Microlocal Analysis and Adiabatic Problems: The Case of Perturbed Periodic Schrödinger Operators

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Microlocal analysis is a powerful technique to deal with multiscale and adiabatic problems in Quantum Mechanics. We illustrate this general claim in the specific case of a perturbed periodic Schrödinger operator, namely the operator defined in a dense subspace of $L^2(\mathbb{R}^d)$ by

$$H_\varepsilon = \frac{1}{2}\sum_{j=1}^{d}\left(-i\frac{\partial}{\partial x_j} - A_j(\varepsilon x)\right)^2 + V(x) + \varphi(\varepsilon x), \tag{1}$$

where $V : \mathbb{R}^d \to \mathbb{R}$ is a $\mathbb{Z}^d$-periodic function, $V \in L^2_{\mathrm{loc}}(\mathbb{R}^d)$, corresponding to the interaction of the test electron with the ionic cores of a crystal, while $A_j \in C_{\mathrm{b}}^\infty(\mathbb{R}^d)$ and $\varphi \in C_{\mathrm{b}}^\infty(\mathbb{R}^d)$ represent some perturbing external electromagnetic potentials. The parameter $\varepsilon \ll 1$ corresponds to the separation of space-scales.

Since the unperturbed Hamiltonian $H_{\mathrm{per}} = -\frac{1}{2}\Delta + V$ is periodic, it can be decomposed as a direct integral of simpler operators, thus exhibiting a *band structure*, analogous to the one appearing in the Born-Oppenheimer problem.

We are interested to the behavior of the solutions to the dynamical Schrödinger equation $i\varepsilon\,\partial_t\psi_\varepsilon(t) = H_\varepsilon\psi_\varepsilon(t)$ in the limit $\varepsilon \to 0$. We show that by using microlocal analysis with operator-valued symbols one can decouple the dynamics corresponding to different bands and determine a simpler approximate dynamics for each band [3]. Further developments have been obtained, more recently, in [1, 5].

The Bloch-Floquet transform. The $\mathbb{Z}^d$-symmetry of the unperturbed Hamiltonian operator $H_{\mathrm{per}} = -\frac{1}{2}\Delta + V$ can be used to decomposed it as a direct integral of simpler operators. To fix the notation, let Y be a fundamental domain for the action of the translation group $\Gamma = \mathbb{Z}^d$ on $\mathbb{R}^d$, and let $\mathbb{B}$ be a fundamental domain for the action of the dual lattice $\Gamma^* := \left\{\kappa \in (\mathbb{R}^d)^* : \kappa\cdot\gamma \in 2\pi\mathbb{Z} \quad \forall\gamma \in \Gamma\right\}$ on the dual

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space $(\mathbb{R}^d)^*$ ("momentum space"). We also introduce the tori $\mathbb{T}^d_Y = \mathbb{R}^d/\Gamma$ and $\mathbb{T}^* = (\mathbb{R}^d)^*/\Gamma^*$. The formula

$$(\widetilde{\mathcal{U}}\psi)(k,y) = \sum_{\gamma\in\Gamma} \mathrm{e}^{-ik\cdot(y+\gamma)}\,\psi(y+\gamma), \qquad y \in \mathbb{R}^d, k \in (\mathbb{R}^d)^*, \psi \in \mathcal{S}(\mathbb{R}^d)$$

extends to a unitary operator $\widetilde{\mathcal{U}} : L^2(\mathbb{R}^d) \longrightarrow L^2(\mathbb{B}) \otimes L^2(\mathbb{T}^d_Y) \simeq L^2(\mathbb{B}, L^2(\mathbb{T}^d_Y))$, called (modified) Bloch-Floquet transform. Hereafter $\mathcal{H}_{\mathrm{f}} := L^2(\mathbb{T}^d_Y)$.

The advantage of this construction is that, after conjugation, H_{per} becomes a fibered operator, namely

$$\widetilde{H}_{\mathrm{per}} := \widetilde{\mathcal{U}}\, H_{\mathrm{per}} \widetilde{\mathcal{U}}^{-1} = \int_{\mathbb{B}}^{\oplus} H_{\mathrm{per}}(k)\, dk \;\text{ in } L^2(\mathbb{B}, \mathcal{H}_{\mathrm{f}}) \simeq \int_{\mathbb{B}}^{\oplus} \mathcal{H}_{\mathrm{f}}\, dk =: \mathcal{H},$$

$$H_{\mathrm{per}}(k) = \frac{1}{2}(-i\nabla_y + k)^2 + V(y) \;\text{ acting on }\; \mathcal{D} \subseteq L^2(\mathbb{T}^d_Y, dy) = \mathcal{H}_{\mathrm{f}}$$

where $\mathcal{D}$ is a dense subspace of $\mathcal{H}_{\mathrm{f}}$. The operator $H_{\mathrm{per}}(k)$ has compact resolvent, and we label its eigenvalues as $E_0(k) \leq E_1(k) \leq \ldots$. Notice that the eigenvalues are Γ^*-periodic. We assume that a solution of the eigenvalue problem $H_{\mathrm{per}}(k)\,\chi_n(k,y) = E_n(k)\,\chi_n(k,y)$ is known, and we denote by $P_n(k)$ the eigenprojector corresponding to the n-th eigenvalue, while $P_n = \int_{\mathbb{B}}^{\oplus} P_n(k)\, dk$. The set $\mathcal{E}_n = \{(k, E_n(k)) \in \mathbb{T}^* \times \mathbb{R}\}$ is called the n-th Bloch band.

The perturbed dynamics. We consider a Bloch band $\mathcal{E}_n$ which is separated by a gap from the rest of the spectrum, *i. e.*

$$\inf\{|E_n(k) - E_m(k)| : k \in \mathbb{T}^*, m \neq n\} > 0, \tag{2}$$

and the corresponding subspace

$$\mathrm{Ran} P_n = \{\Psi \in \mathcal{H} : \Psi(k,y) = \varphi(k)\,\chi_n(k,y) \text{ for } \varphi \in L^2(\mathbb{B}, dk)\}.$$

In the unperturbed case, $A = 0$ and $\phi = 0$, the subspace $\mathrm{Ran} P_n$ is exactly invariant, in the sense that $(1 - P_n)\, e^{-i\widetilde{H}_{\mathrm{per}}t/\varepsilon}\, P_n \Psi = 0$ for all $\Psi \in \mathcal{H}$. Moreover, the dynamics of $\Psi \in \mathrm{Ran} P_n$ is particularly simple, namely

$$\left(e^{-i\widetilde{H}_{\mathrm{per}}t/\varepsilon}\Psi\right)(k,y) = \left(e^{-iE_n(k)t/\varepsilon}\varphi(k)\right)\chi_n(k,y).$$

Thus a natural question arises: to what extent such properties survive in the perturbed case? More precisely,

(i) Does exist a subspace of $\mathcal{H}$ which is almost-invariant with respect to the dynamics, up to errors of order ε^N?
(ii) Is there any simple (and numerically convenient) way to approximately describe the dynamics inside the almost invariant subspace?

The microlocal approach. Microlocal analysis is a useful tool to answer these questions. In a nutshell, one checks that by modified BF transform one has

$$\widetilde{H}_\varepsilon := \widetilde{\mathcal{U}}\ H_\varepsilon\, \widetilde{\mathcal{U}}^{-1} = \big(-i\nabla_y + k - A(i\varepsilon\nabla_k)\big)^2 + V(y) + \phi(i\varepsilon\nabla_y).$$

The latter operator "looks like" the ε-Weyl quantization of an operator-valued symbol

$$\begin{aligned} h : \mathbb{T}^* \times \mathbb{R}^d &\longrightarrow \text{Operators}(\mathcal{H}_\mathrm{f}) \\ (k, r) &\longmapsto \big(-i\nabla_y + k - A(r)\big)^2 + V(y) + \phi(r). \end{aligned}$$

This observation naturally leads to exploit techniques related to matrix-valued pseudo-differential operators [2, 4]. Obviously, to perform this program one has to circumvent some technical *scholia* (*unbounded*-operator-valued symbols, covariance, ...), for whose solution we refer to [3]. As an answer to question (i), we have the following

Theorem 1. *Let $\mathcal{E}_n$ be an isolated Bloch band, see (2). Then there exists an orthogonal projection $\Pi_{n,\varepsilon} \in \mathcal{B}(\mathcal{H})$ such that for every $N \in \mathbb{N}$ there exist C_N such that*

$$\big\|[\widetilde{H}_\varepsilon, \Pi_{n,\varepsilon}]\big\|_{\mathcal{B}(\mathcal{H})} \le C_N\, \varepsilon^N$$

and $\Pi_{n,\varepsilon}$ is $\mathcal{O}(\varepsilon^\infty)$-close to the ε-Weyl quantization of a symbol with principal part $\pi_0(k, r) = P_n(k - A(r))$.

As for question (ii), one preliminarily notices that there is no natural identification between $\mathrm{Ran}\,\Pi_{n,\varepsilon}$ and $L^2(\mathbb{T}^*, dk)$, so no evident reduction of the number of degrees of freedom. To circumvent this obstacle, one constructs an intertwining unitary operator (which is an additional unknown in the problem) $U_{n,\varepsilon} : \mathrm{Ran}\,\Pi_{n,\varepsilon} \to L^2(\mathbb{T}^*, dk)$. The freedom to choose $U_{n,\varepsilon}$ can be exploited to obtain a simple and physically transparent representation of the dynamics, as in the following result [3].

Theorem 2. *Let $\mathcal{E}_n$ be an isolated Bloch band. Define the effective Hamiltonian as the operator $\hat{H}_{\text{eff,"}} := U_{n,\varepsilon}\,\Pi_{n,\varepsilon}\,H_\varepsilon\,\Pi_{n,\varepsilon}\,U_{n,\varepsilon}^{-1}$ acting in $L^2(\mathbb{T}^*, dk)$. Then:*

(i) (approximation of the dynamics) *for any $N \in \mathbb{N}$ there is C_N such that*

$$\Big\|\Big(\varepsilon^{-i\widetilde{H}_\varepsilon t/\varepsilon} - U_{n,\varepsilon}^{-1}\ \varepsilon^{-i\,\hat{H}_{\text{eff,"}}\ t/\varepsilon}\,U_{n,\varepsilon}\Big)\,\Pi_{n,\varepsilon}\Big\|_{\mathcal{B}(\mathcal{H})} \le C_N\,\varepsilon^N\,(1 + |t|).$$

(ii) (explicit description of the approximated dynamics) *the operator $\hat{H}_{\text{eff,"}}$ is $\mathcal{O}(\varepsilon^\infty)$-close to the ε-Weyl quantization of the symbol $h_\varepsilon^{\text{eff}} : \mathbb{T}^* \times \mathbb{R}^d \to \mathbb{C}$, with leading orders*

$$h_0^{\text{eff}}(k, r) = E_n(k - A(r)) + \phi(r)$$

$$h_1^{\text{eff}}(k, r) = (\nabla\phi(r) - \nabla E_n(\kappa)\wedge B(r)) + \mathcal{A}_n(\kappa) - B(r)\cdot M_n(\kappa)$$

where $\kappa(k,r) = k - A(r)$, $B_{jl} = \partial_j A_l - \partial_l A_j$, $\mathcal{A}_n(k) = i \, \langle \chi_n(k) \,|\, \nabla \chi_n(k) \rangle_{\mathcal{H}_\mathrm{f}}$ *is called* Berry connection *and*

$$M_n(k) = \frac{i}{2} \left\langle \nabla \chi_n(k) \wedge | \, (H_{\mathrm{per}}(k) - E_n(k)) \nabla \chi_n(k) \right\rangle_{\mathcal{H}_\mathrm{f}} .$$

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