Effective dynamics for Bloch electrons

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1. The problem

• **The framework.** We consider the Schrödinger equation

$$\mathrm{i}\,\varepsilon\,\partial_t\,\psi(x,t) \;=\; \Big(\tfrac{1}{2}\big(-\mathrm{i}\nabla_x - A(\varepsilon x)\big)^2 + V_\Gamma(x) + \phi(\varepsilon x)\Big)\psi(x,t) \\ =: H^\varepsilon\psi(x,t) \qquad (1)$$

for $\psi \in L^2(\mathbb{R}^d)$, where V_Γ is periodic with respect to some regular lattice $\Gamma \subset \mathbb{R}^d$, ϕ and A are external electric and magnetic potentials and $\varepsilon \ll 1$ expresses the slow space-variation of the potentials.

• **Separation of space-scales.** The separation of scales in the problem plays a fundamental role in the understanding of the dynamics.

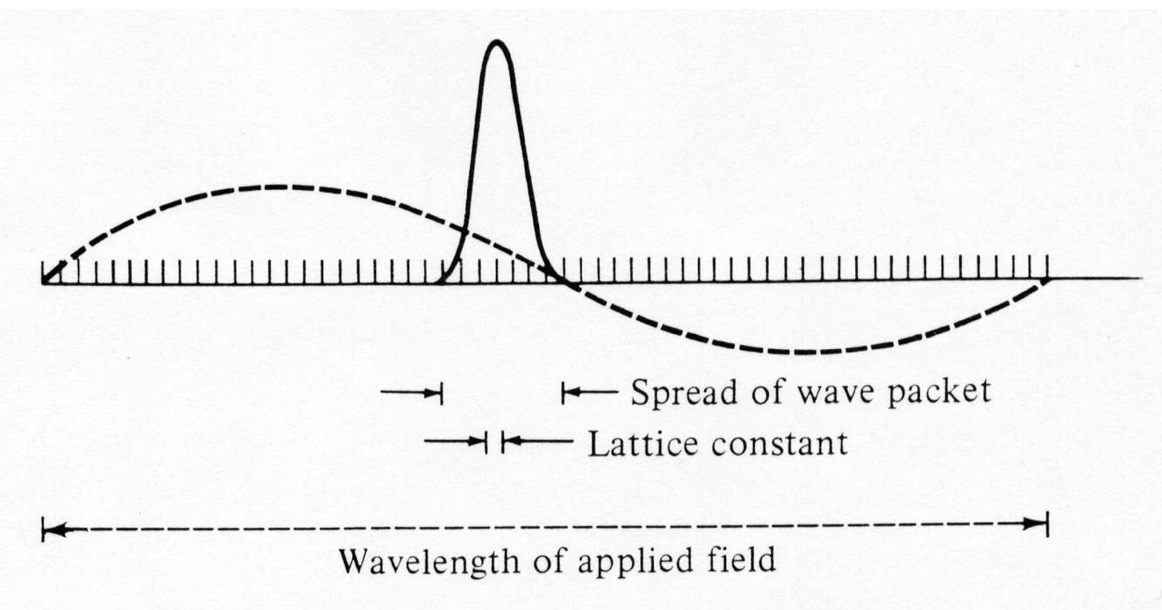

Fig. 1: Separation of space-scales in the perturbed periodic problem.

• **Semiclassical model.** In solid state physics, the motion of semiclassical wave packets is described by the dynamical system

$$\dot r = \nabla E_n(\kappa)\,, \qquad \dot\kappa = -\nabla\phi(r) + \dot r \times B(r)\,,$$

where $\kappa = k - A(r)$, r and k represent the position and the crystal-momentum of the electron, and $E_n(k)$ is the n^{th} Bloch band.

• **The goals.**

1. to give a mathematical **justification** of the semiclassical model
2. to compute **higher-order** corrections in ε to the semiclassical model

◇ A full account of our results is given in arXiv:math-ph/0212041, to appear in Comm. Math. Phys.

2. The mathematical setup

• **The Zak transform** allows to separate slow and fast degrees of freedom,

$$(\mathcal{U}\psi)(k,y) := \sum_{\gamma\in\Gamma} \mathrm{e}^{-\mathrm{i}(y+\gamma)\cdot k}\psi(y+\gamma), \ \ (k,y) \in M^* \times \mathbb{T}^d,$$

$$\mathcal{U} : L^2(\mathbb{R}^d) \to \mathcal{H}_\tau \cong L^2(M^*) \otimes L^2(\mathbb{T}^d)\,,$$

where M^* is the first Brillouin zone. In the Zak representation the periodic Hamiltonian is fibered over M^*:

$$\mathcal{U}\,\left(-\tfrac{1}{2}\Delta + V_\Gamma\right)\mathcal{U}^{-1} = \int_{M^*}^{\oplus} \mathrm{d}k\, H_{\mathrm{per}}(k),$$

$$H_{\mathrm{per}}(k) = \tfrac{1}{2}\big(-\mathrm{i}\nabla_y + k\big)^2 + V_\Gamma(y)\,, \quad k \in M^*.$$

• **The Bloch bands.**

Let E_n be an isolated not degenerate Bloch band. Choose a system of smooth and periodic Bloch functions $\{\varphi_n(k)\}_{k\in M^*}$,

$$H_{\mathrm{per}}(k)\varphi_n(k) = E_n(k)\varphi_n(k).$$

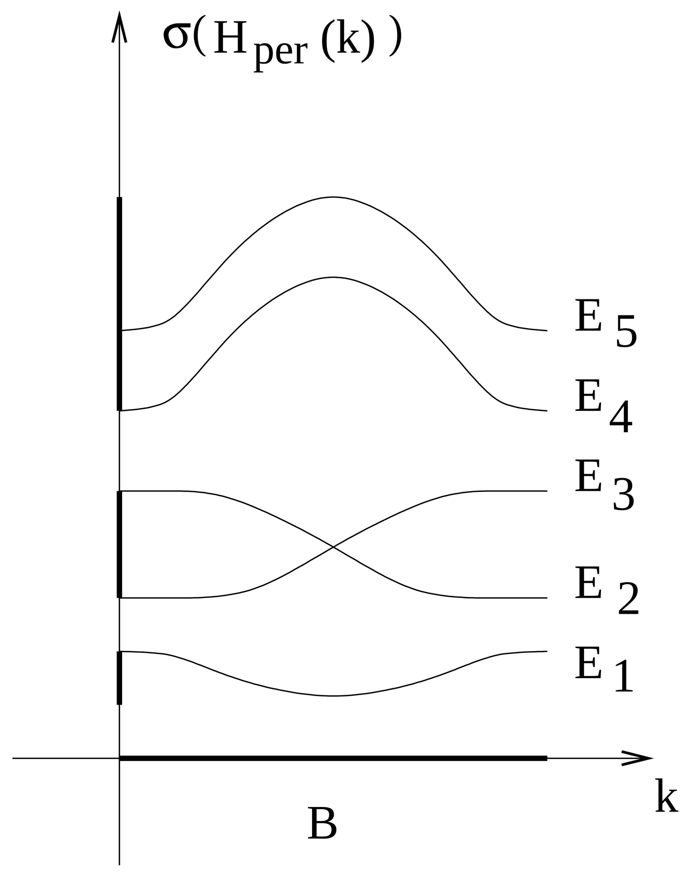

Fig. 2: A schematic picture of Bloch bands (for $d \geq 2$). The bands E_1, E_4 and E_5 are isolated.

3. The result

The electron acquires a k-dependent effective electric moment given by the **Berry connection**

$$\mathcal{A}_n(k) = \mathrm{i}\left\langle \varphi_n(k), \nabla\varphi_n(k)\right\rangle,$$

with curvature $\Omega_n(k) = \nabla \times \mathcal{A}_n(k)$, and an effective magnetic moment given by the **Rammal-Wilkinson term**

$$\mathcal{M}(k)_n = \tfrac{\mathrm{i}}{2}\left\langle \nabla\varphi_n(k),\ \times (H_{\mathrm{per}}(k) - E(k))\nabla\varphi_n(k)\right\rangle.$$

The **ε-corrected semiclassical equations** reads

$$\dot r = \nabla_\kappa\Big(E_n(\kappa) - \varepsilon\,B(r)\cdot\mathcal{M}_n(\kappa)\Big) - \varepsilon\,\dot\kappa \times \Omega_n(\kappa)\,, \\ \dot\kappa = -\nabla_r\Big(\phi(r) - \varepsilon\,B(r)\cdot\mathcal{M}_n(\kappa)\Big) + \dot r \times B(r)\,. \qquad (2)$$

The relation between (1) and the flow $\Phi^t_{n,\varepsilon}$ of (2) in the coordinates (k,r) is given by the following theorem.

• **Theorem.** *To any isolated Bloch band corresponds an orthogonal projector Π^ε_n defining an* ***almost-invariant subspace****, i.e. $[H^\varepsilon, \Pi^\varepsilon_n] = \mathcal{O}(\varepsilon^\infty)$. Moreover, let $a \in C^\infty_{\mathrm{b}}(\mathbb{R}^{2d})$ be Γ^*-periodic in the second argument, i.e. $a(r, k+\gamma^*) = a(r,k)$ for all $\gamma^* \in \Gamma^*$, and $\hat a = a(\varepsilon x, -\mathrm{i}\nabla_x)$ be its Weyl quantization. Then for each finite time-interval $I \subset \mathbb{R}$ there is a constant $C < \infty$ such that for $t \in I$*

$$\left\| \Pi^\varepsilon_n \left(\mathrm{e}^{\mathrm{i}H^\varepsilon t/\varepsilon}\,\hat a\,\mathrm{e}^{-\mathrm{i}H^\varepsilon t/\varepsilon} - \widehat{a\circ\Phi^t_{n,\varepsilon}}\right)\Pi^\varepsilon_n \right\|_{\mathcal{B}(L^2(\mathbb{R}^d))} \leq \varepsilon^2 C\,.$$

• **Strategy of the proof.** Apply space-adiabatic perturbation theory [6] to the τ-equivariant unbounded-operator valued symbol

$$H_0(k,r) = \frac{1}{2}\left(-\mathrm{i}\nabla_y + k - A(r)\right)^2 + V_\Gamma(y) + \phi(r)$$

whose Weyl quantization $H_0(k, \mathrm{i}\varepsilon\nabla_k)$ equals $\mathcal{U}H^\varepsilon\mathcal{U}^*$ acting on $\mathcal{H}_\tau$.

• **Generalizations.** Arbitrary dimension $d \in \mathbb{N}$, degenerate bands, families of Bloch bands.

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