}^{(s)}u)(x)$$

(in this case all eigenvalues of $\mathbf{M}^{(\alpha)}(x)$, except zero, equal $\mu_\alpha|x_\alpha|^{-1}$) so that

$$|(\overset{o}{\chi}_\alpha\, (\varepsilon)K_j^{(\alpha)}u)(x)| \le C|(G_\alpha(\varepsilon)u)(x)|, \quad \varepsilon \le \epsilon_\alpha.$$

Therefore the H- and H_α-smoothness of the operators $\overset{o}{\chi}_\alpha\, (\varepsilon)K_j^{(\alpha)}$ is ensured again by Theorem 3.5. This concludes the proof of the required factorization of the right side of (4.4) into a product of H- and H_a-smooth operators.□

Let us now introduce the observable

$$M^\pm = M^\pm(\Lambda) := W^\pm(H,H;ME(\Lambda)). \tag{4.7}$$

Existence of these wave operators can be verified similarly to Theorem 4.2. Actually, let us consider

$$HM - MH = [T,M] + \sum_\alpha [V^\alpha, M].$$

The main contribution to $[T,M]$ is determined by the operator $L = K_2^*K_1$, where K_j are constructed by the formulas (4.5) in terms of eigenvalues $\lambda_n(x)$ and eigenvectors $p_n(x)$ of the matrix $\mathbf{M}(x)$. For any $\varepsilon > 0$ H-smoothness of the operators $\overset{o}{\chi}_0\, (\varepsilon)K_j$ is ensured by H-smoothness of the operator $G_0(\varepsilon)$. Similarly, H-smoothness of $\overset{o}{\chi}_\alpha\, (\epsilon_\alpha)K_j$ is ensured by H-smoothness of $G_\alpha(\epsilon_\alpha)$. Remaining terms in $[T,M]$ are estimated by Proposition 2.13. Finally, we apply Proposition 3.4 to the commutators $[V^\alpha, M]$. Note that potentials V^α may contain long-range parts since the short-range assumption was used in Theorem 4.2 only for the estimate of the term $V^\beta M^{(a)}$, $\beta \neq a$, which is absent now. Thus we have

Proposition 4.3 *Let M be the same operator as in section 3. Suppose that functions (2.5) satisfy Assumptions 2.2 and 2.3. Then the wave operators (4.7) exist.*

The operator $M^\pm(\Lambda)$ is, clearly, self-adjoint, bounded and commutes with H. Our goal is to show that it is invertible on the subspace $E(\Lambda)\mathcal{H}$. In fact, we shall see that $\pm M^\pm(\Lambda)$ is positively definite.

Let us give a classical interpretation of this assertion for a particle (of mass 1/2) in an external field. In this case the observable $U^*(t)MU(t)$ corresponds, in the Heisenberg picture of motion, to the projection $\mathcal{M}(t) =$

$|x(t)|^{-1}\langle\xi(t), x(t)\rangle$ of the momentum $\xi(t)$ of a particle on a vector $x(t)$ of its position. For positive energies λ and large t we have that $\xi(t) \sim \xi_\pm, \xi_\pm^2 = \lambda$, and $x(t) \sim 2\xi_\pm t + x_\pm$. Therefore $\mathcal{M}(t)$ tends to $\pm\lambda^{1/2}$ as $t \to \pm\infty$.

We shall consider $U(t)$ on elements $f = \varphi(H)g$ where $\varphi \in C_0^\infty(\Lambda)$ and $g \in \mathcal{D}(Q)$. Clearly, for different φ and g such elements are dense in $E(\Lambda)\mathcal{H}$. By Lemma 2.10 applied to $\psi(\lambda) = \exp(-i\lambda t)\varphi(\lambda)$, we have that $U(t)f \in \mathcal{D}(Q)$. Thus $mU(t)f$ are well defined.

Let $f_t = U(t)f$ and $h_t = U(t)h$ where $h \in \mathcal{H}$ is arbitrary. Integrating the identity

$$d(mf_t, h_t)/dt = i([H,m]f_t, h_t) = i([T,m]f_t, h_t) = (Mf_t, h_t),$$

we find that

$$(mf_t, h_t) = (mf, h) + \int_0^t (Mf_s, h_s)ds. \tag{4.8}$$

According to Proposition 4.3

$$|(Mf_s, h_s) - (M^\pm f, h)| \le \varepsilon(s)\|h\|, \tag{4.9}$$

where $\varepsilon(s)$ does not depend on h and tends to zero as $s \to \pm\infty$. Comparing (4.8) and (4.9) we obtain

Lemma 4.4 *Let $f = \varphi(H)g$ where $\varphi \in C_0^\infty(\Lambda)$ and $g \in \mathcal{D}(Q)$. Then*

$$U^*(t)mU(t)f = t\, M^\pm(\Lambda)f + o(|t|), \quad t \to \pm\infty.$$

Since $m \ge 0$, Lemma 4.4 implies that

$$\pm(M^\pm f, f) = \lim_{t\to\pm\infty} |t|^{-1}(mf_t, f_t) \ge 0.$$

The inequality $\pm(M^\pm f, f) \ge 0$ established on the dense set extends by continuity to the whole space $E(\Lambda)\mathcal{H}$. Thus we have

Corollary 4.5 *The operator $M^\pm(\Lambda) \ge 0$.*

To prove that $\pm M^\pm$ is positively definite we use Proposition 2.4. In virtue of the identity $i[H, Q^2] = 2A$, it follows from (2.8) that

$$2^{-1}d^2(Q^2 f_t, f_t)/dt^2 = d(Af_t, f_t)/dt = (i[H,A]f_t, f_t) \ge c\,\|f\|^2,$$
$$f = \varphi(H)g, \quad \varphi \in C_0^\infty(\Lambda_\lambda), \quad g \in \mathcal{D}(Q).$$

Integrating twice this inequality we find that for sufficiently large $|t|$

$$\|Qf_t\| \ge c\,|t|\,\|f\|. \tag{4.10}$$

On the other hand, according to Lemma 4.4

$$\|mf_t\| = \|M^\pm f\|\,|t| + o(|t|). \tag{4.11}$$

By property 2^0, $m(x) \geq m_0|x|$, $m_0 > 0$, $|x| \geq 1$, so that

$$\|Qf_t\|^2 \leq 2\|f_t\|^2 + m_0^{-2}\|mf_t\|^2.$$

Thus comparing (4.10) with (4.11) we obtain the inequality

$$\|M^{\pm}f\| \geq c\,\|f\|, \tag{4.12}$$

where $f = \varphi(H)g$, $g \in \mathcal{D}(Q)$, $\varphi \in C_0^\infty(\Lambda_\lambda)$ and $c = c_\lambda$. This inequality is, of course, true for all $f \in E(\Lambda_\lambda)\mathcal{H}$. The compact set $\bar{\Lambda}$ is covered by finite number of intervals Λ_λ. Since $M^{\pm}$ commutes with $E(\cdot)$, it follows that (4.12) extends to all $f \in E(\Lambda)\mathcal{H}$. Considering now Corollary 4.5 we obtain

Proposition 4.6 *Under the assumptions of Proposition 4.3 for every $f \in E(\Lambda)\mathcal{H}$*

$$\pm(M^{\pm}(\Lambda)f, f) \geq c\,\|f\|^2, \quad c = c(\Lambda) > 0.$$

Corollary 4.7 *In the space $E(\Lambda)\mathcal{H}$ the kernel of $M^{\pm}(\Lambda)$ is trivial and its range*

$$R(M^{\pm}(\Lambda)) = E(\Lambda)\mathcal{H}.$$

5. EXISTENCE AND COMPLETENESS OF WAVE OPERATORS

In this section we give the proof of Theorem 2.7. Its difficult part is, of course, asymptotic completeness. Actually, the relation (2.12) can be reformulated in basically equivalent form without wave operators (2.11). We start with the proof of this form of asymptotic completeness called asymptotic clustering in [10]. Let, as always, Λ be a bounded interval such that $\bar{\Lambda} \cap \Upsilon = \emptyset$ and let M and $M^{(a)}$ be defined by (3.1) and (4.2), respectively. According to (4.1)

$$\sum_a M^{(a)} = M, \quad 0 \leq a \leq \alpha_1. \tag{5.1}$$

Theorem 5.1 *Under the assumptions of Theorem 2.7 for every $f = E(\Lambda)f$ there exist elements $f_a^{\pm}$ such that*

$$U(t)f \sim \sum_a U_a(t)f_a^{\pm}, \quad t \to \pm\infty. \tag{5.2}$$

Proof. – By Corollary 4.7, every $f \in E(\Lambda)\mathcal{H}$ admits the representation $f = M^{\pm}(\Lambda)f^{\pm}$, $f^{\pm} \in E(\Lambda)\mathcal{H}$, so that the asymptotic relation

$$U(t)f \sim MU(t)f^{\pm}, \quad t \to \pm\infty, \tag{5.3}$$

holds. On the other hand, Theorem 4.2 ensures that for every $a = 0, 1, \dots, \alpha_1$

$$M^{(a)}U(t)f^{\pm} \sim U_a(t)f_a^{\pm}, \quad t \to \pm\infty, \tag{5.4}$$

where

$$f_a^{\pm} = W^{\pm}(H_a, H; M^{(a)}E(\Lambda))f^{\pm}.$$

Summing up the relations (5.4) and taking into account (5.1) we find that

$$MU(t)f^{\pm} \sim \sum_a U_a(t)f_a^{\pm}, \quad t \to \pm\infty.$$

Comparing it with (5.3) we arrive at (5.2). □

To complete the proof of Theorem 2.7 we need to establish existence of wave operators (2.11). Note that in the proof of Theorem 5.1 we have used only existence of the second set of wave operators (4.3). Now we rely on existence of $W^{\pm}(H, H_a; M^{(a)}E_a(\Lambda))$. Since elements $f = E_a(\Lambda)f$ are dense in the space $\mathcal{H} = \mathcal{H}^{(ac)}(H_a)$, this is equivalent to existence of the wave operators

$$W^{\pm}(H, H_a; M^{(a)}(H_a + i)^{-1}).$$

Here $-i$ can, of course, be replaced by an arbitrary regular point of H_a. Some minor technical complications below are related to unboundedness of the operators $M^{(a)}$. We start with some simple auxiliary assertions.

Lemma 5.2 *Let $V^\alpha(T^\alpha + I)^{-1}$ be compact in $\mathcal{H}^\alpha$. Then*

$$s - \lim_{|t|\to\infty} V^\alpha U_0(t)(H_0 + i)^{-1} = 0.$$

Proof. – In terms of the tensor product (2.9)

$$V^\alpha U_0(t)(T^\alpha + I)^{-1} = \exp(-iT_\alpha t) \otimes V^\alpha(T^\alpha + I)^{-1} \exp(-iT^\alpha t).$$

According to (2.1), the second factor in the right side converges strongly to zero. Therefore the tensor product also tends strongly to zero. It remains to remark that $(T_\alpha + I)(H_0 + i)^{-1}$ is bounded. □

Lemma 5.3 *Let $\alpha = 1, \dots, \alpha_1$. Suppose that ζ_α is a bounded function such that $\zeta_\alpha(x) = 0$ if $x \in \Gamma_\alpha(\varepsilon)$ for some $\varepsilon > 0$. Then*

$$s - \lim_{|t|\to\infty} \zeta_\alpha U_\alpha(t)P_\alpha = 0, \tag{5.5}$$

$$s - \lim_{|t|\to\infty} \zeta_\alpha \nabla U_\alpha(t)P_\alpha(H_\alpha + i)^{-1} = 0. \tag{5.6}$$

Proof. – It suffices to check (5.5) on elements $f = g \otimes \psi^\alpha$, where ψ^α is an eigenvector of the operator $H^\alpha, H^\alpha \psi^\alpha = \lambda^\alpha \psi^\alpha$, g is an arbitrary element of $\mathcal{H}_\alpha$ and the tensor product is defined by (2.9). Linear combinations of such elements f are dense in the space $P_\alpha \mathcal{H}$. According to (2.10)

$$U_\alpha(t)f = \exp(-i(T_\alpha + \lambda^\alpha))g \otimes \psi^\alpha \tag{5.7}$$

so that

$$\|\zeta_\alpha U_\alpha(t) f\| = \|\Psi_\alpha \exp(-iT_\alpha t) g\|_{\mathcal{H}_\alpha}, \tag{5.8}$$

where

$$\Psi_\alpha^2(x_\alpha) = \int_{X^\alpha} |\zeta_\alpha(x_\alpha, x^\alpha)|^2 |\psi^\alpha(x^\alpha)|^2 dx^\alpha \le C \int_{|x^\alpha| \ge c|x_\alpha|} |\psi^\alpha(x^\alpha)|^2 dx^\alpha,$$

$c = c(\varepsilon) > 0$, by our assumptions on ζ_α. It follows that $\Psi_\alpha(x_\alpha) \to 0$ as $|x_\alpha| \to \infty$ and hence the operator $\Psi_\alpha(T_\alpha + I)^{-1}$ is compact in the space $\mathcal{H}_\alpha$. Therefore (5.8) tends to zero in virtue of (2.1).

Let us split the vector equality (5.6) into two parts corresponding to ∇_{x_α} and ∇_{x^α} (instead of ∇). The operator ∇_{x_α} commutes with $U_\alpha(t) P_\alpha$ and $\nabla_{x_\alpha}(H_\alpha + i)^{-1} \in \mathcal{B}$. So the part of (5.6) for ∇_{x_α} is a consequence of (5.5). To verify the same for ∇_{x^α} we remark that

$$\|\nabla_{x^\alpha} U_\alpha(t) P_\alpha (H_\alpha + i)^{-1}\| \le \|\nabla_{x^\alpha}(H_\alpha + i)^{-1}\| < \infty$$

because $(H_\alpha + i)^{-1}$ commutes with $U_\alpha(t)P_\alpha$ and $\nabla_{x^\alpha}(H_\alpha + i)^{-1} \in \mathcal{B}$. Hence it suffices again to consider this limit on elements $f = g \otimes \psi^\alpha$. In this case $(H_\alpha + i)^{-1} f = \tilde{g} \otimes \psi^\alpha$, where $\tilde{g} = (T_\alpha + \lambda^\alpha + i)^{-1} g \in \mathcal{H}_\alpha$. Thus, by (5.7),

$$\zeta_\alpha \nabla_{x^\alpha} U_\alpha(t) P_\alpha (H_\alpha + i)^{-1} f = \zeta_\alpha \exp(-i(T_\alpha + \lambda^\alpha)) \tilde{g} \otimes \nabla_{x^\alpha} \psi^\alpha.$$

Since $\nabla_{x^\alpha}\psi^\alpha \in \mathcal{H}^\alpha \otimes \mathbb{C}^{d^\alpha}$, this term can be estimated quite similarly to (5.8).□

Corollary 5.4 *For every $\alpha = 1, \dots, \alpha_1$ and $b \neq \alpha$*

$$s - \lim_{|t| \to \infty} M^{(b)} U_\alpha(t) P_\alpha (H_\alpha + i)^{-1} = 0. \tag{5.9}$$

Proof. – According to (4.2)

$$iM^{(b)} = 2(\nabla m^{(b)})\nabla + \Delta m^{(b)}, \tag{5.10}$$

where, by the construction of $m^{(b)}$, the zero-degree homogeneous function $\nabla m^{(b)}$ vanishes in the cone $\Gamma_\alpha(\epsilon_\alpha)$. The contribution to (5.9) of the first term in the right side of (5.10) tends to zero in virtue of (5.6). The term $(\Delta m^{(b)})U_\alpha(t)$ converges strongly to zero because $(\Delta m^{(b)})(x) \to 0$ as $|x| \to \infty$. □

Now we are able to prove

Lemma 5.5 *The wave operators*

$$W^{\pm}(H, H_a; M^{(b)}(H_a + i)^{-1}) \tag{5.11}$$

exist for all $a, b = 0, 1, \ldots, \alpha_1$.

Proof. – According to Theorem 4.2 it suffices to consider the case $a \neq b$ only. Let first $a = 0$ and $b = \beta \neq 0$. By the multiplication theorem (2.4), the wave operator

$$W^{\pm}(H, H_0; M^{(\beta)}(H_\beta + i)^{-1}) = W^{\pm}(H, H_\beta; M^{(\beta)}(H_\beta + i)^{-1})W^{\pm}(H_\beta, H_0)$$

exists. Here we have taken into account that the wave operators in the right side exist in virtue of Theorem 4.2 and Proposition 2.8. Therefore in order to establish existence of $W^{\pm}(H, H_0; M^{(\beta)}(H_0 + i)^{-1})$ it remains to verify that

$$s - \lim_{|t| \to \infty} M^{(\beta)}((H_\beta + i)^{-1} - (H_0 + i)^{-1})U_0(t) = 0. \tag{5.12}$$

In virtue of the resolvent identity this is a direct consequence of Lemma 5.2.

In case $a = \alpha \neq 0$ and $b \neq \alpha$ we proceed from the relation (2.13). Let us apply to it the bounded operator $M^{(\beta)}(H_\alpha + i)^{-1}$. In virtue of Corollary 5.4 it follows that

$$M^{(b)}(H_\alpha + i)^{-1}U_\alpha(t)f \sim M^{(b)}(H_\alpha + i)^{-1}U_0(t)f_0^{\pm}, \quad t \to \pm\infty.$$

Furthermore, according to Lemma 5.2, we can replace (cf. with (5.12)) the operator $(H_\alpha + i)^{-1}$ in the right side by $(H_0 + i)^{-1}$. Therefore the existence of the wave operators (5.11) for $a \neq 0$ is ensured by their existence for $a = 0$.□

Corollary 5.6 *The wave operators* $W^{\pm}(H, H_a; M(H_a + i)^{-1})$ *exist for all* $a = 0, 1, \ldots, \alpha_1$.

Proof. – It suffices to "sum up" the wave operators (5.11) over all $b = 0, 1, \ldots, \alpha_1$ and to take into account the relation (5.1). □

Now we can get rid of the identification M.

Proposition 5.7 *The wave operators* $W^{\pm}(H, H_a)$ *exist for all* $a = 0, 1, \ldots, \alpha_1$.

Proof. – By Proposition 4.3 there exists

$$M_a^{\pm}(\Lambda) = W^{\pm}(H_a, H_a; ME_a(\Lambda))$$

(here it is sufficient to assume that an interval Λ is bounded, $0 \notin \bar{\Lambda}$ and $\sigma^{(p)}(H^\alpha) \cap \bar{\Lambda} = \emptyset$ if $a = \alpha$). By Corollary 4.7, $E_a(\Lambda)\mathcal{H} = R(M_a^{\pm}(\Lambda))$ so that for every $f \in E_a(\Lambda)\mathcal{H}$

$$U_a(t)f \sim MU_a(t)f_a^{\pm}, \quad t \to \pm\infty, \quad f = M_a^{\pm}(\Lambda)f_a^{\pm}, \quad f_a^{\pm} \in E_a(\Lambda)\mathcal{H}.$$

Thus Corollary 5.6 ensures existence of $W^{\pm}(H, H_a; E_a(\Lambda))$ and hence of $W^{\pm}(H, H_a)$. □

Since P_a commutes with $U_a(t)$, we have

Corollary 5.8 *The wave operators (2.11) exist and are isometric on $P_a\mathcal{H}$.*

In order to check that the ranges of the operators (2.11) are orthogonal, we shall show that

$$\lim_{t\to\pm\infty}(U_a(t)P_af_a, U_b(t)P_bf_b) = 0, \quad a \neq b. \tag{5.13}$$

If $b = 0$ (so that $P_b = I$) and $a = \alpha$, then, by Proposition 2.8, the limit (5.13) exists and equals

$$(P_\alpha f_\alpha, W^{\pm}(H_\alpha, H_0)f_0) = 0.$$

Let now $b = \beta$ and $a = \alpha \neq \beta$. The relation (5.5) implies that

$$U_\alpha(t)P_\alpha f_\alpha \sim \chi_\alpha(\varepsilon)U_\alpha(t)P_\alpha f_\alpha, \quad |t| \to \infty, \quad \alpha = 1, \dots, \alpha_1,$$

where $\chi_\alpha(\varepsilon)$ is the characteristic function of the cone $\Gamma_\alpha(\varepsilon)$ and $\varepsilon \in (0,1)$ is arbitrary. So it remains to recall that $\chi_\alpha(\varepsilon)\chi_\beta(\varepsilon) = 0$ if $\alpha \neq \beta$ and $\varepsilon < \epsilon$.

Let us finally verify the relation (2.12). According to (5.2) and (2.13) for every $f \in E(\Lambda)\mathcal{H}$ and some elements $\tilde{f}_0^{\pm}, f_\alpha^{\pm}$ the representation

$$U(t)f \sim U_0(t)\tilde{f}_0^{\pm} + \sum_{\alpha=1}^{\alpha_1} U_\alpha(t)P_\alpha f_\alpha^{\pm}, \quad t \to \pm\infty,$$

holds. Since the wave operators (2.11) exist, it follows that

$$f = W_0^{\pm}\tilde{f}_0^{\pm} + \sum_{\alpha=1}^{\alpha_1} W_\alpha^{\pm} f_\alpha^{\pm}$$

and hence f belongs to the left side of (2.12). Considering that linear combinations of elements $f = E(\Lambda)f$ for all admissible Λ are dense in $\mathcal{H}^{(ac)}(H)$, we conclude the proof of Theorem 2.7.

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REFERENCES

[1] L. D. Faddeev, *Mathematical Aspects of the Three Body Problem in Quantum Scattering Theory*, Trudy MIAN **69**, 1963. (Russian)

[2] J. Ginibre and M. Moulin, Hilbert space approach to the quantum mechanical three body problem, Ann. Inst. H.Poincaré, A **21**(1974), 97-145.

[3] L. E. Thomas, Asymptotic completeness in two- and three-particle quantum mechanical scattering, Ann. Phys. **90** (1975), 127-165.

[4] K. Hepp, On the quantum-mechanical N-body problem, Helv. Phys. Acta **42**(1969), 425-458.

[5] I. M. Sigal, *Scattering Theory for Many-Body Quantum Mechanical Systems*, Springer Lecture Notes in Math. **1011**, 1983.

[6] R. J. Iorio and M. O'Carrol, Asymptotic completeness for multi-particle Schrödinger Hamiltonians with weak potentials, Comm. Math. Phys. **27** (1972), 137-145.

[7] T. Kato, Smooth operators and commutators, Studia Math. **31** (1968), 535-546.

[8] R. Lavine, Commutators and scattering theory I: Repulsive interactions, Comm. Math. Phys. **20**(1971), 301-323.

[9] R. Lavine, Completeness of the wave operators in the repulsive N-body problem, J. Math. Phys. **14** (1973), 376-379.

[10] I. M. Sigal and A. Soffer, The N-particle scattering problem: Asymptotic completeness for short-range systems, Ann. Math. **126** (1987), 35-108.

[11] G. M. Graf, Asymptotic completeness for N-body short-range quantum systems: A new proof, Comm. Math. Phys. **132** (1990), 73-101.

[12] V. Enss, Completeness of three-body quantum scattering, in: *Dynamics and processes*, P. Blanchard and L. Streit, eds., Springer Lecture Notes in Math. **103** (1983), 62-88.

[13] T. Kato, Wave operators and similarity for some non-self-adjoint operators, Math. Ann. **162** (1966), 258-279.

[14] Y. Saito, *Spectral Representation for Schrödinger Operators with Long-Range Potentials*, Springer Lecture Notes in Math. **727**, 1979.

[15] P. Constantin, Scattering for Schrödinger operators in a class of domains with noncompact boundaries, J. Funct. Anal. **44** (1981), 87-119.

[16] E. M. Il'in, Scattering by unbounded obstacles for elliptic operators of second order, Proc. of the Steklov Inst. of Math. **179** (1989), 85-107.

[17] D. R. Yafaev, Remarks on the spectral theory for the multiparticle type Schrödinger operator, J. Soviet Math. **31** (1985), 3445-3459 (translated from Zap. Nauchn. Sem. LOMI **133** (1984), 277-298).

[18] S. Agmon, *Lectures on Exponential Decay of Solutions of Second-Order Elliptic Equations*, Math. Notes, Princeton Univ. Press, 1982.

[19] M. Reed and B. Simon, *Methods of Modern Mathematical Physics* IV, Academic Press, 1978.

[20] E. Mourre, Absence of singular spectrum for certain self-adjoint operators, Comm. Math. Phys. **78** (1981), 391-400.

[21] P. Perry, I. M. Sigal and B. Simon, Spectral analysis of N-body Schrödinger operators, Ann. Math. **144** (1981), 519-567.

[22] R. Froese, I. Herbst, A new proof of the Mourre estimate, Duke Math. J. **49** (1982), 1075-1085.

[23] D. R. Yafaev, *Mathematical Scattering Theory*, Amer. Math. Soc., 1992.

[24] I. Herbst and E. Skibsted, Radiation conditions - the free channel N-body case, Aarhus University preprint, 1991.

[25] P. Deift and B. Simon, A time-dependent approach to the completeness of multiparticle quantum systems, Comm. Pure Appl. Math. **30** (1977), 573-583.

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