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RESONANCE THEORY FOR PERIODIC SCHRÖDINGER OPERATORS

BY

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RÉSUMÉ. — Nous étudions le prolongement analytique de la résolvante $(H-\lambda)^{-1}$ pour un opérateur de Schrödinger périodique H. Nous montrons que $(H-\lambda)^{-1}$ s'étend à travers le spectre de H au complémentaire d'un ensemble discret de points, appelés *singularités de Van Hove* en physique du solide. Les singularités de Van Hove sont les points où la surface de Fermi complexifiée n'est pas lisse et sont en général des points de branchement pour $(H-\lambda)^{-1}$. Nous étudions aussi la relation des singularités de Van Hove avec la structure de bande du spectre, les singularités de la densité d'états et les résonances créées par des impuretés.

ABSTRACT. — We study the problem of analytic extension of the resolvent $(H-\lambda)^{-1}$ for H a periodic Schrödinger operator. We prove that $(H-\lambda)^{-1}$ extends across the spectrum of H to the complementary of a discrete set of points, called *Van Hove singularities* in solid state physics. The Van Hove singularities are roughly the points where the (complex) Fermi surface is not smooth, and are usually branch points of $(H-\lambda)^{-1}$. We study also the relationship of the Van Hove singularities with the band structure of the spectrum, the singularities of the density of states, and the resonances created by impurities.

Introduction

We study in this paper the theory of resonances for Schrödinger operators with periodic potentials. We consider Hamiltonians of the following form :

$$H = -\Delta + V(x) \quad \text{on } \mathbb{R}^n,$$

where V is a real multiplicative potential which is periodic with respect to some lattice T in $\mathbb{R}^n$.

We want to extend the resolvent $(H-\lambda)^{-1}$ from the physical region $\{\lambda \mid \operatorname{Im}\lambda > 0\}$ to the lower half plane across the bands of the spectrum of H, and study the singularities of this extension.

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The existence of such an extension is more or less tacitly assumed in solid state physics when one studies the resonances created by localized impurities. (See for example the book of CALLAWAY [C, chapter 5].)

We will consider two kinds of problems :

i) *local extension problem* : given $\lambda_0 \in \sigma(H)$, extend analytically $(H-\lambda)^{-1}$ to a small neighborhood of λ_0, and describe its singularities;

ii) *global extension problem* : given some open set $\mathcal{U}$ extend analytically $(H-\lambda)^{-1}$ to $\mathcal{U}$ and describe its singularities.

For the *local extension problem*, we prove that any $\lambda_0 \in \sigma(H)$, there exist some neighborhood $\mathcal{U}_{\lambda_0}$ of λ_0, and a finite set Σ of points which we call *Landau resonances* such that $(H-\lambda)^{-1}$ extends holomorphically to the universal covering of $\mathcal{U}_{\lambda_0} \setminus \Sigma$. The Landau resonances are usually branch points of $(H-\lambda)^{-1}$ instead of poles. We decided to call the points of Σ *Landau resonances* by analogy with Landau singularities in Feynman integrals. We learned afterwards that these singularities (at least for the density of states) are known in solid state physics as *Van Hove singularities.*

For the *global extension problem*, we have to add to Σ a closed set of measure zero Σ_∞ which corresponds to a complex essential spectrum (see Definition 4.6). Then $(H-\lambda)^{-1}$ extends holomorphically to the universal covering of $\mathcal{U} \setminus \Sigma \cup \Sigma_\infty$.

The Landau resonances can be described geometrically in the following way : in the study of periodic Schrödinger operators one introduces usually the *Fermi surface* S_λ for $\lambda \in \mathbb{R}$: S_λ is the set of Bloch numbers p such that λ is an eigenvalue of the reduced Hamiltonian H_p obtained by the Floquet-Bloch theory.

The *Bloch variety* is then the set $S = \{(p,\lambda) \mid p \in S_\lambda, \lambda \in \mathbb{R}\}$. The Bloch variety has an extension to complex energies and Bloch numbers, and is a complex analytic set. Then roughly Σ is the set of $\lambda \in \mathcal{U}$ such that the (complex) Fermi surface S_λ is not a union of smooth submanifolds. (See Definition 3.2.) So the Landau resonances have a simple geometric interpretation in terms of singularities of complex Fermi surfaces.

Another new feature of the Landau resonances in contrast to the resonances encountered in two-body Hamiltonians is that they are usually branch points of $(H-\lambda)^{-1}$ instead of poles.

Moreover, it can happen that the singular part of $(H-\lambda)^{-1}$ at a Landau resonance is not a finite rank operator. (See THEOREMS 3.5, 3.6.) In simple cases it is however possible to associate resonant eigenfunctions to the leading singularity of $(H-\lambda)^{-1}$ at a Landau resonance. (See COROLLARY 3.7.)

Σ_∞ looks more like essential spectrum in the sense that Σ_∞ acts as a natural boundary for the extension of $(H - \lambda)^{-1}$ between $L^2_a(\mathbb{R}^n)$ and $H^1_{-a}(\mathbb{R}^n)$ for fixed values of a. Σ_∞ comes in part from the fact that we integrate operator-valued functions and that we have to take care of domain considerations. To make this remark more clear, let us compare H with two-body Schrödinger operators with exponentially decreasing potentials.

In the last case, the resolvent can be extended meromorphically to a strip $\{\lambda \in \mathbb{C} \mid \operatorname{Im} \lambda > -\alpha\}$ for α depending on the rate of decay of the potential. Σ_∞ plays a role similar to $\operatorname{Im} \lambda = -\alpha$ in this problem.

In the last part of the paper we present some applications.

We study first the relationship of real Landau resonances with the band structure of the spectrum. We recover here some results obtained by BENTOSELA [B] in his study of time independent impurity scattering. (See THEOREM 4.1.)

We study then the analyticity properties of the density of states $d\rho/d\lambda$ and prove that $d\rho/d\lambda$ is analytic outside the real Landau resonances.

Finally, we study the resonances created by a localized impurity. We modelize the impurities by adding to V a potential W which is exponentially decreasing. This is not a severe limitation in view of the phenomenon of dielectric screening. (See [C].)

We prove that the impurities add usual poles on $(\mathcal{U} \setminus \Sigma \cup \Sigma_\infty)^*$ to the Landau resonances of $(H - \lambda)^{-1}$. As a consequence, we show that the singular continuous spectrum of $H + W$ is empty and that the eigenvalues can accumulate only at the real Landau resonances which play the role of threshold energies.

The plan of the paper is the following :

- In Section I, we recall the Floquet-Bloch reduction which will be used in the next sections.

- In Section II, we prove the meromorphic extension in the energy and Bloch numbers of the reduced resolvent $(H_p - \lambda)^{-1}$ using Fredholm theory.

- In Section III, we prove the main results of this paper using methods from complex analytic geometry.

- In Section IV, we apply these results to the band structure, to the density of states and to resonances created by impurities.

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1. The Floquet-Bloch reduction

In this section, we recall the Floquet-Bloch reduction of a periodic operator on $\mathbb{R}^n$ to a family of Schrödinger operators on a n-torus. We will follow the exposition of SKRIGANOV [Sk].

On $\mathbb{R}^n$ we consider the following Hamiltonian :

$$H = -\Delta + V(x),$$

where V is a real multiplicative potential which is T-periodic for some lattice T in $\mathbb{R}^n$, *i.e.* :

$$V(x+\tau) = V(x), \qquad \forall \tau \in T.$$

We will assume that V is $-\Delta$ bounded with relative bound strictly less than 1, so that H is self adjoint with domain $H^2(\mathbb{R}^n)$.

We denote by T^* the dual lattice of T, which is defined as follows : if $(a_1, \dots, a_n)$ is a basis for T, a basis for T^* is given by the $(b_1, \dots, b_n)$ such that $\langle a_i, b_j \rangle = 2\pi\delta_{ij}$, where $\langle\ ,\ \rangle$ is the Euclidean scalar product on $\mathbb{R}^n$.

We denote by F_T a fundamental domain of T, F_{T^*} a fundamental domain of T^* which are chosen to be diffeomorphic to the n-torus $\mathbb{T}^n$. μ_T (resp. μ_{T^*}) will be the Lebesgue measure of F_T (resp. F_{T^*}).

For $\varphi \in \mathcal{S}(\mathbb{R}^n)$, the Schwartz space of rapidly decreasing C^∞ functions, and for $p \in F_{T^*}$ we set :

$$K_p\varphi(x) = \mu_T^{1/2} \sum_{\tau \in T} \varphi(x+\tau) e^{i\langle p, x+\tau\rangle}. \tag{1.1}$$

The sum in (1.1) is convergent because of the rapid decay of φ and $K_p\varphi$ is T-periodic and satisfies the equations :

$$K_{p+p'}\varphi(x) = e^{i\langle p', x\rangle} K_p\varphi(x) \quad \text{for } p' \in T^*. \tag{1.2}$$

The family of operators K_p gives a unitary operator W_T :

$$L^2(\mathbb{R}^n) \longrightarrow \mathcal{L} = \int_{F_{T^*}}^{\oplus} L^2(F_T)\,dp$$
$$\varphi \longmapsto K_p\varphi(x).$$

Then since V is T periodic, it is well known that we can decompose H as a direct integral of operators :

$$W_T H W_T^{-1} = \int_{F_{T^*}}^{\oplus} H_p\,dp$$