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Semi-classical asymptotics in magnetic Bloch bands

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This talk is a report on joint work with Mouez Dimassi and Jean-Claude Guillot which will appear in Journal of Physics A. We give a simple method for deriving "semi-classical" dynamics. The semi-classical approximation in solid state physics refers to dynamics for electrons in slowly varying perturbations of periodic fields. Here we are going to construct wave packets for the Schrödinger equation for a periodic electric potential and a constant magnetic field perturbed by slowly varying electric and magnetic potentials. This corresponds to finding asymptotic solutions to

$$-i\frac{\partial u}{\partial t}=\left[\left(-i\frac{\partial}{\partial x}+\frac{\omega\times x}{2}+A(\epsilon x,\epsilon t)\right)^2+V_0(x)+V(\epsilon x,\epsilon t)\right]u,$$

where ω is the constant unperturbed magnetic field and V_0 is the periodic unperturbed electric potential. We assume that $V_0(x+\gamma)=V_0(x)$ for all γ in the lattice Γ_0 in $\mathbb{R}^3$. The perturbations A and V are assumed to be smooth, and we are looking for solutions which are asymptotic to true solutions to any given order in ϵ on any given time interval $-T_0\le t\le T_0$.

Magnetic Band Functions

The construction depends on hypotheses on the band structure in the spectrum of the unperturbed problem. The unperturbed Hamiltonian is (in units which make mass and charge for the electron as well as Planck's constant equal 1)

$$H_0=(-i\frac{\partial}{\partial x}+\frac{\omega\times x}{2})^2+V_0(x).$$

This Hamiltonian commutes with the "magnetic translation operators" T_γ^ω, $\gamma\in\Gamma_0$, given by

$$T_\gamma^\omega u(x)=e^{i\langle\frac{\omega\times x}{2},\gamma\rangle}u(x-\alpha).$$

These operators satisfy

$$T_\alpha^\omega T_\beta^\omega=e^{-\frac{i}{2}\langle\omega,\alpha\times\beta\rangle}T_{\alpha+\beta}^\omega=e^{-i\langle\omega,\alpha\times\beta\rangle}T_\beta^\omega T_\alpha^\omega.$$

We will assume that the lattice Γ_0 has a sublattice Γ such that $e^{-\frac{i}{2}\langle\omega,\alpha\times\beta\rangle}=1$ for all $\alpha,\beta\in\Gamma$. This is a rationality condition on the magnetic field ω and the lattice Γ_0. Then by Bloch-Floquet theory one can decompose H acting on $L^2(\mathbb{R}^3)$ as the direct integral of H restricted to the subspaces $\mathcal{D}(k)$, defined by $T_\gamma^\omega u=e^{ik\cdot\gamma}u$ for all $\gamma\in\Gamma$. These restrictions are self-adjoint with compact resolvents, and hence have the eigenvalues

$$E_1(k)\le E_2(k)\le\cdots$$

Since $\mathcal{D}(k+\gamma^*)=\mathcal{D}(k)$ for all $\gamma^*\in\Gamma^*$, the dual lattice to Γ, $E_n(k+\gamma^*)=E_n(k)$, and we can restrict the E_n to a fundamental domain, M^*, for Γ^*.

For the constructions that we give here the following assumption is essential:

(A) There is an l such that $E_l(k)$ is simple for all $k \in M^*$ i.e.

$$E_{l-1}(k) < E_l(k) < E_{l+1}(k), \ k \in M^*$$

With this assumption we can choose normalized $\Psi(x,k)$ in $\mathcal{D}(k)$, depending real analytically on k such $H\Psi(\cdot,k) = E_l(k)\Psi(\cdot,k)$ and $\Psi(x,k+\gamma^*) = \Psi(x,k)$. As in ordinary Bloch theory it will be more convenient to work with the function $\Phi(x,k) = e^{-ik\cdot x}\Psi(x,k)$ which satisfies $T^\omega_\gamma\Psi = \Psi$ for all $\gamma \in \Gamma$ and

$$H_0(k)\Phi(x) =_{\text{def.}} \Big[(-i\frac{\partial}{\partial x} + \frac{\omega \times x}{2} + k)^2 + V_0(x)\Big]\Phi(x) = E_l(k)\Phi(x).$$

The Ansatz

We have the time-dependent Schrödinger equation with perturbed magnetic and electric potentials:

$$-i\frac{\partial u}{\partial t} = \left[\left(-i\frac{\partial}{\partial x} + \frac{\omega \times x}{2} + A(\epsilon x, \epsilon t)\right)^2 + V_0(x) + V(\epsilon x, \epsilon t)\right] u.$$

With the change of variables

$s = \epsilon t$ (adiabatic scale) and $y = \epsilon x$(long spatial scale),

this becomes

$$-i\epsilon\frac{\partial u}{\partial s} = \left[\left(-i\epsilon\frac{\partial}{\partial y} + \frac{\omega \times y}{2\epsilon} + A(y,s)\right)^2 + V_0(\frac{y}{\epsilon}) + V(y,s)\right] u.$$

For asymptotics as $\epsilon \to 0$ we will use the method of two scale expansions: using x, y, t and s as independent variables, we consider

$$-i\epsilon\frac{\partial v}{\partial s} = \left[\left(-i\epsilon\frac{\partial}{\partial y} - i\frac{\partial}{\partial x} + \frac{\omega \times x}{2} + A(y,s)\right)^2 + V_0(x) + V(y,s)\right] v. \qquad (*)$$

Note that a solution $v(x,y,s,\epsilon)$ of (*) evaluted at $y = \epsilon x$ and $s = t/\epsilon$ becomes a solution of the original Schrödinger equation. Note also that by assuming that v does not depend on the fast time variable t we are considering the adiabatic regime.

We will look for solutions of (*) in the form

$$v(x,y,s,\epsilon) = e^{i\phi(y,s)/\epsilon} m(x,y,s,\epsilon),$$

where

$$m(x,y,s,\epsilon) = m_0(x,y,s) + \epsilon m_1(x,y,s) + \cdots .$$

and m satisfies $T^\omega_\gamma m = m$ for T^ω_γ acting on the x variable. Substituting the Ansatz into (*), we get

$$\frac{\partial \phi}{\partial s} m - i\epsilon \frac{\partial m}{\partial s}$$

$$= \left[\left(-i\epsilon \frac{\partial}{\partial y} - i\frac{\partial}{\partial x} + A_0(x) + k(y,s)\right)^2 + V_0(x) + V(y,s)\right] m$$

$$= \left[\left(-i\frac{\partial}{\partial x} + A_0(x) + k(y,s)\right)^2 + V_0(x) + V(y,s)\right] m$$

$$-i\epsilon \left[2\left(-i\frac{\partial}{\partial x} + A_0(x) + k(y,s)\right)\cdot \frac{\partial}{\partial y} + \frac{\partial}{\partial y}\cdot k(y,s)\right] m - \epsilon^2 \Delta_y m,$$

where $k(y,s)$ is given by:

$$k(y,s) = A(y,s) + \frac{\partial \phi}{\partial y}(y,s).$$

Requiring that the coefficients of powers of ϵ in this expression vanish individually, we get the sequence of equations:

$$\frac{\partial \phi}{\partial s} m_0 = \left[H_0\left(k(y,s)\right) + V(y,s)\right] m_0, \qquad (\epsilon^0)$$

$$\left[H_0\left(k(y,s)\right) + V(y,s) - \frac{\partial \phi}{\partial s}(y,s)\right] m_1 = K m_0 =, \qquad (\epsilon^1)$$

$$\left[H_0\left(k(y,s)\right) + V(y,s) - \frac{\partial \phi}{\partial s}(y,s)\right] m_j = K m_{j-1} + \Delta_y m_{j-2}, \; j = 2,3,..., \qquad (\epsilon^j)$$

Here

$$K = i\left[\frac{\partial H_0}{\partial k}(k(y,s)) \cdot \frac{\partial}{\partial y} + \frac{\partial}{\partial y}\cdot k(y,s) - \frac{\partial}{\partial s}\right]$$

Eichonal equation for ϕ and semi-classical dynamics

Since we have assumed that $E_l(k)$ is simple, the equation "(ϵ^0)" holds if and only if

$$\frac{\partial \phi}{\partial s}(y,s) = E_l\left(A(y,s) + \frac{\partial \phi}{\partial y}(y,s)\right) + V(y,s) \text{ and}$$

$$m_0(x,y,s) = f_0(y,s)\Phi(x,k(y,s)).$$

This implies that these packets will propagate along the trajectories of the Hamiltonian

$$H_{sc}(y,s,\eta,\sigma) = \sigma - E_l(A(y,s)+\eta) - V(y,s).$$

If one makes the substitution $k = A(y,s)+\eta) - V(y,s)$, these Hamiltonian equations take the form

$$\dot{y} = -\frac{\partial E_l}{\partial k}(k), \ \dot{s} = 1$$

$$\dot{k} = -\dot{y} \times B(y,s) + \frac{\partial A}{\partial s}(y,s) + \frac{\partial V}{\partial y}(y,s).$$

Here $B = \nabla_y \times A(y,s)$ is the magnetic field corresponding to $A(y,s)$. This gives the velocity of a wave packet in terms of the gradient of the function $E_l(k)$ in momentum space, and says that the momentum k of a packet is governed by the classical equation of motions associated with the perturbations $A(y,s)$ and $V(y,s)$.

Transport equations

To solve the equations "(ϵ^j)", $j = 1, 2, \ldots$, one only needs to observe that, by the Fredholm alternative, these equations are solvable if and only if their right hand sides are orthogonal to

$$\ker \left[H_0\left(k(y,s)\right) + V(y,s) - \frac{\partial \phi}{\partial s} \right],$$

which is spanned by $\Phi(x, k(y,s))$. For $j = 1$ this condition is given by

$$0 = \langle \Phi, \frac{\partial m_0}{\partial s} - \frac{\partial H_0}{\partial k} \cdot \frac{\partial m_0}{\partial y} - \frac{\partial}{\partial y} \cdot k(y,s) m_0 \rangle. \qquad (T)$$

After a few pages of computation, making heavy use of the relation

$$\left[H_0 - E_l\right] \frac{\partial \Phi}{\partial k} = \left[\frac{\partial E_l}{\partial k} - \frac{\partial H_0}{\partial k}\right] \Phi$$

which one obtains by differentiating $H_0(k)\Phi = E_l \Phi$, the equation (T) simplifies to

$$\frac{\partial f_0}{\partial s} - \frac{\partial E_l}{\partial k}(k(y,s)) \cdot \frac{\partial f_0}{\partial y} - \frac{1}{2}\left(\frac{\partial}{\partial y} \cdot \frac{\partial E}{\partial k}(k(y,s)) f_0 + (iL \cdot B + \langle \Phi, \dot{\Phi} \rangle) f_0 = 0, \quad (T_0)$$

Here

$$L = \operatorname{Im}\left\{ (\langle (H_0 - E)\frac{\partial \Phi}{\partial k_2}, \frac{\partial \Phi}{\partial k_3} \rangle, \langle (H_0 - E)\frac{\partial \Phi}{\partial k_3}, \frac{\partial \Phi}{\partial k_1} \rangle, \langle (H_0 - E)\frac{\partial \Phi}{\partial k_1}, \frac{\partial \Phi}{\partial k_2} \rangle) \right\},$$

and, as the notation suggests, it can be interpreted as an angular momentum. The term $L \cdot B$ has appeared elsewhere, and it is called the Rammal-Wilkinson term. Note that it will contribute to the evolution of the phase of the packet. The term $\dot{\Phi}$ is derivative of $\Phi(\cdot, k(y,s))$ along the trajectories, and it contributes the "Berry phase" evolution.

When (T) holds, the equation "(ϵ^1)" can be solved modulo a multiple of Φ, i.e.

$$m_1(x,y,s) = f_1(y,s)\Phi(x,k(y,s)) + m_1^{\perp}(x,y,s),$$

with

$$\langle \Phi(\cdot,k(y,s)), m_1^{\perp}(x,y,s)\rangle = 0.$$

The function f_1 must be chosen so that the right hand side of "(ϵ^2)" satisfies the compatibility condition. Continuing in this way one finds a sequence of linear first order equations which determine the terms in the expansion of $m = m_0 + \epsilon m_1 + \cdots$.

Gaussian beams

To construct solutions which concentrate on a single trajectory of the effective Hamiltonian H_{sc} we will choose the phase ϕ complex-valued with $\mathrm{Im}\{\phi\} \geq 0$. This is the method of "Gaussian beams" or "coherent states". One chooses a single trajectory $(y(r), r, \eta(r), \sigma(r))$ of the flow of H_{sc} and requires

$$(\phi_y(y(r),r), \phi_s(y(r),r)) = (\eta(r), \sigma(r)).$$

Requiring that ekonal equation hold to high order on $\gamma = \{(y(r),r) : -\infty < r < \infty\}$ then leads to differential equations for the derivatives of ϕ along γ. In particular, the Hessian of ϕ satisfies a matrix Ricatti equation.

Choosing the initial data of the phase function ϕ so that

$$\mathrm{Im}\{\phi(y(0),0)\} \geq 0, \ \mathrm{Im}\{\phi(y(0),0)\} = 0, \ \text{and}$$

$$\mathrm{Im}\{\phi_{yy}\}(y(0),0) \text{ is positive definite,}$$

the conservation laws for Ricatti equations arising from eikonal equations imply that $\mathrm{Im}\{\phi_{yy}\}(y(r),r)$ is positive definite for all r. This localizes the packet to a tubular neighborhood of γ which has radius $O(\epsilon^{1/2})$ and is the basis for the rigorous asymptotics of the packets. As a consequence of this localization, it suffices for the eikonal and transport equations to hold to sufficiently high order on γ for the asymptotics to be valid to any given order. We make these equations hold to the desired orders simply by solving the ODEs for derivatives of ϕ along γ – these are linear for the derivatives of order greater than two – and the linear ODEs along γ for the derivatives of m.