Astérisque

JAMES RALSTON Magnetic breakdown

Astérisque, tome 210 (1992), p. 263-282 http://www.numdam.org/item?id=AST 1992 210 263 0>

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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

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

R(k), must be two dimensional, and it depends analytically on k. Thus one can assume that ψ_1 and ψ_2 belong to this subspace, and this forces b(k) in (5) to be real-valued. This consequence of V(x) = V(-x) is well-known (it is used in [10]), but I am grateful to J. Sjöstrand for explaining it to me. The symmetry has the effect of changing the set of k where $E_n(k) = E_{n+1}(k)$ from just k_0 , as it would be for a generic matrix of the form (5), to a curve through k_0 in the generic case.

Next I assume that we are in the generic case.¹ For this I simply assume that a, b and c have linearly independent gradients at k_0 . Since

$$D \equiv \det \begin{pmatrix} a(k) - \tau & b(k) \\ b(k) & c(k) - \tau \end{pmatrix} = \left(\frac{a+c}{2} - \tau\right)^2 - \left(\frac{a-c}{2}\right)^2 - b^2,$$

we see that $E_n(k) = E_{n+1}(k)$ on the analytic curve $\Gamma = \{k : a - c = b = 0\}$ through k_0 , and the surfaces D = 0 have conic singularities on Γ (see Figure 1). Here we consider τ as a parameter.



Figure 1. The Cone $D(\cdot, \tau) = 0$

The final hypothesis will insure that we are in the situation where magnetic breakdown occurs. One checks easily that on the trajectories of the Hamiltonian $E_n(p+A(y)) - \tau$ the function k = p+A(y)

¹Note that generic here means generic among symmetric real 2×2 matrices scalar at k_0 .

satisfies

$$\dot{k} = \omega \times \frac{\partial E_n}{\partial k}(k).$$

Hence k moves on the intersection of the surfaces D = 0 with a plane $k \cdot \omega = c$. To get magnetic breakdown we need to choose ω so that these planes cut both nappes of the cone D = 0. Thus we assume that the plane $k \cdot \omega = k_0 \cdot \omega$ cuts both nappes of $D(k, \tau_0) = 0$ nontangentially.

With these hypotheses we can put our problem in a standard form. We translate and rotate coordinates in k-space so that the vertex of $D(\cdot, \tau) = 0$ is the origin for all τ , $\omega = \hat{e}_3$ and the Hessian matrix of D in (k_1, k_2) is diagonal at the origin with $\frac{\partial^2 D}{\partial k_1^2}(0) >$ 0. This is possible because the magnetic breakdown hypothesis implies that the Hessian is indefinite. Then, using the Weierstrass preparation theorem (trivially) in k_1 , we have

$$D = ((k_1 - r)^2 - q)Q_0$$

where $r = r(k_2, k_3, \tau)$, $q = q(k_2, k_3, \tau)$ and $Q_0(0, \tau_0) > 0$. Moreover, the preceding choices of coordinates imply $r = \frac{\partial r}{\partial k_2} = q = \frac{\partial q}{\partial k_i} = 0$ at $(0, \tau_0)$, and the Hessian of q is positive definite. Since $\omega = \hat{e}_3$, it will be convenient to choose $A(y) = y_1 \hat{e}_2$ instead of $\frac{1}{2}\omega \times y$ from here on.

II. THE BASIC ANSATZ AND THE EICHONAL

We are now ready to construct asymptotic solutions to (2) in the magnetic breakdown case. We will use the general Ansatz

(6)
$$u = \int_C e^{\frac{-i}{\varepsilon}\varphi} m dz,$$

where $\varphi = \varphi_0(y_1, z) + \tau t + \xi_2 y_3 + \xi_3 y_3$ and C is a contour to be determined. Thus we assume linear dependence of the phase on all space-time variables except y_1 . However, the construction will be uniform in the parameters (ξ_2, τ) on a neighborhood of $((k_0)_2, \tau_0)$ so

that one can construct more general wave packets with (crystal) momentum localized around k_0 by superposition in these parameters.

At this point I could simply write out the rest of the Ansatz in detail, but I would like to try to motivate the choices. When one substitutes (6) into (2), one does not need to set coefficients of powers of ε in the integrand to zero. As long as the coefficients are equal to smooth multiples of $\frac{\partial \varphi}{\partial z}$ one sees by integration by parts that they contribute to terms with an additional power of ε . Since we assume that $m = m_0 + \varepsilon \ m_1 + \cdots$ with

(7)
$$m_{0} = \alpha(y, t, z)\psi_{1}\left(\frac{y}{\varepsilon}, \frac{\partial\varphi}{\partial y} + y_{1}\hat{e}_{1}\right) + \beta(y, t, z)\psi_{2}\left(\frac{y}{\varepsilon}, \frac{\partial\varphi}{\partial y} + y_{1}\hat{e}_{1}\right),$$

the analog for (6) of the eichonal equation (4) is

(8)
$$D\left(\frac{\partial\varphi}{\partial y_1}, \xi_2 + y_1, \xi_3, \tau\right) = \frac{\partial\varphi}{\partial z}R$$

where R is analytic in z. This condition merely says that $D(\partial \varphi / \partial y_1, \xi_2 + y_1, \xi_3, \tau)$ and $\partial \varphi / \partial z$ have the same zeros as functions of z, which is implied by

(9)
$$0 = \left(\frac{\partial \varphi_0}{\partial y_1} - r(\xi_2 + y_1, \xi_3, \tau)\right)^2 - q(\xi_2 + y_1, \xi_3, \tau) \iff \frac{\partial \varphi_0}{\partial z} = 0.$$

A simple way to achieve (9) is to choose φ_0 so that $\partial \varphi_0 / \partial y_1$ is linear in z and $\partial \varphi_0 / \partial z$ has the zero set of a quadratic function of z. A choice with these properties is

$$\varphi_0 = \frac{z^2}{4} - fz - \frac{h}{2}\log z + g,$$

where $f = f(\xi_2 + y_1, \xi_3, \tau)$, $h = h(\xi_3, \tau)$ and $g = g(y_1 + \xi_2, \xi_3, \tau)$. This reduces (9) to

(10)
$$\frac{\partial f}{\partial k_2}\sqrt{f^2 + h} = \sqrt{q}$$

to be solved with h independent of k_2 and $\frac{\partial f}{\partial k_2}(k_0, \tau_0) > 0$. This problem has been treated in a similar setting by Gérard and Grigis in [3] and solved in exactly this setting by Horn [7]. One sees that (10) implies

$$h(k_3, \ \tau) = \frac{1}{\pi i} \int_{\gamma} \sqrt{q(\zeta, k_3, \tau)} d\zeta,$$

where γ encloses the (two) zeros of $q(\zeta, k_3, \tau)$ near $\zeta = 0$. From this it follows that

(11)
$$h(k_3, \tau) = \frac{2\sqrt{2} \det(\operatorname{Hess} D(0, \tau))}{(-\det(\operatorname{Hess} D|_{\hat{e}_3} \cdot k_{=0}(0, \tau)))^{3/2}} k_3^2 + O(k_3^3).$$

As we will see, h determines the strength of the magnetic breakdown. The formula (11) (with a few typographic errors) was already given by Slutskin in [10].

The function f is assumed to be real-valued here. However, if one takes

$$\varphi_{\mathbf{0}} = \frac{z^2}{4} + i\tilde{f}z + \frac{h}{2}\log z + \tilde{g},$$

one is again lead to (10) for \tilde{f} and \tilde{h} . This gives another family of asymptotic solutions which we will not discuss here (see Horn [7]).

We will take $\{te^{3i\pi/4}, t > 0\}$ as the branch cut in the definition of log z and choose $C = \{se^{3i\pi/4} - 1, s \in \mathbb{R}\}$ with the orientation in Figure 2



Figure 2

To see how this Ansatz incorporates the tunnelling effect of magnetic breakdown one can (when h > 0) use the method of steepest descents. Denoting the two zeros of $\frac{\partial \varphi}{\partial z}$ as $z_{\pm} = f \pm \sqrt{f^2 + h}$, one has for f < 0 the steepest descent curves $Re\{\varphi(z)\} = Re\{\varphi(z_+)\}$ and $Re\{\varphi(z)\} = Re\{(\varphi(z_-))\}$ as shown in Figure 3.



Figure 3

Since C can be deformed to Γ_{-} , the method of steepest descent shows that for f < 0, (6) reduces to (3) with $\varphi(y, t) = \varphi(z_{-})$. However, when f > 0 the steepest descent curves become those shown in Figure 4.



Now C cannot be deformed to a steepest descent curve. One can only deform C to the curve Γ indicated by dots in Fig. 4. Now in addition to the contribution from z_{-} there is a contribution from z_{+} . Since $Im\{\varphi(z)\}$ decreases by $\frac{\pi}{2}h$ as one goes along the lower half of the loop, the latter contribution is weaker by a factor of $\exp\left(-\frac{\pi h}{2\varepsilon}\right)$. This is the tunnelling term, and it explains the earlier remark that h measures the strength of magnetic breakdown. Since we are not claiming to construct solutions valid with exponentially small errors, the only rigorous results here on magnetic breakdown will follow from showing that the asymptotics just described hold uniformly for h in $[0, h_0]$. This was carried out in Horn [7]. One notes that

$$F(x) = \int_C e^{-\frac{i}{\varepsilon} \left(\frac{z^2}{4} - xz - \frac{h}{2}\log z\right)} dz$$

is a solution of a second order ordinary differential equation for which one can construct two bases of solutions having simple asymptotics for $h \in [0, h_0]$ when x > 0 and when x < 0 respectively. Using the explicit computation of these basis functions at x = 0 to match them across x = 0, one computes the asymptotics of F for x > 0, uniformly on $(0, h_0)$. The key step is expressing F, properly normalized, in terms of the basis with simple asymptotics for x > 0. The result of this computation is the identity (with $\gamma = h/2\varepsilon$) (11')

$$W_{1}(x) = e^{-\pi\gamma}Y_{1}(x) + (1 - e^{-2\pi\gamma})^{1/2}e^{i\left(\frac{\pi}{4} - \gamma \log \gamma + \gamma + \operatorname{Arg}\Gamma(i\gamma)\right)}W_{2}(x),$$

where

$$\begin{split} W_1(x) &= e^{-\pi\gamma}(\varepsilon h)^{-1/2} \int_C e^{\frac{-i}{\varepsilon}(\frac{z^2}{4} - xz - \frac{h}{2}\log z)} dz \\ Y_1 &= (\varepsilon h)^{-1/2} \int_{C'} e^{\frac{-i}{\varepsilon}(\frac{z^2}{4} - xz - \frac{h}{2}\log z)} dz, \quad \text{and} \\ W_2(x) &= \varepsilon^{-1/2} e^{\frac{\pi\gamma}{2}} e^{i(\gamma\log h - \gamma - \frac{\pi}{2})} \int_C e^{\frac{-i}{\varepsilon}(\frac{z^2}{4} + ixz + \frac{h}{2}\log z - x^2)} dz. \end{split}$$

Here $C' = \{se^{3i\pi/4} + 1, s \in R\}$ with the orientation in Figure 2. The choice of normalizing factors here makes the asymptotics of W_1 as $\varepsilon \to 0$ with h > 0 fixed and x < 0 match the asymptotics of W_2 as $\varepsilon \to 0$ with h > 0 fixed and x > 0. These asymptotics give terms of order zero as do the asymptotics of Y_1 . Since modulo terms of order ε one can assume m is of the form a + bz in (6), the function u in our Ansatz can be expressed in terms of $W_1(f)$ and $W'_1(f)$. Thus the identity (11') is a computation of magnetic breakdown: note that the coefficient of Y_1 is the tunnelling coefficient, and by Stirling's formula the coefficient of W_2 tends to 1 as $\gamma \to \infty$. Once again this formula appears in Slutskin [10, formula (32)]. The computation of tunnelling strength is also related to that given by Hagedorn in [5]. Since we do not justify exponentially small terms here, (11') gives information to us when $\frac{h}{2\varepsilon} = 0(1)$, i.e. in the regime where $k_3 = O(\varepsilon^{1/2})$ and tunnelling is significant.

The functions W_1 , W_2 and Y_1 are related to parabolic-cylinder or Weber functions, but I feel that the integral representation is more transparent.

III. THE TRANSPORT EQUATIONS

If one makes the choice in (7) for m_0 , the terms of order ε^0 in the integrand resulting from substituting (6) into (2) will contribute

terms of order ε after integration by parts provided

(12)
$$\begin{pmatrix} a & b \\ b & c \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \tau \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

at z_{\pm} . Here, as always from here on, the entries a, b, c are evaluated at $k = \frac{\partial \varphi}{\partial y} + y_1 \hat{e}_2$. We will need to solve such equations systematically in this section. One way to do this is as follows. For any analytic function g(z) we set

$$g^{s} = \frac{1}{2}g(z_{+}) + \frac{1}{2}g(z_{-})$$
 and $g^{a} = \frac{g(z_{+}) - g(z_{-})}{(z_{+} - z_{-})}$.

Then g^s and g^a are analytic functions of f and h, $g(z_{\pm}) = g^s \pm \sqrt{f^2 + h}g^a$, and

$$g(z) = g^s + (z - f)g^a \mod z \frac{\partial \varphi}{\partial z}$$

Using the same notation for matrices and setting $A_0 = \begin{pmatrix} a - \tau & b \\ b & c - \tau \end{pmatrix}$, one sees that (12) holds at z_{\pm} , if and only if

$$0 = \begin{pmatrix} A_0^s & (f^2 + h)A_0^a \\ A_0^a & A_0^s \\ \beta & \beta & \beta \\ \alpha^c \\ \beta^a \end{pmatrix}.$$

Setting

$$U = \begin{pmatrix} I & 0 \\ -\frac{1}{2}(f^2 + h)^{-1/2}I & I \end{pmatrix} \begin{pmatrix} I & (f^2 + h)^{1/2}I \\ 0 & I \end{pmatrix}$$

and $M_0 = \begin{pmatrix} A_0^s & (f^2+h)A_0^a \\ A_0^a & A_0^s \end{pmatrix}$, we have $\begin{pmatrix} A_0(z_+) & 0 \\ 0 & A_0(z_-) \end{pmatrix} = UM_0U^{-1}$. Hence M_0 has rank at most 2. However, when f = h = 0 and $\tau = \tau_0$

$$A_{\mathbf{0}}^{a} = \begin{pmatrix} \frac{\partial a}{\partial k_{1}}(k_{\mathbf{0}}) & \frac{\partial b}{\partial k_{1}}(k_{\mathbf{0}}) \\ \frac{\partial b}{\partial k_{1}}(k_{\mathbf{0}}) & \frac{\partial c}{\partial k_{1}}(k_{\mathbf{0}}) \end{pmatrix}$$

and, since $\frac{\partial^2 D}{\partial k_1^2}(k_0, \tau_0) > 0$, it follows that A_0^a is nonsingular at the base point. Thus M_0 has rank exactly 2 near the base point and (12) holds if and only if

$$A_0^a \begin{pmatrix} \alpha^s \\ \beta^s \end{pmatrix} + A_0^s \begin{pmatrix} \alpha^a \\ \beta^a \end{pmatrix} = 0.$$

In other words for each choice of $\begin{pmatrix} \alpha^a \\ \beta^a \end{pmatrix}$ there is a unique $\begin{pmatrix} \alpha \\ \beta \end{pmatrix}$ mod $z \frac{\partial \varphi}{\partial z}$ satisfying (12). One checks easily that a convenient basis for these solutions is

$$v_1 = \begin{pmatrix} -b \\ a - \tau \end{pmatrix}, \qquad v_2 = \begin{pmatrix} c - \tau \\ -b \end{pmatrix},$$

and hence the general choice for m_0 is $m_0 = (-b\delta + (c - \tau)\gamma)\psi_1 + ((a - \tau)\delta - b\gamma)\psi_2$, where γ and δ are arbitrary functions of (y, t, z). With this choice of m_0 we assume that m in (6) has the form $m = m_0(y/\varepsilon, y, t, z) + \varepsilon m_1(y/\varepsilon, y, t, z) + \cdots$ where $m_1(x, y, z) = \alpha_1\phi_1\left(x, \frac{\partial\varphi}{\partial y} + y_1\hat{e}_2\right) + \beta_1\psi_2\left(x, \frac{\partial\varphi}{\partial y} + y_1\hat{e}_2\right) + \tilde{m}_1(x, y, z)$. The function \tilde{m}_1 is assumed to be orthogonal to $\psi_1\left(x, \frac{\partial\varphi}{\partial y} + y_1\hat{e}_2\right)$ and $\psi_2\left(x, \frac{\partial\varphi}{\partial y} + y_1\hat{e}_2\right)$ in x over a fundamental domain in the lattice.

The "transport" equations arise as follows. When we substitute (6) into (2) and eliminate terms of order ε^0 from the integrand by integration by parts, we need to solve inhomogeneous problems $L(k)\tilde{m_1} - \tau \tilde{m_1} = g$ to eliminate the terms of order ε . The condition that the inhomogeneous terms be orthogonal to ψ_1 and ψ_2 over a fundamental domain leads to the transport equations

$$\begin{pmatrix} \frac{\partial a}{\partial k_1} & \frac{\partial b}{\partial k_1} \\ \frac{\partial b}{\partial k_1} & \frac{\partial c}{\partial k_1} \end{pmatrix} \begin{bmatrix} \begin{pmatrix} c-\tau & -b \\ -b & a-\tau \end{pmatrix} \begin{pmatrix} \gamma \\ \delta \end{bmatrix}_{y_1} - \begin{bmatrix} \begin{pmatrix} c-\tau & -b \\ -b & a-\tau \end{pmatrix} \begin{pmatrix} \gamma \\ \delta \end{bmatrix}_t$$

(13)
$$- R \begin{pmatrix} \gamma \\ \delta \end{pmatrix}_{z} + D \begin{pmatrix} \gamma \\ \delta \end{pmatrix} + \begin{pmatrix} a - \tau & b \\ b & c - \tau \end{pmatrix} \begin{pmatrix} \gamma_{0} \\ \delta_{0} \end{pmatrix}$$
$$= \begin{pmatrix} 0 \\ 0 \end{pmatrix} \mod z \frac{\partial \varphi}{\partial z}.$$

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Here R is from (8), D is a very complicated (but real-analytic) matrix, and $(\gamma_0, \delta_0) = (i\alpha_1, i\beta_1) + (f_1, f_2)$, where (f_1, f_2) are determined by (γ, δ) . Hence we can treat (γ_0, δ_0) as an arbitrary vector which determines $A_0\begin{pmatrix}\alpha_1\\\beta_1\end{pmatrix}$. Thus, solving (13), determines (α_1, β_1) up to a solution of (12). Expanding this solution in terms of v_1 and v_2 , we get higher order transport equations for the resulting coefficients when we try to eliminate the terms of order ε^2 . Thus provided we can solve (13) and the analogous inhomogeneous equation we will be able to eliminate terms of all orders in ε .

To reduce (13) to an equation for γ^s , δ^s , γ^a and δ^a we set

$$B = \begin{pmatrix} \frac{\partial a}{\partial k_1} & \frac{\partial b}{\partial k_1} \\ \frac{\partial b}{\partial k_1} & \frac{\partial c}{\partial k_1} \end{pmatrix} \quad \text{and} \quad A_1 = \begin{pmatrix} c - \tau & -b \\ -b & a - \tau \end{pmatrix},$$

and we assume that γ and δ are linear in z, so that $R\left(\frac{\gamma}{\delta}\right)_z \mod z \frac{\partial \varphi}{\partial z}$ does not bring in new terms. This is no loss of generality in the *Ansatz* since one can always reduce γ and δ to linear functions in z by integration by parts, changing m_1 . With these definitions we have

$$(14) \qquad \begin{pmatrix} B^{s} & (f^{2}+h)B^{a} \\ B^{a} & B^{s} \end{pmatrix} \begin{bmatrix} \begin{pmatrix} A^{s}_{1} & (f^{2}+h)A^{a}_{1} \\ A^{a}_{1} & A^{s}_{1} \end{bmatrix} \begin{pmatrix} \gamma^{s} \\ \gamma^{a} \\ \delta^{a} \end{pmatrix} \end{bmatrix}_{y_{1}}$$
$$- \begin{bmatrix} \begin{pmatrix} A^{s}_{1} & (f^{2}+h)A^{a}_{1} \\ A^{a}_{1} & A^{s}_{1} \end{bmatrix} \begin{pmatrix} \gamma^{s} \\ \delta^{s} \\ \gamma^{a} \\ \delta^{a} \end{pmatrix} \end{bmatrix}_{t} + E \begin{pmatrix} \gamma^{s} \\ \delta^{s} \\ \gamma^{a} \\ \delta^{a} \end{pmatrix}$$
$$+ \begin{pmatrix} A^{s}_{0} & (f^{2}+h)A^{a}_{0} \\ A^{a}_{0} & A^{s}_{0} \end{bmatrix} \begin{pmatrix} \gamma^{s} \\ \delta^{s} \\ \gamma^{a} \\ \delta^{a} \\ \delta^{a} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}.$$

Here E is a new complicated matrix. Since $A_1 = JA_0J^{-1}$ for $J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$, the coefficient

$$M_{1} = \begin{pmatrix} A_{1}^{s} & (f^{2} + h)A_{1}^{a} \\ A_{1}^{a} & A_{1}^{s} \end{pmatrix}$$

has the properties of M_0 . In particular it has rank 2 near the base point and A_1^a is nonsingular.

Making the change of variables

$$\begin{pmatrix} \gamma^{s} \\ \delta^{s} \\ \gamma^{a} \\ \delta^{a} \end{pmatrix} = \begin{pmatrix} I \\ 0 \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} + \begin{pmatrix} (A_{1}^{a})^{-1}A_{1}^{s} \\ -I \end{pmatrix} \begin{pmatrix} w \\ x \end{pmatrix},$$

the transport equation (14) becomes

(15)

$$\begin{pmatrix}
B^{s} & (f^{2} + h)B^{a} \\
B^{a} & B^{s}
\end{pmatrix}
\begin{bmatrix}
\begin{pmatrix}
A^{s}_{1} \\
A^{a}_{1}
\end{pmatrix}
\begin{pmatrix}
u \\
v
\end{pmatrix}
\end{bmatrix}_{y_{1}} -
\begin{bmatrix}
\begin{pmatrix}
A^{s}_{1} \\
A^{a}_{1}
\end{pmatrix}
\begin{pmatrix}
u \\
v
\end{pmatrix}
\end{bmatrix}_{t} \\
+ F\begin{pmatrix}
u \\
v
\end{pmatrix} + G\begin{pmatrix}
w \\
x
\end{pmatrix} = 0 \mod \begin{pmatrix}
A^{s}_{0} \\
A^{a}_{0}
\end{pmatrix},$$

where F and G are 4×2 matrices. Finally, since A_0^a is invertible, we can simply eliminate the last two components in (15) to get the fully reduced transport equations

(16)
$$\hat{B}\begin{pmatrix} u\\v \end{pmatrix}_{y_1} - \hat{A}\begin{pmatrix} u\\v \end{pmatrix}_t + \hat{F}\begin{pmatrix} u\\v \end{pmatrix} = \hat{G}\begin{pmatrix} w\\x \end{pmatrix}$$

where

$$\hat{A} = A_1^s - A_0^s (A_0^a)^{-1} A_1^a \quad \text{and} \\ \hat{B} = B^s A_1^s + (f^2 + h) B^a A_1^a - A_0^s (A_0^a)^{-1} (B^a A_1^s + B^s A_1^a).$$

Restricted to h = 0, i.e. to the plane $k_3 = 0$ passing through the vertex in Figure 1, the matrix A_0^s and hence A_1^s must be divisible by f. This makes the transport system (16) Fuchsian on $k_3 = 0$. Since $k_2 = \xi_2 + y_1$ and $\frac{\partial f}{\partial k_2} > 0$, we can use f in place of y_1 as a coordinate in (16) so that on $k_3 = 0$ (16) takes the form

(17)
$$f\left(\tilde{B}\begin{pmatrix} u\\v \end{pmatrix}_{f} - \tilde{A}\begin{pmatrix} u\\v \end{pmatrix}_{t}\right) + \hat{F}\begin{pmatrix} u\\v \end{pmatrix} = H$$

where $\tilde{B} = 2 \frac{\partial A_0}{\partial k_1} \frac{\partial A_1}{\partial k_2} + O(f)$. Since $\partial^2 D / \partial k_2^2 < 0$, det $\frac{\partial A_0}{\partial k_2} < 0$, and hence \tilde{B} is invertible. Moreover, $f\tilde{B}(A_1^s)^{-1}$ is symmetric with positive determinant near f = 0 and $\tilde{A}(A_1^s)^{-1}$ is symmetric. Hence, an analytic change of dependent variables makes (17) into a Fuchsian symmetric hyperbolic system. The equation (17) has a unique analytic solution for given analytic H, provided the matrix

$$\tilde{B}^{-1}(k_0, \tau_0)\hat{F}(k_0, \tau_0)$$

has no nonpositive integer eigenvalues (this is the "indicial" condition, see Baouendi and Goulaouic [1]). In addition, since (17) can be made symmetric hyperbolic, the work of Tahara [11] (see particularly Theorem 4.1 of part II and the Introduction of III) shows that under the same indicial condition (17) has a unique C^{∞} solution for a given C^{∞} function H(f,t). Thus to exhibit packets undergoing magnetic breakdown we may proceed as follows. Choosing $\hat{G}\begin{pmatrix} w\\ x \end{pmatrix}$ supported in f < 0 with support near t = 0and assuming the indicial condition, we construct $\begin{pmatrix} u\\ v \end{pmatrix}$ depending smoothly on k_3 so that (16) holds to order k_3^{∞} . Since we are only interested in $k_3 = O(\varepsilon^{1/2})$, the errors in solving (16) are $O(\varepsilon^{\infty})$. As mentioned in the introduction, $\begin{pmatrix} u\\ v \end{pmatrix}$ and all its k_3 -derivatives at $k_3 = 0$ are uniquely determined by $\hat{G}\begin{pmatrix} w\\ x \end{pmatrix}$.

To complete this analysis we need to see what form the term $\hat{G}(\frac{w}{x})$ can have. The terms which contribute to $G(\frac{w}{x})$ come from

$$(\langle \psi_1, -(R\gamma\psi_1 + R\delta\psi_2)_z \rangle, \langle \psi_1, -(R\gamma\psi_1 + R\delta\psi_2)_z \rangle)$$

where \langle , \rangle denotes the L²-inner product over a fundamental domain in the lattice. From (8) on sees that

$$R = 2z \left(\frac{\partial f}{\partial k_2}\right)^2 Q_0 \left(\frac{\partial \varphi}{\partial y_1}, \xi_2 + y_1, \xi_3, \tau\right),$$

and, hence R = zP where P is analytic in z and positive at the base point. From this one concludes that

$$G = -\begin{pmatrix} P^{s}I + (zM)^{s} & (f^{2} + h)(P^{a}I + (zM)^{a}) + zPI^{s} \\ P^{a}I + (zM)^{a} & P^{s}I + (zM)^{s} + (zP)^{a}I \end{pmatrix} \begin{pmatrix} (A^{a}_{1})^{-1}A^{s}_{1} \\ -I \end{pmatrix},$$

where M is the matrix

$$P\begin{pmatrix} \langle \psi_1, \ \psi_{1z} \rangle & \langle \psi_1, \ \psi_{2z} \rangle \\ \langle \psi_2, \ \psi_{1z} \rangle & \langle \psi_2, \ \psi_{2z} \rangle \end{pmatrix}.$$

Since $(zC)^s = fC^s + (f^2 + h)C^a$ and $(zC)^a = fC^a + C^s$ for any C, this leads to

$$\begin{split} \hat{G} &= -P^{s}((A_{1}^{a})^{-1}A_{1}^{s} + 2A_{0}^{s}(A_{0}^{a})^{-1} - fI) \\ &- P^{a}(fA_{0}^{s}(A_{0}^{a})^{-1} - (f^{2} + h)I) \\ &- (fM^{s} + (f^{2} + h)M^{a})(A_{1}^{a})^{-1}A_{1}^{s} + (f^{2} + h)(fM^{a} + M^{s}) \\ &+ A_{0}^{s}(A_{0}^{a})^{-1}(fM^{a} + M^{s})(A_{1}^{a})^{-1}A_{1}^{s}. \end{split}$$

Since $A_i^s = f \tilde{A}_i + k_3 \tilde{B}_i$, \tilde{A}_i and \tilde{B}_i analytic,

$$\begin{split} \hat{G} &= -P^s((A^a_1)^{-1}A^s_1 + 2A^s_0(A^a_0)^{-1} - fI) \\ &+ fk_3H + f^2L + k_3^2N \end{split}$$

where K, L and N are analytic matrix functions. To understand the leading term, $\hat{G}_0 = -P^s((A_1^a)^{-1}A_1^s + 2A_0^s(A_0^a)^{-1} - fI)$, one can use the following. Choosing v_{\pm} such that $A_0(z_{\pm})v_{\pm} = 0$, and $\|v_{\pm}\| = 1$, one has

$$A_0^s(A_0^a)^{-1}v_{\pm} = \pm \sqrt{f^2 + h}v_{\pm}.$$

Also one checks $A_0^s(A_0^a)^{-1}(A_1^a)^{-1}A_1^s = -(f^2+h)I$. Using these facts, it is easy to compute

$$\hat{G}_0 v_{\pm} = -P^s (-f \pm \sqrt{f^2 + h}) v_{\pm}.$$

Note that by (11) $h = k_3^2 \tilde{h}$, where \tilde{h} is analytic and nonzero at $k_3 = 0$.

To see how \hat{G} degenerates on $k_3 = 0$ one begins by noting that v_+ and v_- are discontinuous on h = 0 at f = 0. However, since $f^{-1}A_0^s(A_0^a)^{-1}$ is analytic on h = 0 with eigenvalues ± 1 , we can choose \tilde{v}_{\pm} analytic such that $A_0^s(A_0^a)^{-1}\tilde{v}_{\pm} = \pm f\tilde{v}_{\pm}$. Therefore, up to order f^2 , \hat{G} is the projection onto \tilde{v}_- along \tilde{v}_+ multiplied by $-2fP^s$ on h = 0. Thus one can choose (w, x) so that $\hat{G}(\frac{w}{x})$ is approximately $f\tilde{v}_-$ near $f = k_3 = 0$.

References

- [1] M. S. Baouendi and C. Goulaouic, "Cauchy problems with characteristic initial hypersurface," CPAM 26 (1973), 455-475.
- [2] V. Buslaev, "The quasi-classical approximation for equations with periodic coefficients," Uspekhi Mat. Nauk 42 (1987), 77-98.
- [2a] V. Buslaev, "On spectral properties of adiabatically perturbed Schrödinger operators with periodic potentials," Seminaire EDP 1990-91, Ecole Polytechnique, Expose 23, April 1991.
 - [3] C. Gerard and A. Grigis, "Precise estimates of tunnelling and eigenvalues near a potential barrier," J. Diff. Eq. 72 (1988), 149-177.
 - [4] J.-C. Guillot, J. Ralston and E. Trubowitz, "Semi-classical asymptotics in solid state physics," *Commun. Math. Phys.* 116 (1988), 401.
 - [5] G. A. Hagedorn, "Electron energy level crossings in the timedependent Born-Oppenheimer approximation," *Theoretica Chimica Acta* 77 (1990), 163-190.
 - [6] B. Helffer and J. Sjöstrand, "On diamagnetism and de Haasvan Alphen effects," Ann. Inst. H. Poincaré 52 (1990), 303-375.
 - [7] W. Horn, "Semi-classical constructions in solid state physics," Comm. in P.D.E. 16 (1991), 255-290.
 - [8] C. März, "Spectral asymptotics for Hill's equation near the potential maximum," to appear Asymptotic Analysis.
 - [9] J. Sjöstrand, "Density of states oscillations for magnetic Schrödinger operators," preprint Orsay, 1991.

- [10] A. A. Slutskin, "Dynamics of conduction electrons under magnetic breakdown conditions," *Soviet Physics JETP* 26 (1968), 474-482.
- [11] H. Tahara, "Singular hyperbolic systems I, II, III," J. Fac. Sci. Tokyo, Sec. IA Math. 26 (1979), 213-238, 26 (1979), 391-412, 27 (1980), 465-507.

Department of Mathematics UCLA Los Angeles, California 90024-1555