Gaussian Beam Construction for Adiabatic Perturbations

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1 Introduction

The quantum dynamics of a Bloch electron in a crystal subject to external electric and magnetic fields, $\nabla_y V(y)$ and $\nabla_y \times A(y)$, which vary slowly on the scale of the crystal lattice, is governed by the Schrödinger equation

$$D_t u = P_\epsilon u, \quad u_{|t=0} = u_\epsilon(y),\ D = \frac{1}{i}\partial \tag{1}$$

$$P_\epsilon = (\epsilon D_y + A(y))^2 + V_0(\frac{y}{\epsilon}) + V(y).$$

Here V_0 is periodic with respect to the crystal lattice $\Gamma \subset R^3$, and it models the electric potential generated by the lattice of atoms in the crystal.

There has been a growing interest in the rigorous study of dynamics of Bloch electrons in the presence of slowly varying external perturbations (see [1,3,4,5,6,7,11,12,14,16,18,20,22,27]). Since the work of Peierls [21] and Slater [26], it is well known that, if ϵ is sufficiently small, then solutions of (1) for suitable initial data u_ϵ are in some sense governed by the "semi-classical" Hamiltonian

$$H(y,\eta) = \lambda(\eta + A(y)) + V(y).$$

Here $\lambda(\xi)$ is one of the "band functions" describing the Floquet spectrum of the unperturbed Hamiltonian $P_0 = -\Delta_x + V_0(x),\ x = y/\epsilon$.

The purpose of this paper is to construct nontrivial asymptotic solutions of (1) which are concentrated near $\gamma = \{(y(s), s),\ -\infty < s < +\infty\}$, the projection into space-time of a trajectory of the Hamiltonian H. We can allow A and V to have a slow time dependence as well, i.e. $A = A(\epsilon x, \epsilon t)$ and $V = V(\epsilon x, \epsilon t)$, which changes H to

$$H(y, \eta, s) = \lambda(\eta + A(y, s)) + V(y, s).$$

This construction was presented in [7] with only a sketch of the "Gaussian beam" method which gives asymptotic solutions over arbitrarily long time intervals. We give the details of that method here.

2 Preliminaries

Let $\Gamma = \oplus_{i=1}^{3} Z a_i$ be the lattice generated by the basis a_1, a_2, a_3, $a_i \in R^3$. The reciprocal lattice Γ^* is defined as the lattice generated by the dual basis $\{a_1^*, a_2^*, a_3^*\}$ determined by $a_i \cdot a_j^* = 2\pi\delta_{ij}$, $i, j = 1, 2, 3$. Let E be a fundamental domain for Γ, and let E^* be a fundamental domain for Γ^*. If we identify opposite edges of E (resp. E^*) then it becomes a flat torus denoted by $T = R^3/\Gamma$ (resp. $T^* = R^3/\Gamma^*$).

Let V_0 be a real-valued potential, C^∞ and Γ-periodic. For k in R^3, we define

$$P_k = (D_x + k)^2 + V_0(x).$$

as an unbounded operator on $L^2(T)$ with domain $H^2(T)$. The hamiltonian P_k is a semi-bounded and self-adjoint. Since the resolvent of $(D_x + k)^2$ is compact, the resolvent of P_k is also compact, and therefore P_k has a complete set of (normalized) eigenfunctions $\Phi_n(\cdot, k) \in H^2(T^*)$, $n \in N$, called Bloch functions. The corresponding eigenvalues accumulate at infinity and we enumerate them according to their multiplicities,

$$\lambda_1(k) \leq \lambda_2(k) \leq \ldots.$$

Since $e^{-ix\gamma^*} P_k e^{ix\gamma^*} = P_{\gamma^* + k}$, $\lambda_n(k)$ is periodic with respect to Γ^*. The function $\lambda_n(k)$ is called a band function and the closed intervals $\Lambda_n := \lambda_n(T^*)$ are called bands.

Standard perturbation theory shows that $\lambda_n(k)$ is a continuous function of k and is real analytic in a neighborhood of any k such that

$$\lambda_{n-1}(k) < \lambda_n(k) < \lambda_{n+1}(k). \tag{2}$$

We make the following hypothesis on the spectrum of the unperturbed Schrödinger operator

(H1) *For a given n_0 we will assume that $\lambda_{n_0}(k)$ satisfies (2) for all k*

Under this assumption we can choose the eigenfunction $\Phi_{n_0}(x,k)$ associated to $\lambda_{n_0}(k)$ to be a real-analytic function of k with values in $H^2(T)$.

Turning now to equation (1), we assume that $A(y,s)$ and $V(y,s)$ are smooth and that the derivatives $\partial^{\alpha}_{y,s}A$ and $\partial^{\beta}_{y,s}V$ are bounded on $R^3 \times R$ for $|\alpha| \geq 1$ and $|\beta| \geq 0$. To construct asymptotic solutions of (1) we use, as in [4,7,8,11,12], the two-scale expansion method in which the electron coordinate x and the slowly varying space variable $y = \epsilon x$ are regarded as independent variables, and we introduce the slow time variable $s = \epsilon t$. Thus, we consider the following equation in the independent variables x, y and s:

$$\epsilon D_s v = Pv, \text{ where}$$

$$Pv = \left[(\epsilon D_y + D_x + A(y,s))^2 + V_0(x) + V(y,s)\right] v \tag{3}$$

Note that, if in the solution $v(x,y,s,\epsilon)$ of (3) we let $x = y/\epsilon$ and $t = s/\epsilon$ then it becomes a solution of (1). In the variable x, $v(x,y,s,\epsilon)$ is required to be periodic.

We look for approximate solution to (3), which have the form :

$$v(x,y,s,\epsilon) = e^{i\phi(y,s)/\epsilon}\Big[m_0(x,y,s) + \epsilon m_1(x,y,s) + \cdots + \epsilon^N m_N(x,y,s)\Big] \tag{4}$$

Now substituting (4) into (3) and collecting terms which are the same order in ϵ, we get

$$(\epsilon D_s - P)v = e^{i\phi(y,s)/\epsilon}\Big[c_0(x,y,s) + \epsilon c_1(x,y,s) + \cdots + \epsilon^{N+2} c_{N+2}(x,y,s)\Big] \tag{5}$$

where

$$c_0(x,y,s) = \left[\frac{\partial\phi}{\partial s} - H_0\left(k(y,s)\right) - V(y,s)\right] m_0, \tag{6}$$

$$c_1(x,y,s) = Km_0 - \left[H_0\left(k(y,s)\right) + V(y,s) - \frac{\partial\phi}{\partial s}(y,s)\right] m_1, \tag{7}$$

and for $j = 2, 3, ..., N+2$

$$c_j(x,y,s) = Km_{j-1} + \Delta_y m_{j-2} - \left[H_0\left(k(y,s)\right) + V(y,s) - \frac{\partial\phi}{\partial s}(y,s)\right] m_j.$$

Here

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

and

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

Notice that, when ϕ is real-valued, (4) is the standard ansatz of geometric optics. In the construction of geometric optics solutions one requires that

$$c_0(x,y,s) = 0, \quad \text{(eikonal equation)} \tag{E}$$

$$c_j(x,y,s) = 0, \quad \text{(transport equations).} \tag{T_j}$$

One can solve these equations locally by applying the classical "method of characteristics". However, as is well known, if we try to construct WKB-solutions globally (that is in some large given region) ϕ may develop singularities at "caustics", and the transport equations then become undefined. The consideration of these difficulties, beginning with Keller [17] and Maslov [19], lead to the development of the theory of Fourier integral operators, e.g. as given by Hörmander [15].

Instead of Fourier integral operators we are going to use "Gaussian Beams", as in [2,22,23]. Let us explain briefly the main idea of this construction.

Given $T > 0$, we want to find $\phi, m_0, ..., m_N$ such that

$$\|(\epsilon D_s - P)v\|_{L^2(R^3/\Gamma\times R^3\times[-T,T])} = \mathcal{O}(\epsilon^N). \tag{8}$$

Since we are going to choose ϕ so that

$$\Im\phi \geq c\, d((y,s),\gamma)^2,$$

in view of (4) it suffices, assuming for instance that the intersection of the support of $c_i(x,y,s)$ with $|s| < T$ is compact, to have $(y,s) \to c_i(x,y,s)$ vanish to high order on γ uniformly with respect to $x \in R^3/\Gamma$.

In fact, (8) will follow from the obvious equality

$$d((y,s),\gamma)^m |e^{i\phi/\epsilon}| = \mathcal{O}(\epsilon^{m/2})$$

which implies that, when $c_j(x,y,s)$ vanishes to order m on γ uniformly in x,

$$\int_{|s|<T} |c_j(x,y,s)e^{i\phi/\epsilon}|^2 dy = \mathcal{O}(\epsilon^{m+3/2}),$$

uniformly on x.

3 Construction of the phase function

From now on we assume that (H1) holds, and we let Φ_{n_0} be the normalized eigenfunction corresponding to $\lambda_{n_0}(k)$:

$$H_0(k)\Phi_{n_0} = \lambda_{n_0}(k)\Phi,$$

$$\langle \Phi_{n_0}, \Phi_{n_0} \rangle = 1.$$

In view of (H1) we can assume that both $\lambda_{n_0}(k)$ and $\Phi_{n_0}(x,k)$ are real-analytic in k. From here on we will suppress the index n_0, since it remains fixed throughout the construction.

Equation (E) tells us that for all (y,s), $m_0(x,y,s)$ is an eigenfunction of $H_0(k(y,s))$ with eigenvalue $\frac{\partial \phi}{\partial s}(y,s) - V(y,s)$. Hence, under assumption (H1), we can satisfy (E) by choosing

$$G(y,s) := \frac{\partial \phi}{\partial s}(y,s) - \lambda\left(A(y,s) + \frac{\partial \phi}{\partial y}(y,s)\right) + V(y,s) = 0, \text{(eikonal equation)}, \tag{9}$$

and setting

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

Set

$$h(y,s,\eta,\sigma) = \sigma - \lambda\left(A(y,s) + \eta\right) - V(y,s),$$

and let $(y(s), s, \eta(s), \sigma(s))$ be a trajectory of the hamiltonian flow generated by $h(y,s,\eta,\sigma)$, i.e.,

$$\dot{y} = -\frac{\partial \lambda}{\partial k}(A(y,s)+\eta), \quad \dot{s} = 1 \tag{10}$$

and

$$\dot{\eta} = -\sum_{i=1}^{3} \dot{y}_i \frac{\partial A_i}{\partial y}(y,s) + \frac{\partial V}{\partial y}(y,s), \;\; \dot{\sigma} = -\dot{y}\cdot\frac{\partial A}{\partial s}(y,s) + \frac{\partial V}{\partial s}(y,s). \tag{11}$$

The physical significance of these equations becomes clearer when they are rewritten in the coordinates $(y,s,k,\sigma) = (y,s,\eta + A(y),\sigma)$. It follows from (9) that

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

$$
\begin{aligned}
\dot{k} &= \dot{\eta} + \sum_{i=1}^{3} \frac{\partial A}{\partial y_i}(y,s)\dot{y}_i + \frac{\partial A}{\partial s}(y,s)\dot{s} \\
&= \sum_{i=1}^{3} \Big(\frac{\partial A}{\partial y_i}(y,s) - \frac{\partial A_i}{\partial y}(y,s) \Big) \dot{y}_i + \frac{\partial A}{\partial s}(y,s) + \frac{\partial V}{\partial y}(y,s) \\
&= -\dot{y} \times B(y,s) + \frac{\partial A}{\partial s}(y,s) + \frac{\partial V}{\partial y}(y,s).
\end{aligned}
$$

Here $B = \nabla_y \times A(y,s)$ is the magnetic field corresponding to $A(y,s)$.
Remark. *Notice that, the classical flow exists for all s. Indeed, the hamiltonian vector field $(\partial_{\eta,\sigma} h, -\partial_{y,s} h)$ is uniformly bounded with respect to (y,s,η,σ), and hence no classical trajectory can blow up in a finite time.*

From now on, we fix a trajectory $\{(y(s), s, \eta(s), \sigma(s)),\ -\infty < s < +\infty\}$ with initial data $(y_0, 0, \eta_0, \sigma_0)$ satisfying $h(y_0, 0, \eta_0, \sigma_0) = 0$. We denote by γ its projection into the (y,s)-space.

As was indicated above, we are not going to attempt to solve (9) exactly. We only need to have $G(y,s)$ vanish to high order on γ. More precisely, we are going to prove :

Theorem 1. *Let $\phi_0(y)$ be a smooth function such that the Hessian, $\Im \partial_y^2 \phi_0(y_0)$, is positive definite. Then, given N and $T > 0$, there is a smooth function $\phi(y,s)$ such that $\phi(y,0) - \phi_0(y)$ vanishes to order N at y_0, and $\phi(y,s)$ has the properties:*
i) the gradient of ϕ satisfies $(\partial_y \phi(y(s),s), \partial_s \phi(y(s),s)) = (\eta(s), \sigma(s))$

ii) in a small neighborhood Ω of γ we have

$$
G(y,s) = \mathcal{O}(d((y,s),\gamma)^N), \ \text{and} \tag{12}
$$

iii)

$$
\Im \phi(y,s) > C d((y,s),\gamma)^2 \tag{13}
$$

uniformly on $(y,s) \in \Omega \cap \{|s| < T\}$.

Proof. In this section and the next we will use the following coordinates $Y = (y_1, y_2, y_3, s)$ and $Z = (\eta_1, \eta_2, \eta_3, \sigma)$. With this notation, the condition that (12) holds to third order on $(y(s), s)$ is

$$
\frac{\partial G}{\partial Y_i} = \frac{\partial h}{\partial Y_i} + \sum_{l=1}^{4} \frac{\partial h}{\partial Z_l} \frac{\partial^2 \phi}{\partial Y_i \partial Y_l} = 0, \tag{14}
$$

$$\frac{\partial^2 G}{\partial Y_i \partial Y_j} = \frac{\partial^2 h}{\partial Y_i \partial Y_j} + \sum_{l=1}^{4} \Big[\frac{\partial^2 h}{\partial Y_i \partial Z_l} \frac{\partial^2 \phi}{\partial Y_i \partial Y_l} + \frac{\partial^2 h}{\partial Y_i \partial Z_l} \frac{\partial^2 \phi}{\partial Y_j \partial Y_l} \Big] + \tag{15}$$

$$\sum_{l=1}^{4} \sum_{m=1}^{4} \Big[\frac{\partial^2 h}{\partial Z_l \partial Z_m} \frac{\partial^2 \phi}{\partial Y_m \partial Y_j} \frac{\partial^2 \phi}{\partial Y_i \partial Y_l} + \sum_{l=1}^{4} \frac{\partial h}{\partial Z_l} \frac{\partial^3 \phi}{\partial Y_i \partial Y_j \partial Y_l} = 0,$$

Remembering the equations (10-11), (14) is just the compatibility condition

$$(\dot{\eta}(s), \dot{\sigma}(s)) = ((\partial_y \phi(y(s), s))_s, (\partial_s \phi(y(s), s))_s).$$

To study (15), we introduce the matrices $M(s)$, $A(s)$, $B(s)$ and $C(s)$ defined by

$$(M(s))_{ij} = \frac{\partial^2 \phi}{\partial Y_i \partial Y_j}(y(s), s),\ (A(s))_{ij} = \frac{\partial^2 h}{\partial Y_i \partial Y_j}(y(s), s, \eta(s), \sigma(s)),$$

$$(B(s))_{ij} = \frac{\partial^2 h}{\partial Y_i \partial Z_j}(y(s), s, \eta(s), \sigma(s)),\ (C(s))_{ij} = \frac{\partial^2 h}{\partial Z_i \partial Z_j}(y(s), s, \eta(s), \sigma(s)).$$

By observing that $\sum_{l=1}^{4} \frac{\partial h}{\partial Z_l} \frac{\partial^3 \phi}{\partial Y_i \partial Y_j \partial Y_l} = \frac{d}{ds}\Big[\frac{\partial^2 \phi}{\partial Y_i \partial Y_j}(y(s), s)\Big]$, (15) becomes

$$\dot{M}(s) + M(s)C(s)M(s) + M(s)B^t(s) + B(s)M(s) + A(s) = 0, \tag{16}$$

which is a nonlinear Ricatti equation. The initial value $M(0) = \partial^2_{y,s}\phi(y_0, 0)$ is determined by the requirement $\partial^2_y \phi(y_0, 0) = \partial^2_y \phi_0(y_0)$ and conclusion i) of the Theorem which implies $M(0)\dot{y}(0) = \dot{\eta}(0)$. Note that this makes $\Im M(0)$ positive semi-definite with null space spanned by $(\dot{y}(0), 1)$.

Since (16) is a nonlinear ODE, one has no assurance that solutions will exist for all s. However, with the choice of $M(0)$ in the preceding paragraph we will have that here. To see this, we proceed as in [23].

Lemma 1. *Let A, B and C be as above and assume that the initial value $M(0)$ is a symmetric matrix, $M(0) = M(0)^t$, such that $\Im M(0)$ is positive semi-definite with null space spanned by $(\dot{y}(0), 1)$. Then (16) has a solution defined for all s. Moreover, $M(s) = M(s)^t$, and $\Im M(s)$ is positive semi-definite with null space spanned by $(\dot{y}(s), 1)$.*

Proof. Consider the system of equations

$$\begin{aligned} \dot{Y} &= B(s)Y + A(s)Z \\ \dot{Z} &= -C(s)Y - B^t(s)Z \end{aligned} \tag{17}$$

Let $(Y^1(s), Z^1(s))$ and $(Y^2(s), Z^2(s))$ be solutions of (17) and set

$G_1(s) = \sigma((Y^1(s), Z^1(s)), (Y^2(s), Z^2(s))) =_{\rm def} Y^2(s) \cdot Z^1(s) - Y^1(s) \cdot Z^2(s)$, and

$G_2(s) = \sigma_C((Y^1(s), Z^1(s)), (Y^2(s), Z^2(s))) =_{\rm def} \overline{Y}^2(s) \cdot Z^1(s) - Y^1(s) \cdot \overline{Z}^2(s)$.

Since $A(s) = A^t(s)$ and $C(s) = C^t(s)$, we have

$$\dot{G}_i(s) = 0, \ i = 1, 2.$$

Hence, the flow defined by (17) preserves both the canonical 2-form σ and the complexified form σ_C.

Now let $(Y^i(s), Z^i(s))$ be the solution of (17) with initial data $(\hat{e}_i, M(0)\hat{e}_i)$, where $\hat{e}_i, \ i = 1, .., 4$, is the standard basis for R^4. We denote by $K(s)$ and $H(s)$ the 4×4 matrices with columns

$$Y^1(s), Y^2(s), Y^3(s), Y^4(s) \text{ and } Z^1(s), Z^2(s), Z^3(s), Z^4(s).$$

respectively. We claim that $K(s)$ is invertible for all s. To see this suppose $\sum_{i=1}^4 a_i Y^i(s_0) = 0$, and let $w(s) = \sum_{i=1}^4 a_i (Y^i(s), Z^i(s))$. Since σ_C is constant on pairs of solutions of (17), we obtain

$$0 = \sigma_C(w(s_0), w(s_0)) = \sigma(w(0), w(0))$$

$$= \sum_{i,j=1}^{4} a_i \overline{a}_j \sigma_C((Y^i(0), Z^i(0)), (Y^i(0), Z^i(0))) = -2i \langle \Im M(0) v_0 \cdot v_0 \rangle,$$

where $v_0 = \sum_{i=1}^4 a_i Y^i(0)$. Since $\Im M(0)$ is positive semi-definite with null space spanned by $(\dot{y}(0), 1)$, it follows that $v_0 = c(\dot{y}(0), 1)$ for some scalar c. Differentiating (10-11) with respect to s shows that $((\dot{y}(s), 1), (\dot{\eta}(s), \dot{\sigma}(s))$ is a solution of (17), and uniqueness for the initial value problem implies

$$\sum_{i=1}^{4} a_i Y^i(s_0) = (c\dot{y}(s_0), c).$$

Thus $c = 0$ which implies $v_0 = 0$ and hence $a_i = 0, \ i = 1, .., 4$, since $\{Y^i, \ i = 1, .., 4\}$ is the standard basis for R^4. Thus $K(s)$ is invertible for all s, and we define $M(s) = H(s)K(s)^{-1}$. We have

$$\dot{M} = \dot{N}Y^{-1} - NY^{-1}\dot{Y}Y^{-1} = (-CY - B^t N)Y^{-1} - NY^{-1}(BY + AN)Y^{-1}$$

$$= -C - B^t M - MB - MAM.$$

On the other hand, by definition of $K(s)$ and $H(s)$, $M(s)Y^i(s) = Z^i(s)$. Combining this with the fact that σ and σ_C are constant in s, we deduce that the matrix $M(s)$ has the properties that $M(0)$ has for $s = 0$. In particular, $M(s) = M(s)^t$ and $\Im M(s)$ is positive definite on the orthogonal complement of $(\dot{y}(s), 1)$. This completes the proof of this lemma.

In view of the preceding lemma, if we require $\partial_Y \phi(Y(s)) = (\eta(s), \sigma(s))$ and $\partial_Y^2 \phi(Y(s)) = M(s)$, (12) holds for $N = 3$. Next we determine the higher order derivatives of ϕ on γ by setting higher order derivatives of G equal to zero on γ. However, the differential equations along γ that we obtain for $\partial^\alpha \phi(y(s), s)$ for $|\alpha| > 2$ will be linear. From $\partial_y^\alpha G = 0$ on γ with $|\alpha| \geq 3$ we obtain

$$\partial_Z h \cdot \partial_Y(\partial_y^\alpha \phi) + \sum_{|\beta|=|\alpha|} c_{\alpha,\beta} \partial_y^\beta \phi + d_\alpha = 0,$$

where $c_{\alpha,\beta}$ and d_α depend on $\partial_Y^\delta \phi(y(s), s)$ for $|\delta| < |\alpha|$. Taking into account the Hamiltonian equations (10-11), we get

$$\frac{d}{ds}[\partial_y^\alpha \phi(y(s), s)] + \sum_{|\beta|=|\alpha|} c_{\alpha,\beta} \partial_y^\beta \phi(y(s), s) + d_\alpha = 0 \tag{18}$$

on $(y(s), s)$. This gives us a linear system for the partial derivatives of a fixed order $\{\partial_y \phi(y(s), s), |\alpha| = m\}$. The remaining partial derivatives of ϕ on γ are determined by the relations

$$\frac{d}{ds}[\partial^\beta \phi(y(s), s)] = \partial_y(\partial^\beta \phi)(y(s), s) \cdot \dot{y}(s) + (\partial_s \partial^\beta \phi)(y(s), s)$$

We we solve the system (18) starting with $m = 3$, then $m = 4$ and so on. Since the equations are linear, we have solutions defined for $-\infty < s < \infty$.

Now, given the formal Taylor series of ϕ on γ, and using that $\Im M(s) = \Im \partial_{y,s}^2 \phi(y(s), s)$ is positive definite on the orthogonal complement of $(\dot{y}(s), 1)$, we construct ϕ satisfying all the properties of Theorem 1 from its Taylor series on γ.

4 Propagation of the Amplitude

In the following, we assume that ϕ has been chosen so that (12) holds for given N. We will denote $H_0(k)$, $\Phi(x, k)$ and $\lambda(k)$ simply by H_0, Φ and λ

respectively. We will use the Einstein summation convention (like indices are summed from 1 to 3).

Recall that

$$m_0(x, y, s) = f_0(y, s)\Phi(x, k(y, s)). \tag{19}$$

On the other hand, since $x \to m_1(x, \cdot, \cdot)$ is required to be Γ-periodic, it is natural to write

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

with

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

Substituting (19) and the definition of $m_1^{\perp}$ into (7) and using (9), we obtain

$$c_1(x, y, s) = Km_0 - G(y, s)m_1(x, y, s) - \Big[H_0(k(y, s)) - \lambda(k(y, s))\Big]m_1^{\perp}. \tag{20}$$

Since we have already made $G(y, s)m_1(x, y, s)$ vanish to arbitrary order on γ, we can omit it, and consider the equation

$$0 = c_1(x, y, s) = Km_0 - \Big[H_0(k(y, s)) - \lambda(k(y, s))\Big]m_1^{\perp}. \tag{21}$$

By the Fredholm alternative, the equation (21) has a solution m_1 if and only if the term involving m_0 in (21) is orthogonal to

$$\ker\left[H_0\left(k(y, s)\right) - \lambda(k(y, s))\right].$$

In view of the definition of K and (H1) this is equivalent to

$$0 = \langle Km_0, \Phi\rangle = \langle \Phi, \frac{\partial m_0}{\partial s} - \frac{\partial H_0}{\partial k} \cdot \frac{\partial m_0}{\partial y} - \frac{\partial}{\partial y} \cdot k(y, s)m_0\rangle. \tag{22}$$

Since $\lambda(k)$ is simple eigenvalue, we may assume that $\Phi(\cdot, k)$ is analytic in k. Thus, taking the gradient with respect to k in

$$\Big[H_0 - \lambda\Big]\frac{\partial \Phi}{\partial k} = \Big[\frac{\partial \lambda}{\partial k} - \frac{\partial H_0}{\partial k}\Big]\Phi,$$

and taking the inner product with Φ we get

$$\frac{\partial \lambda}{\partial k} = \langle \Phi, \frac{\partial H_0}{\partial k}\Phi\rangle. \tag{23}$$

Here we have used the fact that $\langle\Phi(\cdot,k),\Phi(\cdot,k)\rangle = 1$.

Substituting (19) into the right hand side of (22) and using (23), we get the transport equation for f_0

$$0 = \frac{\partial f_0}{\partial s} - \frac{\partial\lambda}{\partial k}\cdot\frac{\partial f_0}{\partial y} + n(y,s)f_0, \tag{24}$$

where n is the function given by

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

The real and imaginary parts of n were computed in [7, §5]

$$\Re n = -\frac{1}{2}\frac{\partial}{\partial y}\cdot\frac{\partial\lambda}{\partial k}(k(y,s)),$$

$$\Im n = -\frac{i}{2}\langle(H_0-\lambda)\frac{\partial\Phi}{\partial k_j},(M\frac{\partial\Phi}{\partial k})_j\rangle + i\langle\frac{\partial\lambda}{\partial k_j}\Phi,\frac{\partial\Phi}{\partial y_j}\rangle - i\langle\Phi,\frac{\partial\Phi}{\partial s}\rangle,$$

where M is the anti-symmetric matrix corresponding to the magnetic field $B = \nabla_y\times A(y,s)$:

$$\begin{pmatrix} 0 & B_3 & -B_2 \\ -B_3 & 0 & B_1 \\ B_2 & -B_1 & 0 \end{pmatrix}$$

Introducing

$$L = \Im\Big\{(\langle(H_0-\lambda)\frac{\partial\Phi}{\partial k_2},\frac{\partial\Phi}{\partial k_3}\rangle,\langle(H_0-\lambda)\frac{\partial\Phi}{\partial k_3},\frac{\partial\Phi}{\partial k_1}\rangle,\langle(H_0-\lambda)\frac{\partial\Phi}{\partial k_1},\frac{\partial\Phi}{\partial k_2}\rangle)\Big\}$$

one can write

$$\Im n = L\cdot B - i\langle\Phi,\dot\Phi\rangle$$

L is an angular momentum which satisfies the usual commutation relations.

As in section 2, we want to choose f_0 so that the right hand side of (24) vanishes on γ to order N. Differentiating the coefficient of the right hand side of (24), and setting the derivatives equal to zero on γ, we obtain linear differential equation for $\partial_Y^\alpha f_0$ with an inhomogeneous term involving the derivatives of f_0 up to order $|\alpha|-1$:

$$\frac{\partial}{\partial s}(\partial_Y^\alpha f_0) - \frac{\partial\lambda}{\partial k}\cdot\frac{\partial}{\partial y}(\partial_Y^\alpha f_0) + n(y,s)\partial_Y^\alpha f_0 + C(f_0,\partial_Y f_0,...,\partial_Y^{\alpha-1}f_0) = 0,$$

with $C = 0$ for $\alpha = 0$. We recall that $Y = (y_1, y_2, y_3, s)$. Along $Y(s) = (y(s), s)$ the above differential equation takes the form

$$\frac{d}{ds}[\partial_Y^\alpha f_0(Y(s))] + n(Y(s))\partial_Y^\alpha f_0(Y(s)) + C(f_0, \partial_Y f_0, ..., \partial_Y^{\alpha-1} f_0)(Y(s)) = 0,$$

Since the coefficient $C(f_0, \partial_Y f_0, ..., \partial_Y^{\alpha-1} f_0)$ depends on all the partials up to order $|\alpha| - 1$ and this equation is linear, we can solve it recursively for all s. Thus, we may assume that f_0 is chosen so that for all $M \in N$,

$$\langle Km_0, \Phi\rangle = \mathcal{O}_M(d((y, s), \gamma)^M), \tag{25}$$

uniformly on $\Omega \cap |s| < T$.

Next we set

$$m_1^\perp = (H - \lambda)^{-1}\Big[Km_0 - \langle Km_0, \Phi\rangle\Phi\Big], \tag{26}$$

where $(H - \lambda)^{-1}$ denotes the inverse which maps the orthogonal complement of Φ in $L^2(E)$ into itself. In view of hypothesis (H1), the right-hand side of (26) is well defined and depends smoothly on (x, y, s). To complete the construction of m_1, we have to compute f_1. As in the case of the equation $c_1 = 0$, modulo a negligible term the equation $c_2 = 0$ has a solution m_2 if and only if

$$\langle Km_1 + \Delta m_0, \Phi\rangle = 0, \tag{27}$$

which yields

$$\langle \Phi, K(f_1\Phi)\rangle = \langle \Phi, Km_1^\perp + \Delta_y m_0\rangle. \tag{28}$$

Clearly, the left-hand side of (28) equals that of (23) with f_1 instead of f_0. Thus, (23) yields

$$\frac{\partial f_1}{\partial s} - \frac{\partial E}{\partial k}\cdot\frac{\partial f_1}{\partial y} - \frac{1}{2}(\frac{\partial}{\partial y}\cdot\frac{\partial E}{\partial k})f_1 + (iL\cdot B + \langle\Phi, \dot{\Phi}\rangle)f_1 = -i\langle\Phi, Km_1^\perp + \Delta_y m_0\rangle.$$

Thus the problem of making $\langle Km_1 + \Delta m_0, \Phi\rangle$ vanish to high order on γ is also reduced to solving linear ordinary differential equation along $Y(s)$. Hence, we may assume that $f_1(y, s)$ is constructed such that

$$\langle Km_1 + \Delta m_0, \Phi\rangle = \mathcal{O}(d((y, s), \gamma)^M, \tag{29}$$

uniformly on $(y, s) \in \Omega \cap \{|s| < T\}$.

Summing up (20), (21), (22), (25), (26), (27) and (29) we have constructed m_0, m_1 such that

$$c_0(x,y,s) = G(y,s)f_0(y,s)\Phi(x,k(y,s)) = \mathcal{O}(d((y,s),\gamma)^N, \tag{30}$$

$$c_1(x,y,s) = G(y,s)m_1(x,y,s) + \langle Km_0, \Phi\rangle\Phi(x,k(y,s)) = \mathcal{O}(d((y,s),\gamma)^N, \tag{31}$$

uniformly on $x \in T$ and $(y,s) \in \Omega \cap \{|s| < T\}$.

The situation for the equations $c_j(x,y,s) = 0$, $j \geq 2$ is quite similar: we set

$$m_j(x,y,s) = f_j(y,s)\Phi(x,k(y,s)) + m_j^\perp,$$

with

$$m_j^\perp = (H_0 - \lambda)^{-1}\Big[Km_{j-1} + \Delta m_{j-2} - \langle Km_{j-1} + \Delta m_{j-2}, \Phi\rangle\Phi\Big].$$

This shows that $m_j^\perp$ only depends on m_{j-1} and m_{j-2}. Next, the function f_j is determined from the equation

$$\langle Km_j + \Delta m_{j-1}, \Phi\rangle = 0,$$

which leads to a linear differential equation for f_j with an inhomogeneous term involving m_{j-1} and m_{j-2}.

5 Main results

Before stating the main results of this paper let us specify the form of the initial u_ϵ in (1). Recall that ϕ_0 was an arbitrary smooth function such that $\Im\partial_y^2\phi_0(y_0)$ was positive definite. For any $f \in C_0^\infty(R^3)$ we can carry out the preceding construction with

$$u_\epsilon(y) = f(y)e^{\frac{i\phi_0(y)}{\epsilon}}\Phi(\frac{y}{\epsilon}, A(y,0) + \frac{\partial\phi_0}{\partial y}(y)).$$

Theorem 2. *Given $T > 0$ and $N \in N$, there exists $\epsilon_0 > 0$ and an approximate solution $\psi_\epsilon(s)$ concentrated near the projection of the null-bicharacteristc of the hamiltonian $h(y,s,\eta,\sigma) = \sigma - \lambda\,(A(y,s)+\eta) - V(y,s)$ with initial data $(y_0, 0, \partial\phi_0(y_0), \sigma_0)$ such that for all $\epsilon \in]0, \epsilon_0[$*

$$\|\psi_\epsilon(y,0) - u_\epsilon(y)\| = \mathcal{O}(\epsilon), \tag{32}$$

$$\|(\epsilon D_t - P_\epsilon)\psi_\epsilon\| = \mathcal{O}_N(\epsilon^N), \tag{33}$$

uniformly on $t \in [-T,T]$.

Proof Let $\gamma = \{(y(s), s, \eta(s), \sigma(s)), -\infty < s < \infty\}$ be the null bicharacteristic of $h(y, s, \eta, \sigma)$ with initial data $y(0) = y_0, \eta(0) = \partial_y \phi_0(y_0)$, and let $\phi(y, s)$ be the corresponding function given by Theorem 1 with $\partial_y^\alpha \phi(y_0, 0) = \partial_y^\alpha \phi_0(y_0)$.

The results of section 4 yield

$$\psi_\epsilon(y, s) = f(y, s)e^{i\phi(y,s)/\epsilon}\Phi(\frac{y}{\epsilon}, A(y, s) + \frac{\partial \phi}{\partial y}(y, s)) + \mathcal{O}(\epsilon).$$

On the other hand, from the estimates (13) and (30) we have

$$\|f(\cdot, 0)e^{i\frac{\phi(\cdot,0)}{\epsilon}}\Phi(x, A(\cdot, 0)+\frac{\partial \phi}{\partial y}(\cdot, 0))-f(\cdot)e^{i\frac{\phi_0(\cdot)}{\epsilon}}\Phi(x, A(y, 0)+\frac{\partial \phi_0}{\partial y}(\cdot))\|_{L^2(R_y^3)} = \mathcal{O}(\epsilon^M),$$

uniformly on $x \in T$. Clearly (32) follows from the two above equalities.

In sections 2, 3 and 4, we have constructed functions $\psi(x, y, s, \epsilon)$ for each M of the form

$$\psi(x, y, s, \epsilon) = e^{i\frac{\phi(y,s)}{\epsilon}}\Big[m_0(x, y, s) + \epsilon m_1(x, y, s) + ... + \epsilon^M m_M(x, y, s)\Big]$$

so that

$$(\epsilon D_s - P)\psi = e^{i\phi(y,s)/\epsilon}\Big[c_0(x, y, s) + ... + \epsilon^{M+2}c_{M_1+2}(x, y, s)\Big],$$

with

$$c_j(x, y, s) = \mathcal{O}(d((y, s), \gamma)^M,$$
$$\Im\phi(y, s) \geq C(d((y, s), \gamma)^2,$$

uniformly on $x \in T$. Consequently,

$$\|(\epsilon D_s - P)\psi(x, \cdot, s, \epsilon)\|^2_{L^2(R_y^3)} =$$

$$\int e^{-2\Im\phi(y,s)/\epsilon}|c_0(x, y, s) + ... + \epsilon^{M+2}c_{M+2}(x, y, s)|^2 dy = \mathcal{O}(\epsilon^{M+3/2}) \qquad (34)$$

uniformly on $x \in T$. Here we have used the remarks in the end of section 2.

Set $\psi_\epsilon(y, s) = \psi(\frac{y}{\epsilon}, y, s, \epsilon)$. Since

$$(\epsilon D_s - P_\epsilon)\psi_\epsilon = \Big[(\epsilon D_s - P)\psi\Big](\frac{y}{\epsilon}, y, s, \epsilon),$$

(33) follows from (34).

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