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JAMES RALSTON Magnetic breakdown

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Magnetic Breakdown James Ralston

This paper treats a problem in quantum mechanics by what might be called the "classical" method of semi-classical analysis. One makes an Ansatz and solves eichonal and transport equations to determine phases and amplitudes. However, the problem has some nonclassical aspects. First, the small parameter in the problem is not Planck's constant but the magnetic field strength, ε . When one scales variables so that powers of ε appear where they should in semi-classical analysis, the electric potential becomes a periodic function of x/ε . This complicates the Ansatz, and makes the wave function one is trying to construct vector-valued rather than scalar. In most regions one can uncouple the components and construct the wave function one component at a time. That case was discussed in [2] and [4].

In the situation called "magnetic breakdown" one can only uncouple a two component system, and the matrix of the zero magnetic field operator on this system has a codimension two eigenvalue crossing of the form discussed in [5]. The eichonal equation becomes one treated by Horn in [7], and, after several reductions, the transport equations become a 2×2 first order hyperbolic system which degenerates on the set where the eigenvalues cross and uncoupling is impossible. Much of the analysis here is devoted to deriving that system and showing that it has solutions. However, the solutions do not add much to one's qualitative understanding of magnetic breakdown. Perhaps the oddest feature of the ultimate transport equations is that one cannot solve the initial value

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problem for them. Their solutions are uniquely determined by the inhomogeneous terms. Fortunately, since it would be embarassing to devote so much effort to constructing the zero function, one can prescribe nonzero inhomogeneous terms for the top order transport.

I should emphasize that the constructions here are time-dependent. One could construct asymptotic solutions to the time-independent Schrödinger equation by suppressing the time dependence in the Ansatz as was done in the construction of quasimodes in [2], [4] and [7]. However, for questions related to the spectral density an approach like that of Helffer and Sjöstrand [6], [9] would be more effective.

I. Hypotheses and Preliminaries

We consider the Schrödinger equation for a single electron in a crystal lattice of ions in a constant magnetic field. That is, we consider the Schrödinger equation with a smooth, periodic electric potential V(x) and a linear magnetic potential $\varepsilon A(x)$:

(1)
$$i\varepsilon \frac{\partial u}{\partial t} = \left(i\frac{\partial}{\partial x} + \varepsilon A(x)\right)^2 u + V(x)u, \quad x \in \mathbb{R}^3.$$

Here $A(x) = \frac{\omega \times x}{2}$, $|\omega| = 1$, and the magnetic field is given by $B = \nabla \times \varepsilon A = \varepsilon \omega$. The periodicity condition on V is $V(x+\ell) = V(x)$ for all ℓ in a three-dimensional lattice L. The Schrödinger equation takes the form (1) in suitable distance, energy and time scales - Ångstroms for distance and roughly electron volts for energy. These units make $\varepsilon = 1.5 \times 10^{-9}g$, where g is the magnetic field strength in gauss. Thus ε is the natural small parameter here. In what follows we will put (1) in the form

(2)
$$i\varepsilon \frac{\partial u}{\partial t} = \left(i\varepsilon \frac{\partial}{\partial y} + A(y)\right)^2 u + V\left(\frac{y}{\varepsilon}\right)u,$$

by making the change of variables $y = \varepsilon x$.

The article [4] discussed asymptotic solutions of (2) of the form

(3)
$$u = e^{-i\varphi(y,t)/\varepsilon} m(y/\varepsilon, y, t, \varepsilon)$$

where $m(x, y, t, \varepsilon) = m(x + \ell, y, t, \varepsilon)$, $\forall \ell \in L$, and $m = m_0(x, y, t) + \varepsilon m_1(x, y, t) + \cdots$. Substituting the Ansatz (3) into (2), equating coefficients of powers of ε to zero and solving the resulting equations, one constructs asymptotic solutions to all orders in ε . The leading amplitude is given by

$$m_{\mathbf{0}}(x, y, t) = h(y, t)\psi_{n}\left(x, \frac{\partial\varphi}{\partial y} + A(y)\right),$$

where $\psi_n(x, k)$ is an eigenfunction of the operator

$$L(k) = \left(i\frac{\partial}{\partial x} + k\right)^2 + V(x)$$

with the lattice periodicity condition, belonging to the eigenvalue $E_n(k)$. The phase φ must be a solution of the Hamilton-Jacobi equation

(4)
$$\frac{\partial \varphi}{\partial t} = E_n \left(\frac{\partial \varphi}{\partial y} + A(y) \right).$$

The only hypothesis needed to solve the transport equations and carry out the construction to all orders in ε is that $E_n(k)$ must be a *simple* eigenvalue of L(k) for the values of $k = \frac{\partial \varphi}{\partial y}(y, t) + A(y)$ which arise from propagating the support of h(y, 0) along the trajectories of the Hamiltonian $E_n(p + A(y)) - \tau$ associated with (4).

In this article I want to consider the situation when $E_n(k)$ is not simple on one of those trajectories. In this case the wave packets $u(y, t, \varepsilon)$ can no longer just propagate along the trajectories of $E_n(p + A(y)) - \tau$, and one is in the situation called "interband magnetic breakdown" in the physics literature. This terminology refers to the way that packets can now "tunnel" to trajectories of $E_{n+1}(p+A(y))-\tau$, an effect that becomes more evident as the magnetic field strength increases. I should mention that there is also a phenomenon known as "intraband magnetic breakdown" associated with k_0 such that $E_n(k_0)$ is simple, but $\nabla E_n(k_0) \times \omega = 0$. The construction of time-dependent wave packets in this situation is included in the preceding, but when one studies the spectrum near $E_n(k_0)$ there are effects caused by tunnelling between the branches of the curve $\{E_n(k) = E_n(k_0), \ \omega \cdot (k - k_0) = 0\}$. Quasimodes for this case were constructed in Horn [7], using the same Ansatz we will use for interband magnetic breakdown here. The effect of such points on the spectral density (they turn out to be negligible) was analyzed by Sjöstrand in [9]. Closely related spectral problems are discussed in [2], [2a], [3] and [8].

I am going to make a number of assumptions to simplify the constructions. First E_n is only a double eigenvalue, i.e.

$$E_{n-1}(k_0) < E_n(k_0) = \tau_0 = E_{n+1}(k_0) < E_{n+2}(k_0).$$

The point k_0 is going to be the base point in what follows. Since L(k) is analytic in k, this implies that, for δ sufficiently small, when $|k - k_0| < \delta$, the span, R(k), of the eigenvectors of L(k) belonging to eigenvalues in $|\tau - \tau_0| < \delta$ has a basis $\{\psi_1(x,k), \psi_2(x,k)\}$ which is orthonormal and real analytic in k. The restriction of L(k) to R(k) has the matrix

(5)
$$\begin{pmatrix} a(k) & b(k) \\ \overline{b}(k) & c(k) \end{pmatrix}$$

in terms of this basis, where the entries are real-analytic and a and c are real.

Next the potential is assumed to have the symmetry V(x) = V(-x). This symmetry is typical of metals. With this symmetry L(k) commutes with the involution $[If](x) = \overline{f}(-x)$. The 1-eigenspace of I, considered as a real-linear transformation of