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MICROLOCAL ESTIMATES OF THE STATIONARY SCHRÖDINGER EQUATION IN SEMI-CLASSICAL LIMIT

by

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Abstract. — We give a new proof for microlocal resolvent estimates for semi-classical Schrödinger operators, extending the known results to potentials with local singularity and to those depending on a parameter. These results are applied to the study of the stationary Schödinger equation with the approach of semi-classical measures. Under some weak regularity assumptions, we prove that the stationary Schrödinger equation tends to the Liouville equation in the semi-classical limit and that the associated semi-classical measure is unique with support contained in an outgoing region.

Résumé **(Estimations microlocales de l'équation de Schrödinger stationnaire en limite semi-classique)**

Nous présentons une nouvelle démonstration pour les estimations microlocales de l'opérateur de Schrödinger semi-classique, qui permet de généraliser les résultats connus aux potentiels avec singularité locale et aux potentiels dépendant d'un paramètre. Nous appliquons ces résultats à l'étude de l'équation de Schödinger stationnaire par l'approche de mesure semi-classique. Sous des hypothèses faibles sur la régularité du potentiel, nous montrons que l'équation de Schrödinger stationnaire converge vers l'équation de Liouville en limite semi-classique et que la mesure semi-classique est unique et de support inclus dans une région sortante.

1. Introduction

Microlocal resolvent estimates for two-body Schrödinger operators were firstly studied by Isozaki and Kitada in [**19, 24**] for smooth potentials. These results are useful in the study of scattering problems. For semi-classical Schrödinger operators, under a non-trapping assumption on the classical Hamiltonian, microlocal resolvent estimates were obtained in [**36**]. The method of [**36**] consists in comparing the total resolvent with the free one, using the global parametrix in form of Fourier integral operators. Here we want to give a more elementary proof of such results which allows to treat

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potentials with local singularity or depending on a parameter. We will apply these estimates to study the semi-classical measure of stationary Schrödinger equation, which is motivated by the recent works on the high frequency Helmholtz equation with a source term having concentration or concentration-oscillation phenomena.

Let $P(h) = -h^2\Delta + V(x)$ with V a smooth long-range potential verifying $V \in C^\infty(\mathbb{R}^d;\mathbb{R})$ and for some $\rho > 0$

$$|\partial^\alpha V(x)| \leq C_\alpha \langle x\rangle^{-\rho-|\alpha|}, \quad x \in \mathbb{R}^n, \tag{1.1}$$

for any $\alpha \in \mathbb{N}^n$. Here $h > 0$ is a small parameter and $\langle x\rangle = (1+|x|^2)^{1/2}$. $P(h)$ is self-adjoint in $L^2(\mathbb{R}^n)$. Let $R(z,h) = (P(h)-z)^{-1}$ for $z \notin \sigma(P(h))$. Let $b_\pm(.,.)$ be bounded smooth symbols with supp $b_\pm \subset \{(x,\xi) \in \mathbb{R}^{2n};\ \pm x\cdot\xi > -(1-\epsilon)|x||\xi|\}$ for some $\epsilon > 0$. Denote by $b_\pm(x,hD)$ the h-pseudo-differential operators with symbol $b_\pm$ defined by

$$(b_\pm(x,hD)u)(x) = \frac{1}{(2\pi h)^d}\int_{\mathbb{R}^n} e^{ix\cdot\xi/h} b_\pm(x,\xi)\hat{u}(\xi)\ d\xi, \tag{1.2}$$

where $u \in \mathcal{S}(\mathbb{R}^d)$ and $\hat{u}$ is the Fourier transform of u. We denote by $b^w(x,hD)$ the Weyl quantization of b

$$(b^w_\pm(x,hD)u)(x) = \frac{1}{(2\pi h)^n}\int_{\mathbb{R}^{2d}} e^{i(x-y)\cdot\xi/h} b_\pm((x+y)/2,\xi)u(y)\ d\xi dy. \tag{1.3}$$

At the level of principal symbols in the semi-classical limit $h \to 0$, the two quantizations are equivalent.

Let $p(x,\xi)$ denote the classical Hamiltonian $p(x,\xi) = \xi^2 + V(x)$ and

$$t \to (x(t;y,\eta), \xi(t;y,\eta))$$

be solutions of the Hamiltonian system associated with $p(x,\xi)$:

$$\left\{\begin{array}{rcl} \frac{\partial x}{\partial t} &=& \partial_\xi p(x,\xi), \quad x(0;y,\eta) = y, \\ \frac{\partial \xi}{\partial t} &=& -\partial_x p(x,\xi), \quad \xi(0;y,\eta) = \eta. \end{array}\right. \tag{1.4}$$

$E > 0$ is called a non-trapping energy for the classical Hamiltonian $p(x,\xi) = |\xi|^2 + V(x)$ if

$$\lim_{|t|\to\infty} |x(t;y,\eta)| = \infty, \quad \forall\ (y,\eta) \in p^{-1}(E). \tag{1.5}$$

The one-sided microlocalized resolvent estimate says that if $E > 0$ is a non-trapping energy, then one has for any $s > 1/2$

$$\|\langle x\rangle^{s-1} b_\mp(x,hD)R(E \pm i0,h)\langle x\rangle^{-s}\| \leq C_s h^{-1} \tag{1.6}$$

uniformly in $h > 0$ small enough. Here

$$R(E \pm i0,h) = \lim_{\epsilon\downarrow 0}(P(h) - E \mp i\epsilon)^{-1},$$

and $\|\cdot\|$ denotes the norm of bounded operators on $L^2(\mathbb{R}^n)$. Recall that without microlocalization, one can only have an estimate like

$$\|\langle x\rangle^{-s} R(E \pm i0, h)\langle x\rangle^{-s}\| \leq C_s h^{-1}. \tag{1.7}$$

See [**33**]. With microlocalization, one can overcome some difficulties related to the lack of decay. There are also two-sided microlocal resolvent estimates in semi-classical limit. See [**37**] for potentials satisfying (1.1).

The recent interest in uniform resolvent estimates arises from the study of propagation of semi-classical measure related to the high frequency Helmoltz equation. Recall that the Helmholtz equation describes the propagation of light wave in material medium. It appears in the design of very high power laser devices such as Laser Méga-Joule in France or the National Ignition Facility in the USA. The laser field, $A(x)$, can be very accurately modelled and computed by the solution of the Helmholtz equation

$$\Delta A(x) + k_0^2(1 - N(x))A(x) + ik_0\nu(x)A(x) = 0 \tag{1.8}$$

where k_0 is the wave number of laser in vacuum, $N(x)$ is a smooth positive function representing the electronic density of material medium and $\nu(x)$ is positive smooth function representing the absorption coefficient of the laser energy by material medium. Since laser can not propagate in the medium with the electronic density bigger than 1, it is assumed that $0 \leq N(x) < 1$. The equation (1.8) may be posed in an unbounded domain with a known incident excitation A_0. The equation is then complemented by a radiation condition. The highly oscillatory behavior of the solution to the Helmholtz equation makes the numerical resolution of (1.8) unstable and rather expensive. See [**3**]. Fortunately, the wave length of laser in vacuum, $\frac{2\pi}{k_0}$, is much smaller than the scale of N. It is therefore natural and important to study the Helmholtz equation in the high frequency limit $k_0 \to \infty$. To be simple, instead of studying boundary value problem related to a non-self-adjoint operator, one studies the high frequency Helmholtz equation with a source term

$$(\Delta + \epsilon^{-2}n(x)^2 + i\epsilon^{-1}\alpha_\epsilon)u_\epsilon(x) = -S_\epsilon(x) \tag{1.9}$$

in $\mathbb{R}^d$, $d \geq 1$. Here $n(x)$ is the refraction index, $\epsilon \sim \frac{1}{k_0} > 0$ is regarded as a small parameter, $\alpha_\epsilon \geq 0$ and

$$\lim_{\epsilon\to 0} \alpha_\epsilon = \alpha \geq 0. \tag{1.10}$$

In [**4, 8, 40**], α_ϵ is assumed to be a regularizing parameter :

$$\text{if } \alpha = 0, \exists\gamma \in]0,1[\text{ such that } \alpha_\epsilon \geq \epsilon^\gamma. \tag{1.11}$$

Motivated by this model, we study in this work the Schrödinger equation

$$(-h^2\Delta + V(x) - (E + i\kappa))u_h = S^h(x) \tag{1.12}$$

by the Wigner's approach or the approach of semi-classical measures. Here $E > 0$, $\kappa = \kappa(h) \geq 0$ and $\kappa \to 0$ as $h \to 0$. To prove the existence of a limiting Liouville equation when $h \to 0$, we assume that $\alpha_h = \kappa h^{-1}$ satisfies (1.10) with $\epsilon = h \to 0$. The condition (1.11) is not needed in this work: when $\kappa = 0$, u_h is defined as the unique outgoing (or incoming) solution of (1.12) for each $h \in]0,1]$. Note that (1.12) is a scattering problem, since the behavior of $(-h^2\Delta + V - (E + i\kappa))^{-1}$ for κ near 0 is closely related to the long-time behavior of the unitary group

$$U(t,h) = e^{-itP(h)/h}$$

as $t \to \infty$.

In the study of semi-classical measures associated to u_h, the uniform resolvent estimate plays an important role. See [**4, 9, 8, 10, 40**]. Under some technical conditions, the microlocal estimates are used in [**40**] to overcome the difficulty due to the lack of decay for the source term with concentration-oscillation over a hyperplane.

In these notes, we recall in Section 2 some abstract results on the uniform limiting absorption principle. In Section 3, we give a new proof of microlocal resolvent estimates in the semi-classical limit, using the Mourre's method and symbolic calculus of h-pseudo-differential operators. For fixed h, related ideas have appeared in [**12, 21, 34, 38**]. Our approach combines these ideas and the method used in the semi-classical resolvent estimates [**11, 13, 33, 38**]. The same ideas can be applied to potentials with singularities and potentials depending on a parameter. In Subsection 4.3, we apply the results on uniform resolvent estimates to the study of the equation (1.12) with the second hand side concentrated near one point. We prove that the outgoing solution of (1.12), when microlocalized in an incoming region, is uniformly bounded in L^2. The convergence of (1.12) to the limiting Liouville equation is proved under the assumption on the uniform continuity of V, ∇V and $x \cdot \nabla V$. The microlocal estimates for (1.12) give rise to some strong radiation property of the semi-classical measure associated with u_h, from which we derive the uniqueness of the semi-classical measure. The decay of the potential V is not needed. The results of Subsection 4.3 hold for a large class of N-body potentials of the form

$$V(x) = \sum_a V_a(x^a),$$

where x^a is part of the variables $x \in \mathbb{R}^d$.

The pre-requests of these lecture notes are contained in the books [**18, 31**] and [**32**]. The symbolic and functional calculi for h-pseudo-differential operators will be frequently used and can be found in [**31**]. To be self-contained, some known results are recalled here. In particular, the results of Section 2 are contained in a joint work with P. Zhang [**40**] and those of Subsections 4.1 and 4.2 are based on [**14, 16, 26**].

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2. Some abstract results

2.1. Mourre's method depending on a parameter. — We first state a parameter dependent version of Mourre's method which is an important tool in quantum scattering theory. Given two families $\{P_\epsilon\}$, $\{A_\epsilon\}$, $\epsilon \in]0,1]$, in some Hilbert space H, we shall say A_ϵ is uniformly conjugate operator of P_ϵ on an interval $I \subset \mathbb{R}$ if the following properties are satisfied:

1. Domains of P_ϵ and A_ϵ are independent of ϵ: $D(P_\epsilon) = D_1, D(A_\epsilon) = D_2$. For each ϵ, $D = D_1 \cap D_2$ is dense in D_1 in the graph norm
$$\|u\|_{\Gamma_\epsilon} = \|P_\epsilon u\| + \|u\|.$$
2. The unitary group $e^{i\theta A_\epsilon}$, $\theta \in \mathbb{R}$ is bounded from D_1 into itself and
$$\sup_{\epsilon\in]0,1],|\theta|\le 1} \|e^{i\theta A_\epsilon} u\|_{\Gamma_\epsilon} < \infty, \quad \forall u \in D_1.$$
3. The quadratic form $i[P_\epsilon, A_\epsilon]$ defined on D is bounded from below and extends to a self-adjoint operator B_ϵ with $D(B_\epsilon) \supset D_1$ and B_ϵ is uniformly bounded from D_1 to H, *i.e.* $\exists C > 0$ such that
$$\|B_\epsilon u\| \le C\|u\|_{\Gamma_\epsilon}, \quad u \in D_1$$
uniformly in ϵ.
4. The quadratic form defined by $i[B_\epsilon, A_\epsilon]$ on D extends to a uniformly bounded operator from D_1 to H.
5. (Uniform Mourre's estimate) There is $m_\epsilon > 0$ such that

$$E_I(P_\epsilon) i[P_\epsilon, A_\epsilon] E_I(P_\epsilon) \ge m_\epsilon E_I(P_\epsilon) \tag{2.13}$$

Remark that the usual Mourre's estimate is of the form

$$E_I(P) i[P, A] E_I(P) \ge E_I(P)(c_0 + K) E_I(P), \tag{2.14}$$

for some $c_0 > 0$ and K a compact operator. If $E \notin \sigma_p(P)$, $E_I(P)$ tends to 0 strongly, as the length of I tends to 0. So, one can take $\delta > 0$ small enough so that $E_I(P) i[P, A] E_I(P) \ge c_1 E_I(P)$ for $I = [E - \delta, E + \delta]$ with $\delta > 0$ sufficiently small and for some $c_1 > 0$. For Mourre's method independent of parameter, see [**21, 22, 27, 28**] and also [**2**] for more information.

In some estimates, we need the following condition on multiple commutators:

(2.15) $\quad (P_\epsilon + i)^{-1} B_j(\epsilon)(P_\epsilon + i)^{-1}$ extends to uniformly bounded operators on H

for $1 \le j \le n$, $n \in \mathbb{N}^*$. Here $B_0(\epsilon) = B_\epsilon$ and $B_j(\epsilon) = [B_{j-1}(\epsilon), A_\epsilon]$ for $j \ge 1$. The following parameter-dependent estimates are useful in many situations.