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ON EFFECTIVE HAMILTONIANS FOR ADIABATIC PERTURBATIONS

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Abstract

We construct almost invariant subspaces and the corresponding effective Hamiltonian for magnetic Bloch bands. We assume that the magnetic and electric potentials are slowly varying perturbations of the potential of a constant magnetic field and a periodic lattice potential, respectively.

1. Introduction

In [5] we constructed wave packets for adiabatic perturbations of Schrödinger operators in periodic media. The recent work of Panati-Spohn-Teufel, [14], led us to consider the relation of those constructions to effective Hamiltonians. In §3 we sketch a simple derivation of effective Hamiltonians for these problems, and in §4 we show how one could predict the form of the effective Hamiltonians from the wave packets in [5].

The main simplification in our method is the omission of the Floquet-Bloch transformation. This transformation has many nice properties. In particular, it is unitary, and this makes it useful in studying spectral properties of operators. In the work of Helffer-Sjöstrand [10] and Gérard-Martinez-Sjöstrand [8] this transformation was used quite effectively in the computation of spectra, both of perturbed and effective Hamiltonians. However, if one is simply interested in effective Hamiltonians, the Floquet-Bloch transformation requires that one transform the Hamiltonian by a Fourier integral unitary operator only to transform it back at the end of the calculation.

The method that we use here applies when the eigenspaces of the unperturbed Hamiltonian depend smoothly on quasi-momentum and form trivial bundles over a fundamental domain for the dual lattice.

2. Preliminaries

The Hamiltonian for an electron in a crystal lattice Γ in $\mathbb{R}^3$ in the presence of a constant magnetic field $\omega = (\omega_1, \omega_2, \omega_3)$ is given by

$$H_0 = \frac{1}{2m}\left(-ih\frac{\partial}{\partial x} + e\frac{\omega \times x}{2}\right)^2 + V(x), \tag{1}$$

where V is a smooth, real-valued potential, periodic with respect to Γ. Here m and e are the mass and charge of the electron. To simplify notation we will use units in which $h = 2m = e = 1$.

We will assume that Γ is generated by the basis $\{e_1, e_2, e_3\}$ for $\mathbb{R}^3$,

$$\Gamma = e_1\mathbb{Z} + e_2\mathbb{Z} + e_3\mathbb{Z}, \tag{2}$$

and let E be the fundamental domain $\{\sum_{j=1}^3 t_j e_j, t_j \in [0,1)\}$. We will use the dual lattice $\Gamma^* = e_1^*\mathbb{Z} + e_2^*\mathbb{Z} + e_3^*\mathbb{Z}$, where $e_j^* \cdot e_k = 2\pi\delta_{jk}$, with the fundamental domain $E^* = \{\sum_{j=1}^3 t_j e_j^*, t_j \in [0,1)\}$.

To realize H_0 as a self-adjoint operator in $L^2(\mathbb{R}^3)$ we define it first on the Schwartz functions $\mathcal{S}(\mathbb{R}^3)$, and then take the Friedrichs extension. The resulting operator commutes with the magnetic translations introduced by Zak [19],

$$T_\gamma f(x) = e^{i\langle \omega \times x, \gamma\rangle/2} f(x - \gamma) \tag{3}$$

for $\gamma \in \Gamma$. We assume that

$$\langle \omega, \Gamma \times \Gamma\rangle \subset 4\pi\mathbb{Z}.$$

With this assumption $G = \{T_\gamma, \gamma \in \Gamma\}$ is an abelian group, and we can reduce H_0 by the eigenspaces of G, i.e. setting

$$\mathcal{D}_k = \{u \in H^2_{loc}(\mathbb{R}^3), T_\gamma u = e^{-ik\cdot\gamma}u, \gamma \in \Gamma\}, \tag{4}$$

considered as a subspace of $L^2(E)$, H_0 restricted to $\mathcal{D}_k$ is self-adjoint with compact resolvant. We denote its spectrum by

$$E_1(k) \leq E_2(k) \leq \dots$$

Then by standard results the spectrum of H_0 as an operator in $L^2(\mathbb{R}^3)$ is equal to

$$\cup_{k\in E^*} \cup_{m=1}^{\infty} E_m(k).$$

Note that, since $\mathcal{D}_{k+\gamma^*} = \mathcal{D}_k$ for $\gamma^* \in \Gamma^*$, $E_m(k+\gamma^*) = E_m(k)$.

Standard perturbation theory shows that the function $E_m(k)$ is continuous for $k \in \mathbb{R}^3$ and real analytic in a neighborhood of any k such that

$$E_{m-1}(k) < E_m(k) < E_{m+1}(k) \tag{5}$$

The closed interval $\Lambda_m = \cup_{k\in E^*} E_m(k)$ is known as the "m-th magnetic Bloch band" in the spectrum of H_0.

In what follows it will be convenient to replace H_0 acting on $\mathcal{D}_k$ by

$$H_0(k) = e^{-ik\cdot x} H_0 e^{ik\cdot x} = \left(-i\frac{\partial}{\partial x} + \frac{\omega \times x}{2} + k\right)^2 + V(x)$$

with the domain

$$\mathcal{D} = \{u \in H^2_{loc}(\mathbb{R}^3), T_\gamma u = u, \gamma \in \Gamma\}.$$

for all k. As with $\mathcal{D}_k$, we consider $\mathcal{D}$ as a subspace of $L^2(E)$.

Assumption A. *For a given m we will assume that E_m satisfies (5) for all k.* Under this assumption we can choose the eigenfunction $\Psi(x,k)$ associated to $E_m(k)$ to be a real-analytic function of k with values in $\mathcal{D}$, such that $\int_E |\Psi(x,k)|^2 dx = 1$, and

$$H_0(k)\Psi(k) = E_m(k)\Psi(k) \text{ for all k .}$$

Assumption B. We assume that

$$\Psi(x, k+\gamma^*) = e^{i\gamma^*\cdot x}\Psi(x,k), \gamma^* \in \Gamma^*.$$

This assumption makes the complex line bundle of the eigenspaces a trivial bundle over the torus the torus, $\mathbb{R}^3/\Gamma^*$. In general one has

$$\Psi(x, k+\gamma^*) = e^{i(\gamma^*\cdot x+\theta(k,\gamma^*))}\Psi(x,k), \gamma^* \in \Gamma^*,$$

where $\theta(k,\gamma^*)$ is real-valued, and determines the structure of the family of eigenspaces as a complex line bundle. Since

$$\theta(k, m_1e_1^* + m_2e_2^* + m_3e_3^*) = m_1\theta(k,e_1^*) + m_2\theta(k,e_2^*) + m_3\theta(k,e_3^*),$$

when $\theta(k,\gamma^*)$ is nonzero, the derivatives of Ψ with k may be unbounded and Ψ may not belong to the class of symbolds $\mathcal{B}$ which we introduce below. Thus we need Assumption B.

Remark 1. The general method of constructing effective Hamiltonians which we give here will apply under the weaker hypothesis: for a given m there exist p and q such that

$$E_{m-p-1}(k) < E_{m-p}(k) \text{ and } E_{m+q}(k) < E_{m+q+1}(k) \text{ for all } k,$$

and the corresponding eigenspaces form a trivial bundle over $\mathbb{R}^3/\Gamma^*$. However, in this case the effective Hamiltonian will be a matrix operator acting on functions with values in $\mathbb{C}^{p+q+1}$, as in [7],[8] and [14].

3. Main Result

The adiabatically perturbed Hamiltonian is

$$H_\epsilon = \left(-i\frac{\partial}{\partial x} + \frac{\omega\times x}{2} + A(\epsilon x)\right)^2 + V(x) + W(\epsilon x),$$

where W and $A = (A_1, A_2, A_3)$ are smooth, and bounded together with all of their derivatives. As before, we define H_ϵ first on $\mathcal{S}(\mathbb{R}^3)$, and then take the Friedrichs extension to get a self-adjoint operator in $L^2(\mathbb{R}^3)$.

The essential step in applying multi-scale techniques is simply to consider $y = \epsilon x$ as a new independent variable in H_ϵ. Let

$$\tilde{H}_\epsilon = \left(-i\frac{\partial}{\partial x} - i\epsilon\frac{\partial}{\partial y} + \frac{\omega\times x}{2} + A(y)\right)^2 + V(x) + W(y).$$

Then, for $u(x,y)$ we can define $w(x) = u(x, \epsilon x)$ and conclude that

$$[\tilde{H}_\epsilon u](x, \epsilon x) = [H_\epsilon w](x). \tag{6}$$

The identity (6) enables us to solve the Schrödinger equation for H_ϵ uniformly in ϵ by solving the Schrödinger equation for $\tilde{H}_\epsilon$ uniformly in (y, ϵ). The latter might sound more difficult, but it turns out not to be.

Let $\mathcal{B}$ denote the subspace of $C^\infty(\mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{R}^3)$ consisting of functions of the form

$$P(x,y,k,\epsilon) = P_0(x,y,k) + \epsilon P_1(x,y,k) + \cdots + \epsilon^N P_N(x,y,k)$$

such that $P(x+\gamma, y, k, \epsilon) = e^{i\langle \omega \times x, \gamma \rangle/2} P(x,y,k,\epsilon)$ and

$$\sup_{y,k} \|\partial_y^\alpha \partial_k^\beta P_j(\cdot, y, k)\|_{L^2(E)} < \infty, \text{ for all } \alpha, \beta \in \mathbb{N}^3.$$

To $P \in \mathcal{B}$ we associate the ϵ-pseudo-differential operator

$$P(x, y, \epsilon D_y, \epsilon) f(x,y,\epsilon) = (2\pi\epsilon)^{-3} \int e^{ik\cdot(y-z)/\epsilon} P(x,y,k,\epsilon) f(z) dz dk, \, f \in \mathcal{S}(\mathbb{R}^3).$$

Note that here we are using the standard quantization – as opposed to the Weyl quantization. Our main result is the following:

Theorem. *For every $N \in \mathbb{N}$ there exist $P_N = F_0 + \epsilon F_1 + \cdots + \epsilon^N F_N \in \mathcal{B}$ and $H^N_{eff} = h_0 + \epsilon h_1 + \cdots + \epsilon^N h_N \in \mathcal{B}$, with the h_j's independent of x, such that*

$$\tilde{H}_\epsilon(P_N(x,y,\epsilon D_y,\epsilon)u) - P_N(x,y,\epsilon D_y,\epsilon)(H^N_{eff}(y,\epsilon D_y)u) = \mathcal{O}(\epsilon^{N+1}) \tag{7}$$

for $u \in \mathcal{S}(\mathbb{R}^3)$. Moreover, considered as an operator from $L^2(\mathbb{R}^3)$ into $L^2(E \times \mathbb{R}^3)$, P_N is approximately isometric, i.e. $P_N^* P_N = I + \mathcal{O}(\epsilon^{N+1})$.

We interpret H^N_{eff} as the effective Hamiltonian up to order ϵ^N. The leading term in its symbol is $h_0(y,k) = E_m(k + A(y)) + W(y)$. This is the well-known "Peierls substitution", [15]. The symbol of h_1 is given by

$$h_1(y,k) = \frac{1}{2i} \frac{\partial}{\partial y} \cdot \frac{\partial E_m(k+A(y))}{\partial k} - L \cdot B - i\langle \Psi(\cdot, k + A(y)), \dot{\Psi}(\cdot, k + A(y)) \rangle. \tag{8}$$

Here $B(y) = \nabla \times A(y)$ and

$$L = \mathrm{Im}\left(\langle M(y,k)\frac{\partial\Psi}{\partial k_2}, \frac{\partial\Psi}{\partial k_3}\rangle, \langle M(y,k)\frac{\partial\Psi}{\partial k_3}, \frac{\partial\Psi}{\partial k_1}\rangle, \langle M(y,k)\frac{\partial\Psi}{\partial k_1}, \frac{\partial\Psi}{\partial k_2}\rangle\right).$$

with $M(y,k) = \tilde{H}_0(k) - h_0(y,k)$. The function $\dot{\Psi}(x, k + A(y))$ is given by

$$\dot{\Psi}(x, k + A(y)) = \frac{\partial\Psi(x, k + A(y))}{\partial y} \cdot \dot{y} + \frac{\partial\Psi(x, k + A(y))}{\partial k} \cdot \dot{k}$$

and $\dot{y}$ and $\dot{k}$ are defined by the Hamiltonian system

$$\dot{y} = \frac{\partial(E_m(k + A(y)) + W(y))}{\partial k} \qquad \dot{k} = -\frac{\partial(E_m(k + A(y)) + W(y))}{\partial y}.$$

Thus one recognizes $i\langle\Psi(\cdot, k + A(y)), \dot{\Psi}(\cdot, k + A(y))\rangle$ as the term generating the Berry phase precession, cf. [13], [17]. The vector L is an angular momentum and $L \cdot B$ contributes the "Rammal-Wilkinson" term to the energy, cf. [1]. Comparing (8) with [14, (22)] (in the case $l = 1$), one sees that they agree completely when one takes into account the difference in the choice of sign in the magnetic potential, $A(y)$, and the use of Weyl quantization in [14]. The sign of the Berry phase term in (8) may appear inconsistent with [5, (29)], but it is not. In [5] $(\dot{y}, \dot{k})$ was the vector field from the Hamiltonian $-E_m(k + A(y))$.

The proof of the theorem is given in [6], and it is short. One treats x as a parameter, and uses the ϵ-pseudo-differential calculus in y to construct the symbols of the pairs (h_0, F_0), $(h_1, F_1), \ldots$, successively so that (7) holds to order $\mathcal{O}(\epsilon^{N+1})$.

Relation to Wave Packets. In [5] and [9], instead of introducing effective Hamiltonians, we constructed wave packets. These packets are nonetheless related to effective Hamiltonians in that one can compute what the effective Hamiltonian must be – assuming that there is one – from the packets. To see this one can proceed as follows. The packets have the form (here $s = \epsilon t$ and $W(y) = 0$)

$$u(x, y, s, \epsilon) = e^{i\phi(y,s)/\epsilon}[f(y, s)\Psi(x, \frac{\partial\phi}{\partial y} + A(y)) + \mathcal{O}(\epsilon)],$$

where ϕ and f are solutions of

$$\begin{aligned}\frac{\partial\phi}{\partial s} &= E_m(\frac{\partial\phi}{\partial y} + A(y)) \text{ and} \\ \frac{\partial f}{\partial s} &= \frac{\partial E_m}{\partial k}(\frac{\partial\phi}{\partial y} + A(y)) \cdot \frac{\partial f}{\partial y} + (D - iL \cdot B + \langle\Psi, \dot{\Psi}\rangle)f.\end{aligned} \tag{9}$$

Here all functions of (k, y) are evaluated at $k = \tilde{k}(y, s) = \partial_y\phi$, and $D = (1/2)\partial_y \cdot (\partial_k E_m(\partial_y\phi + A(y)))$. Assuming that the evolution of f is governed by an effective Hamiltonian $H_{eff} = h_0(y, \epsilon D_y) + \epsilon h_1(y, \epsilon D_y) + \mathcal{O}(\epsilon^{\in})$, we must have (on bounded intervals in s)

$$[e^{isH_{eff}/\epsilon}(e^{i\phi(\cdot,0)/\epsilon}f(\cdot, 0)](y, s) = e^{i\phi(y,s)/\epsilon}f(y, s) + \mathcal{O}(\epsilon^{\in}). \tag{10}$$

Differentiating (10) with respect to s, one concludes

$$\frac{i}{\epsilon}H_{eff}(e^{i\phi(y,s)/\epsilon}f(y, s)) = (\frac{i}{\epsilon}\frac{\partial\phi}{\partial s}f + \frac{\partial f}{\partial s})e^{i\phi(y,s)/\epsilon} + \mathcal{O}(\epsilon). \tag{11}$$

Using the symbol expansion from the pseudo-differential calculus

$$e^{-i\phi/\epsilon}H_{eff}(e^{i\phi/\epsilon}f) = h_0(y, \tilde{k}) +$$

$$\epsilon[\frac{1}{i}\frac{\partial h_0}{\partial k}(y, \tilde{k}) \cdot \frac{\partial f}{\partial y}(y) + \frac{1}{2i}\sum_{j,l}\frac{\partial^2 h_0}{\partial k_j \partial k_l}(y, \tilde{k})\frac{\partial^2\phi}{\partial y_j \partial y_l}(y) + h_1(y, \tilde{k})]f(y) + \mathcal{O}(\epsilon^{\in}). \tag{12}$$

Substituting (12) into (11) and comparing the result with (9), one recovers the formulas given earlier for $h_0(y, k)$ and $h_1(y, k)$.

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