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# Semiclassical asymptotics in magnetic Bloch bands 

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#### Abstract

This paper gives a simple construction of wave packets localized near semiclassical trajectories for an electron subject to external electric and magnetic fields. We assume that the magnetic and electric potentials are slowly varying perturbations of the potential of a constant magnetic field and a periodic lattice potential, respectively.


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## 1. Introduction

In this paper we present a multiple-scale method for deriving semiclassical dynamics. In [8] this method was used to construct wave packets for the Schrödinger equation with a periodic potential perturbed by a weak, constant magnetic field. In this paper a constant magnetic field and a periodic electric field are the unperturbed fields, and we consider their slowly varying perturbations. This means that the electric and magnetic potentials have the form

$$
\mathcal{V}=V_{0}(x)+V(\epsilon x, \epsilon t) \quad \text { and } \quad \mathcal{A}=\frac{\omega \times x}{2}+A(\epsilon x, \epsilon t)
$$

respectively, where $V_{0}$ is periodic. We are interested in the asymptotic solutions of the Schrödinger equation with these potentials as $\epsilon \rightarrow 0$. Note that this implies that the fields resulting from the perturbation terms are both slowly varying and relatively small. Since we assume that $A$ and $V$ are smooth functions, the multi-scale approach leads to asymptotics to all orders in $\epsilon$ over any fixed time interval $[0, T]$. The wave packets that we construct are localized in spacetime near the semiclassical trajectories, but their supports are large relative to the lattice spacing.

We think that this method gives an easy derivation of rigorous semiclassical asymptotics. The dynamics we obtain is quite different from that derived by Chang and Niu in [14, 15]. While the relevant hypotheses are not given explicitly in these papers, it is possible that this results from different assumptions on the strength of the perturbations (see remark 2).

## 2. The unperturbed Hamiltonian

Semiclassical dynamics involve the spectral-band functions for the unperturbed Hamiltonian. In this section, we will define the magnetic Bloch bands, and state our assumptions on the unperturbed Hamiltonian. We first give a brief review of the magnetic translation operators [20].

The Hamiltonian for an electron in a crystal lattice $\Gamma_{0}$ of $\mathbf{R}^{3}$ in the presence of a constant magnetic field $\omega=\left(\omega_{1}, \omega_{2}, \omega_{3}\right)$ is given by

$$
H_{0}=\frac{1}{2 m}\left(-\mathrm{i} h \frac{\partial}{\partial x}+e \frac{\omega \times x}{2}\right)^{2}+V_{0}(x)
$$

where $V_{0} \in C^{\infty}\left(\mathbf{R}^{3} ; \mathbf{R}\right)$ is periodic with respect to $\Gamma_{0}$. Here $m$ and $e$ are the electron mass and charge, respectively. To simplify the notation, we will use the system of units in which $h=2 m=e=1$ from now on.

In general, $H_{0}$ will not commute with ordinary translations, but it will commute with magnetic translations $T_{\alpha}^{\omega}, \alpha \in \Gamma_{0}$, given by

$$
T_{\alpha}^{\omega} u(x)=\mathrm{e}^{\mathrm{i}\left|\frac{\omega x x}{2}, \alpha\right\rangle} u(x-\alpha) .
$$

The $T_{\alpha}^{\omega}$ satisfy the commutation relations:

$$
\begin{equation*}
T_{\alpha}^{\omega} T_{\beta}^{\omega}=\mathrm{e}^{-\frac{1}{2}\langle\omega, \alpha \times \beta\rangle} T_{\alpha+\beta}^{\omega}=\mathrm{e}^{-\mathrm{i}\langle\omega, \alpha \times \beta\rangle} T_{\beta}^{\omega} T_{\alpha}^{\omega} . \tag{1}
\end{equation*}
$$

Throughout this work, we assume that

$$
\left\langle\omega, \Gamma_{0} \times \Gamma_{0}\right\rangle \subset 2 \pi \mathbf{Q} .
$$

Then we can find a sublattice $\Gamma$ of $\Gamma_{0}$ such that

$$
\begin{equation*}
\langle\omega, \Gamma \times \Gamma\rangle \subset 4 \pi \mathbf{Z} \tag{2}
\end{equation*}
$$

In the following, we denote by $\Gamma^{*}:=\left\{\gamma^{*} \in \mathbf{R}^{3} ; \gamma \cdot \gamma^{*} \in 2 \pi \mathbf{Z}, \forall \gamma \in \Gamma\right\}$ the dual lattice of $\Gamma$. A fundamental domain of $\Gamma$ is denoted by $M$, and of $\Gamma^{*}$ by $M^{*}$. Note that (2) implies

$$
\begin{equation*}
T_{\alpha}^{\omega} T_{\beta}^{\omega}=T_{\alpha+\beta}^{\omega} \quad \forall \gamma, \beta \in \Gamma \tag{3}
\end{equation*}
$$

We now introduce the magnetic Bloch-Floquet transformation:

$$
U u(x, k)=\sum_{\alpha \in \Gamma} \mathrm{e}^{\mathrm{i}(x-\alpha) \cdot k} T_{\alpha}^{\omega} u(x) \quad x, k \in \mathbf{R}^{3} .
$$

By (3), we get

$$
\begin{aligned}
& T_{\alpha}^{\omega} U u(x, k)=U u(x, k) \\
& U u\left(x, k+\alpha^{*}\right)=\mathrm{e}^{\mathrm{i} x \cdot \alpha^{*}} U u(x, k)
\end{aligned}
$$

from which we can prove easily that $U$ extends to a unitary operator

$$
L^{2}\left(\mathbf{R}^{3}\right) \rightarrow \int_{M^{*}}^{\oplus} \mathcal{H}_{\omega} \mathrm{d} k=L^{2}\left(M^{*} ; \mathcal{H}_{\omega}\right)
$$

where $\mathcal{H}_{\omega}=\left\{u \in L_{\text {loc }}^{2}\left(\mathbf{R}^{3}\right) ; T_{\gamma}^{\omega} u=u, \forall \gamma \in \Gamma\right\}$. Moreover, one has

$$
\begin{equation*}
U H_{0} U^{-1}=\int_{M^{*}}^{\oplus} H_{0}(k) \mathrm{d} k \tag{4}
\end{equation*}
$$

where by definition the last expression is the self-adjoint operator with domain $L^{2}\left(M^{*} ; \mathcal{H}_{\omega}^{2}\right)$, given by

$$
\begin{equation*}
H_{0}(k) u(x)=\left[\left(-\mathrm{i} \frac{\partial}{\partial x}+\frac{\omega \times x}{2}+k\right)^{2}+V_{0}(x)\right] u(x) \tag{5}
\end{equation*}
$$

for all $k \in M^{*}$ and all $u \in \mathcal{H}_{\omega}^{2}:=\left\{u \in \mathcal{H}_{\omega} ; \partial^{\alpha} u \in \mathcal{H}_{\omega},|\alpha| \leqslant 2\right\}$.

Since the resolvent of $H_{0}(k)$ is compact, $H_{0}(k)$ has a complete set of (normalized) eigenfunctions $\Phi_{l}(\cdot, k) \in \mathcal{H}_{\omega}^{2}, l \in \mathbf{N}$, called magnetic Bloch states. The corresponding eigenvalues accumulate at infinity and we enumerate them according to their multiplicities,

$$
E_{1}(k) \leqslant E_{2}(k) \leqslant \cdots
$$

Since $\mathrm{e}^{-\mathrm{i} x \gamma^{*}} H_{0}(k) \mathrm{e}^{\mathrm{i} x \gamma^{*}}=H_{0}\left(\gamma^{*}+k\right), E_{l}(k)$ is periodic with respect to $\Gamma^{*}$. Ordinary perturbation theory shows that $E_{j}(k)$ are continuous functions in $k$ for every fixed $j$. The closed intervals $\Lambda_{j}:=E_{j}\left(M^{*}\right)$ are called magnetic Bloch bands. Combining this with (4), we get

$$
\sigma\left(H_{0}\right)=\bigcup_{l=1}^{\infty} \Lambda_{l} \quad \Lambda_{l}=E_{l}\left(M^{*}\right)
$$

We make the following hypothesis on the spectrum of the unperturbed magnetic Schrödinger operator:
(H) There exists $l$ such that $E_{l}(k)$ is simple for all $k \in M^{*}$, i.e.

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

## 3. The perturbed Hamiltonian

As stated in the introduction, we consider the time-dependent Schrödinger equation with perturbed magnetic and electric potentials:

$$
\begin{equation*}
-\mathrm{i} \frac{\partial u}{\partial t}=\left[\left(-\mathrm{i} \frac{\partial}{\partial x}+\frac{\omega \times x}{2}+A(\epsilon x, \epsilon t)\right)^{2}+V_{0}(x)+V(\epsilon x, \epsilon t)\right] u . \tag{6}
\end{equation*}
$$

With the change of variables

$$
s=\epsilon t \quad(\text { adiabatic scale }) \quad \text { and } \quad y=\epsilon x \quad \text { (long spatial scale) }
$$

equation (6) becomes

$$
\begin{equation*}
-\mathrm{i} \epsilon \frac{\partial u}{\partial s}=\left[\left(-\mathrm{i} \epsilon \frac{\partial}{\partial y}+\frac{\omega \times y}{2 \epsilon}+A(y, s)\right)^{2}+V_{0}\left(\frac{y}{\epsilon}\right)+V(y, s)\right] u . \tag{7}
\end{equation*}
$$

When $\epsilon \rightarrow 0$, there are two spatial scales in equation (7): the first one of the order of the linear dimensions $\gamma$ of the periodicity cell and the second of order $\gamma / \epsilon$ on which the perturbations of the potentials vary appreciably. This makes it possible to use the method of two scale expansions ( $x=y / \epsilon$ and $y$ are regarded as independent variables) (cf Buslaev [4], Guillot-Ralston-Trubowitz [8], Gérard-Martinez-Sjöstrand [7], Horn [10], Ralston [18] and Dimassi-Sjöstrand [5]). More precisely, one can consider the following equation in the independent variables $x$ and $y$ :

$$
\begin{equation*}
-\mathrm{i} \epsilon \frac{\partial v}{\partial s}=\left[\left(-\mathrm{i} \epsilon \frac{\partial}{\partial y}-\mathrm{i} \frac{\partial}{\partial x}+\frac{\omega \times x}{2}+A(y, s)\right)^{2}+V_{0}(x)+V(y, s)\right] v \tag{8}
\end{equation*}
$$

Note that, if in the solution $v(x, y, s, \epsilon)$ of (8) we let $x=y / \epsilon$, then it becomes a solution of (7). In the variable $x, v(x, y, s, \epsilon)$ is required to be in $\mathcal{H}_{\omega}^{2}$.

Now if (8) is regarded as an $\epsilon$-pseudodifferential operator on $y$ with operator-valued symbol, one looks for a local solution of the form

$$
\begin{equation*}
v(x, y, s, \epsilon)=\mathrm{e}^{\mathrm{i} \phi(y, s) / \epsilon} m(x, y, s, \epsilon) \tag{9}
\end{equation*}
$$

where

$$
\begin{equation*}
m(x, y, s, \epsilon)=m_{0}(x, y, s)+\epsilon m_{1}(x, y, s)+\cdots \tag{10}
\end{equation*}
$$

Inserting (9) in (8), we get

$$
\begin{align*}
\frac{\partial \phi}{\partial s} m-\mathrm{i} \epsilon \frac{\partial m}{\partial s} & =\left[\left(-\mathrm{i} \epsilon \frac{\partial}{\partial y}-\mathrm{i} \frac{\partial}{\partial x}+A_{0}(x)+k(y, s)\right)^{2}+V_{0}(x)+V(y, s)\right] m \\
= & {\left[\left(-\mathrm{i} \frac{\partial}{\partial x}+A_{0}(x)+k(y, s)\right)^{2}+V_{0}(x)+V(y, s)\right] m }  \tag{11}\\
& -\mathrm{i} \epsilon\left[2\left(-\mathrm{i} \frac{\partial}{\partial x}+A_{0}(x)+k(y, s)\right) \cdot \frac{\partial}{\partial y}+\frac{\partial}{\partial y} \cdot k(y, s)\right] m-\epsilon^{2} \Delta_{y} m
\end{align*}
$$

where

$$
\begin{equation*}
k(y, s)=A(y, s)+\frac{\partial \phi}{\partial y}(y, s) \tag{12}
\end{equation*}
$$

Substituting (10) into the last expression in (11) and requiring that each term in the resulting asymptotic expansion vanishes, we get the sequence of equations:
$\frac{\partial \phi}{\partial s} m_{0}=\left[H_{0}(k(y, s))+V(y, s)\right] m_{0}$
$K m_{0}=\left[H_{0}(k(y, s))+V(y, s)-\frac{\partial \phi}{\partial s}(y, s)\right] m_{1}$
$K m_{j-1}+\Delta_{y} m_{j-2}=\left[H_{0}(k(y, s))+V(y, s)-\frac{\partial \phi}{\partial s}(y, s)\right] m_{j} \quad j=2,3, \ldots$.
Here

$$
K=\mathrm{i}\left[\frac{\partial H_{0}}{\partial k}(k(y, s)) \cdot \frac{\partial}{\partial y}+\frac{\partial}{\partial y} \cdot k(y, s)-\frac{\partial}{\partial s}\right]
$$

## 4. Eikonal equation and semiclassical dynamics

From now on we assume that $(\mathrm{H})$ holds. We let $\Phi_{l}$ be the normalized eigenfunction corresponding to $E_{l}(k)$ :

$$
\begin{align*}
& H_{0}(k) \Phi_{l}=E_{l}(k) \Phi_{l}  \tag{14}\\
& \left\langle\Phi_{l}, \Phi_{l}\right\rangle=1 \tag{15}
\end{align*}
$$

Since $l$ is fixed we shall suppress the subscript $l$ in $E_{l}(k)$ and $\Phi_{l}$.
Equation (13) 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 (H), we can satisfy (13) by choosing
$\frac{\partial \phi}{\partial s}(y, s)=E\left(A(y, s)+\frac{\partial \phi}{\partial y}(y, s)\right)+V(y, s) \quad$ (eikonal equation)
and setting

$$
\begin{equation*}
m_{0}(x, y, s)=f_{0}(y, s) \Phi(x, k(y, s)) \tag{17}
\end{equation*}
$$

Since (16) is derived from the Hamiltonian

$$
h(y, s, \eta, \sigma)=\sigma-E(A(y, s)+\eta)-V(y, s)
$$

we see that the equations of motion of the magnetic Bloch electron are

$$
\begin{equation*}
\dot{y}=-\frac{\partial E}{\partial k}(A(y, s)+\eta) \quad \dot{s}=1 \tag{18}
\end{equation*}
$$

and
$\dot{\eta}=-\sum_{i=1}^{3} \dot{y}_{i} \frac{\partial A_{i}}{\partial y}(y, s)+\frac{\partial V}{\partial y}(y, s) \quad \dot{\sigma}=-\dot{y} \cdot \frac{\partial A}{\partial s}(y, s)+\frac{\partial V}{\partial s}(y, s)$.
It is convenient to rewrite the above equations in the new set of coordinates $(y, s, k, \sigma)=$ ( $y, s, \eta+A(y), \sigma)$. It follows from (18) and (19) that

$$
\begin{align*}
\dot{y} & =-\frac{\partial E}{\partial k}(k) \quad \dot{s}=1  \tag{20}\\
\dot{k} & =\dot{\eta}+\sum_{i=1}^{3} \frac{\partial A}{\partial y_{i}}(y, s) \dot{y}_{i}+\frac{\partial A}{\partial s}(y, s) \dot{s} \\
& =\sum_{i=1}^{3}\left(\frac{\partial A}{\partial y_{i}}(y, s)-\frac{\partial A_{i}}{\partial y}(y, s)\right) \dot{y}_{i}+\frac{\partial A}{\partial s}(y, s)+\frac{\partial V}{\partial y}(y, s) \\
& =-\dot{y} \times B(y, s)+\frac{\partial A}{\partial s}(y, s)+\frac{\partial V}{\partial y}(y, s) . \tag{21}
\end{align*}
$$

Here $B=\nabla_{y} \times A(y, s)$ is the magnetic field corresponding to $A(y, s)$.
In (20) we see the formula for the velocity of a wave packet in terms of the gradient of the function $E(k)$ in momentum space, and in (21), the statement that the momentum $k$ of a packet is governed by the classical equation of motion in terms of the additional external magnetic and electric fields $(A(y, s), V(y, s))$.

## 5. Propagation of the amplitude

In the following we will denote $H_{0}(k), \Phi(x, k)$ and $E(k)$ simply by $H_{0}, \Phi$ and $E$, respectively.
By the Fredholm alternative, equation $\left(T_{1}\right)$ has a solution $m_{1}$ if and only if the right-hand side of $\left(T_{1}\right)$ is orthogonal to

$$
\operatorname{ker}\left[H_{0}(k(y, s))+V(y, s)-\frac{\partial \phi}{\partial s}\right]
$$

In view of (17), this is equivalent to

$$
\begin{equation*}
0=\left\langle\Phi, \frac{\partial m_{0}}{\partial s}-\frac{\partial H_{0}}{\partial k} \cdot \frac{\partial m_{0}}{\partial y}-\frac{\partial}{\partial y} \cdot k(y, s) m_{0}\right\rangle . \tag{22}
\end{equation*}
$$

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

$$
\begin{equation*}
\left[H_{0}-E\right] \frac{\partial \Phi}{\partial k}=\left[\frac{\partial E}{\partial k}-\frac{\partial H_{0}}{\partial k}\right] \Phi \tag{23}
\end{equation*}
$$

and taking the inner product with $\Phi$, we get

$$
\begin{equation*}
\frac{\partial E}{\partial k}=\left\langle\Phi, \frac{\partial H_{0}}{\partial k} \Phi\right\rangle \tag{24}
\end{equation*}
$$

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

Substituting (17) into the right-hand side of (22) and using (24), we get the transport equation for $f_{0}$ :

$$
\begin{equation*}
0=\frac{\partial f_{0}}{\partial s}-\frac{\partial E}{\partial k} \cdot \frac{\partial f_{0}}{\partial y}+h(y, s) f_{0} \tag{25}
\end{equation*}
$$

where $h$ is the function given by

$$
\begin{equation*}
h(y, s)=\left\langle\Phi, \frac{\partial \Phi}{\partial s}\right\rangle-\left\langle\Phi, \frac{\partial H_{0}}{\partial k} \cdot \frac{\partial \Phi}{\partial y}\right\rangle-\frac{\partial}{\partial y} \cdot k(y, s) \tag{26}
\end{equation*}
$$

In order to study the transport properties of the magnetic Bloch electron, we must compute the real and imaginary parts of $h(y, s)$.

Differentiating (24) with respect to $y$, and noting that $\frac{\partial H_{0}}{\partial k_{j}}$ is self-adjoint,

$$
\begin{aligned}
\frac{\partial}{\partial y} \cdot \frac{\partial E}{\partial k}(k(y, s)) & =\left\langle\frac{\partial H_{0}}{\partial k} \cdot \frac{\partial}{\partial y} \Phi, \Phi\right\rangle+\left\langle\Phi, \frac{\partial H_{0}}{\partial k} \cdot \frac{\partial}{\partial y} \Phi\right\rangle+2 \frac{\partial}{\partial y} \cdot k(y, s) \\
& =2 \operatorname{Re}\left\langle\Phi, \frac{\partial H_{0}}{\partial k} \cdot \frac{\partial}{\partial y} \Phi\right\rangle+2 \frac{\partial}{\partial y} \cdot k(y, s)
\end{aligned}
$$

and using that $\left\langle\Phi, \frac{\partial \Phi}{\partial s}\right\rangle \in \mathrm{i} \mathbf{R}$ (which follows from $\langle\Phi, \Phi\rangle=1$ ), we obtain from (26)

$$
\begin{equation*}
\operatorname{Re} h(y, s)=-\frac{1}{2} \frac{\partial}{\partial y} \cdot \frac{\partial E}{\partial k}(k(y, s)) . \tag{27}
\end{equation*}
$$

In the following, we are interested in computing the imaginary part of $h(y, s)$. We use the Einstein summation convention (like indices are summed from 1 to 3 ).

Taking the imaginary part of (26) and using (23) as well as $\left\langle\Phi, \frac{\partial \Phi}{\partial s}\right\rangle \in \mathrm{i} \mathbf{R}$, we obtain

$$
\begin{align*}
\operatorname{Im} h=\operatorname{Im} & \left\{\left\langle\Phi,-\frac{\partial H_{0}}{\partial k_{j}} \frac{\partial \Phi}{\partial y_{j}}\right\rangle\right\}+\operatorname{Im}\left\{\left\langle\Phi, \frac{\partial \Phi}{\partial s}\right)\right\} \\
& =\operatorname{Im}\left\{\left\langle-\frac{\partial E}{\partial k_{j}} \Phi, \frac{\partial \Phi}{\partial y_{j}}\right\rangle+\left\langle\left(H_{0}-E\right) \frac{\partial \Phi}{\partial k_{j}}, \frac{\partial \Phi}{\partial y_{j}}\right\rangle\right\}+\operatorname{Im}\left\{\left\langle\Phi, \frac{\partial \Phi}{\partial s}\right\rangle\right\} \\
& =-\frac{\mathrm{i}}{2}\left\langle\left(H_{0}-E\right) \frac{\partial \Phi}{\partial k_{j}},\left(\frac{\partial k_{l}}{\partial y_{j}}-\frac{\partial k_{j}}{\partial y_{l}}\right) \frac{\partial \Phi}{\partial k_{l}}\right\rangle+\mathrm{i}\left\langle\frac{\partial E}{\partial k_{j}} \Phi, \frac{\partial \Phi}{\partial y_{j}}\right\rangle-\mathrm{i}\left\langle\Phi, \frac{\partial \Phi}{\partial s}\right\rangle . \tag{28}
\end{align*}
$$

We further note that

$$
\left(\frac{\partial k_{l}}{\partial y_{j}}-\frac{\partial k_{j}}{\partial y_{l}}\right) \frac{\partial \Phi}{\partial k_{l}}=\left(\frac{\partial A_{l}}{\partial y_{j}}-\frac{\partial A_{j}}{\partial y_{l}}\right) \frac{\partial \Phi}{\partial k_{l}} .
$$

Thus, letting $M$ be the anti-symmetric matrix corresponding to the magnetic field $B=$ $\nabla_{y} \times A(y, s)$,

$$
M=\left(\begin{array}{ccc}
0 & B_{3} & -B_{2} \\
-B_{3} & 0 & B_{1} \\
B_{2} & -B_{1} & 0
\end{array}\right)
$$

(28) becomes

$$
\operatorname{Im} h=-\frac{\mathrm{i}}{2}\left\langle\left(H_{0}-E\right) \frac{\partial \Phi}{\partial k_{j}},\left(M \frac{\partial \Phi}{\partial k}\right)_{j}\right\rangle+\mathrm{i}\left\langle\frac{\partial E}{\partial k_{j}} \Phi, \frac{\partial \Phi}{\partial y_{j}}\right\rangle-\mathrm{i}\left\langle\Phi, \frac{\partial \Phi}{\partial s}\right\rangle .
$$

Let $(y(s), s, \eta(s), \sigma(s))$ be the solution of the Hamilton equations (18) and (19). Along $(y(s), s)$, the above differential equation takes the form

$$
\begin{aligned}
\operatorname{Im} h & =-\frac{\mathrm{i}}{2}\left\langle\left(H_{0}-E\right) \frac{\partial \Phi}{\partial k_{j}},\left(M \frac{\partial \Phi}{\partial k}\right)_{j}\right\rangle-\mathrm{i}\left\langle\Phi, \dot{y} \frac{\partial \Phi}{\partial y_{j}}\right\rangle-\mathrm{i}\left\langle\Phi, \frac{\partial \Phi}{\partial s}\right\rangle \\
& =-\frac{\mathrm{i}}{2}\left\langle\left(H_{0}-E\right) \frac{\partial \Phi}{\partial k_{j}},\left(M \frac{\partial \Phi}{\partial k}\right)_{j}\right\rangle-\mathrm{i}\langle\Phi, \dot{\Phi}\rangle .
\end{aligned}
$$

This, together with (25) and (27), yields
$\frac{\partial f_{0}}{\partial s}-\frac{\partial E}{\partial k} \cdot \frac{\partial f_{0}}{\partial y}-\frac{1}{2}\left(\frac{\partial}{\partial y} \cdot \frac{\partial E}{\partial k}\right) f_{0}+\frac{1}{2}\left\langle\left(H_{0}-E\right) \frac{\partial \Phi}{\partial k_{j}},\left(M \frac{\partial \Phi}{\partial k}\right)_{j}\right\rangle f_{0}+\langle\Phi, \dot{\Phi}\rangle f_{0}=0$.
Setting
$L=\operatorname{Im}\left\{\left(\left\langle\left(H_{0}-E\right) \frac{\partial \Phi}{\partial k_{2}}, \frac{\partial \Phi}{\partial k_{3}}\right\rangle,\left\langle\left(H_{0}-E\right) \frac{\partial \Phi}{\partial k_{3}}, \frac{\partial \Phi}{\partial k_{1}}\right\rangle,\left\langle\left(H_{0}-E\right) \frac{\partial \Phi}{\partial k_{1}}, \frac{\partial \Phi}{\partial k_{2}}\right\rangle\right)\right\}$
we then get

$$
\begin{equation*}
\frac{\partial f_{0}}{\partial s}-\frac{\partial E}{\partial k} \cdot \frac{\partial f_{0}}{\partial y}-\frac{1}{2}\left(\frac{\partial}{\partial y} \cdot \frac{\partial E}{\partial k}\right) f_{0}+(\mathrm{i} L \cdot B+\langle\Phi, \dot{\Phi}\rangle) f_{0}=0 \tag{29}
\end{equation*}
$$

Note that $L$ is an angular momentum which satisfies the usual commutation relations.
The transport equation (29) implies that if we begin with a localized packet, i.e., if we choose $f_{0}(y, 0)$ with a small support, the packet will move along the trajectory predicted by the semiclassical theory given by equations (19) and (20). The coefficient

$$
\frac{1}{2} \frac{\partial}{\partial y} \cdot \frac{\partial E}{\partial k}
$$

ensures that $\int_{\mathbf{R}^{3}}\left|f_{0}(y, s)\right|^{2} \mathrm{~d} y$ does not depend on $s$, and thus

$$
\int_{\mathbf{R}^{3}}|u(y, s, \epsilon)|^{2} \mathrm{~d} y=\int_{\mathbf{R}^{3}}|u(y, 0, \epsilon)|^{2} \mathrm{~d} y+\mathcal{O}(\epsilon) .
$$

The term $i L \cdot B+\langle\Phi, \dot{\Phi}\rangle$, which is derived from the term of order $\epsilon$ in equation (11), plays exactly the role in these constructions that the subprincipal symbol plays in the construction of asymptotic solutions to $P\left(y, \epsilon D_{y}, \epsilon\right) u=0$ (Duistermaat [5]). In physics literature the term $L \cdot B$ is well known (see Bellissard-Rammal [3] and also Bellissard [2], Helffer-Sjöstrand [9]). When $A(y, s)=\frac{\omega_{1} \times y}{2}$, it is called the Rammal-Wilkinson term. The term $\langle\Phi, \dot{\Phi}\rangle$ gives rise to the Berry phase progression [19] in the solution.

Remark 1. Formula (29) is not consistent with formula (6) in [8]. A calculation error in passing from formula (A.3) to (A.4) in the appendix to [8] led to the omission of half of the Berry phase term in formula (6) in [8].

We now derive the transport equation for $m_{1}$. Like $T_{1}, T_{2}$ can be solved for $m_{2}$ if and only if

$$
\begin{equation*}
\left\langle\Phi, K m_{1}+\Delta_{y} m_{0}\right\rangle=0 . \tag{30}
\end{equation*}
$$

On the other hand, since $x \rightarrow m_{1}(x, \cdot, \cdot)$ is required to be in $\mathcal{H}_{\omega}$, we can write

$$
m_{1}(x, y, s)=f_{1}(y, s) \Phi(x, k(y, s))+m_{1}^{\perp}(x, y, s)
$$

with

$$
\left\langle\Phi(\cdot, k(y, s)), m_{1}^{\perp}(x, y, s)\right\rangle=0 .
$$

Inserting the above equation in (30), we get

$$
\begin{equation*}
-\mathrm{i}\left\langle\Phi, K\left(f_{1} \Phi\right)\right\rangle=-\mathrm{i}\left\langle\Phi, K m_{1}^{\perp}+\Delta_{y} m_{0}\right\rangle . \tag{31}
\end{equation*}
$$

Clearly, the left-hand side of (31) equals that of (22) with $f_{1}$ instead of $f_{0}$. Thus, (29) yields
$\frac{\partial f_{1}}{\partial s}-\frac{\partial E}{\partial k} \cdot \frac{\partial f_{1}}{\partial y}-\frac{1}{2}\left(\frac{\partial}{\partial y} \cdot \frac{\partial E}{\partial k}\right) f_{1}+(\mathrm{i} L \cdot B+\langle\Phi, \dot{\Phi}\rangle) f_{1}=-\mathrm{i}\left\langle\Phi, K m_{1}^{\perp}+\Delta_{y} m_{0}\right\rangle$.
Since $m_{1}^{\perp}$ is determined by $T_{1}$, (32) reduces to an inhomogeneous version of the transport equation (29). This gives an equation for $m_{1}$. In the same way, we derive equations for all the terms $m_{j}$.

To solve the eikonal equation (16), we will choose $\phi$ to be complex-valued with $\operatorname{Im}\{\phi\} \geqslant 0$. This is the method used in the construction of Gaussian beams (see Arnaud [1] and Ralston [17]). One chooses a single trajectory $(y(r), r, \eta(r), \sigma(r))$ of the system (18), (19), and requires

$$
\left(\phi_{y}(y(r), r), \phi_{s}(y(r), r)\right)=(\eta(r), \sigma(r)) .
$$

Requiring that (16) hold to high order on $\gamma=\{(y(r), r):-\infty<r<\infty\}$ then leads to differential equations for the derivatives of $\phi$ along $\gamma$. In particular, the Hessian of $\phi$ satisfies a matrix Ricatti equation.

Choosing the initial data of the phase function $\phi$ so that $\operatorname{Im}\{\phi(y(0), 0)\} \geqslant 0$, $\operatorname{Im}\{\phi(y(0), 0)\}=0$ and $\operatorname{Im}\left\{\phi_{y y}\right\}(y(0), 0)$ is positive definite, the conservation laws for Ricatti equations arising from eikonal equations (see [17], section 1) imply that $\operatorname{Im}\left\{\phi_{y y}\right\}(y(r), r)$ is positive definite for all $r$. This localizes the packet to a tubular neighbourhood of $\gamma$ which has radius $O\left(\epsilon^{1 / 2}\right)$ 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 (19) and (20) to hold to sufficiently high order on $\gamma$ 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 $\phi$ along $\gamma$ which arise from (16)-these are linear for the derivatives of order greater than 2-and the linear ODEs along $\gamma$ for the derivatives of $m$ which arise from (25).

Remark 2. As one can see from the discussion in the preceding paragraph, the packets we construct are highly localized (to $O\left(\epsilon^{1 / 2}\right)$ ) near the trajectories in spacetime determined by the dynamic equations (20), (21). One can take superpositions of these packets-for instance over focusing families of trajectories-to construct asymptotic solutions with more complicated behaviour from interference of phases, etc. In $[14,15]$ the authors state that packets will follow trajectories in spacetime determined by equations involving the Ramal-Wilkinson term and the 'Berry curvature' directly. Our analysis has only such terms contributing to the phases of the packets.

## References

[1] Arnaud J A 1973 Hamiltonian theory of beam mode propagation Progress in Optics vol 11 ed E Wolf (Amsterdam: North-Holland) pp 249-304
[2] Bellissard J $1987 C^{*}$ algebra in solid state physics (2D electrons in a uniform magnetic field) Talk given at Warwick Conf. on Operator Algebras (July 1987)
[3] Bellissard J and Rammal R 1990 An algebraic semi-classical approach to Bloch electrons in a magnetic field J. Physique France 511803
[4] Buslaev V S 1987 Semiclassical approximation for equations with periodic coefficients Russ. Math. Surv. 42 97-125
[5] Dimassi M and Sjöstrand J 1999 Spectral Asymptotics in the Semi-Classical Limit (London Math. Soc. Lecture Note Ser. vol 268) (Cambridge: Cambridge University Press)
[6] Duistermaat J J 1974 Oscillatory integrals, Lagrange immersions and unfolding of singularities Commun. Pure Appl. Math. 27 207-81
[7] Gérard C, Martinez A and Sjöstrand J 1991 A mathematical approach to the effective Hamiltonian in perturbed periodic problems Commun. Math. Phys. 142 217-44
[8] Guillot J C, Ralston J and Trubowitz E 1988 Semi-classical methods in solid state physics Commun. Math. Phys. 116 401-15
[9] Helffer B and Sjöstrand J 1988 Analyse semi-classique pour l'équation de Harper Bull. SMF $\mathbf{1 1 6}$ mémoire no 34
[10] Horn W 1991 Semi-classical constructions in solid state physics Commun. P.D.E. 16 255-90
[11] Keller J and Rubinow S 1960 Asymptotic solution of eigenvalue problems Ann. Phys. 924-75
[12] Kohmoto M 1993 Berry's phase of Bloch electrons in electromagnetic fields J. Phys. Soc. Japan 62 659-63
[13] Maslov V P and Fedoriuk M V 1981 Semiclassical Approximation in Quantum Mechanics (Dordrecht: Reidel)
[14] Chang Ming-Che and Niu Qian 1996 Berry phase, hyperorbits, and the Hofstadter spectrum Phys. Rev. Lett. 75 1348-51
[15] Chang Ming-Che and Niu Qian 1996 Berry phase, hyperorbits, and the Hofstadter spectrum: semiclassical dynamics in magnetic Bloch bands Phys. Rev. B 53 7010-22
[16] Peierls R 1933 Zur Theorie des diamagnetimus von Leitungselektronen Z. Phys. 80 763-91
[17] Ralston J 1976 On the construction of quasimodes associated with stable periodic orbits Commun. Math. Phys. 51 219-42
[18] Ralston J 1992 Magnetic breakdown Astérisque 210 263-82
[19] Simon B 1983 Phys. Rev. Lett. 512167
[20] Zak J 1968 Dynamics of electrons in solids in external fields Phys. Rev. 168 686-95

