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Radiative Transport Equation for Bloch Electrons in Electromagnetic Fields

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Abstract The radiative transport equation for the Schrödinger equation in a periodic potential with a weak random potential in electromagnetic fields is derived using asymptotic expansion.

Keywords Radiative transport · Waves in random media · Bloch waves

1 Introduction

The radiative transport equation (RTE) is a linear Boltzmann equation, which describes propagation of energy density in a random medium [1,2]. Rigorous analysis on the transport limit for the Schrödinger equation with random potential has been studied [3,4,5,6,7,8,9,10,11,12]. In particular, the RTE was obtained from the Schrödinger equation with time independent [10] and time dependent [11] random potential. In [12], the RTE was derived from the Schrödinger equation with random and periodic potential. See also recent review [13] and references therein.

In the absence of random potential, the semiclassical equations of motion for the Schrödinger equation with periodic potential and electromagnetic fields has been considered [14,15,16,17,18,19].

In this paper, we consider noninteracting electrons in a periodic potential (Bloch electrons) with a weak random potential and apply electromagnetic fields. For this system, the RTE is derived in the same way as [12] except that we here take electromagnetic fields into account.

This paper is organized as follows. In Sec. 2 a two-scale asymptotic expansion is introduced for the Wigner distribution function. In Sec. 3 Bloch functions are considered. The Wigner distribution function is decomposed in Sec. 4 and Sec. 5.

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making use of the Bloch functions. Finally, we derive the RTE and obtain our main result Eq. (79) in Sec. 6.

2 The Schrödinger Equation

We consider Bloch electrons in an electric field \( E \in \mathbb{R}^3 \) and a magnetic field \( B \in \mathbb{R}^3 \). They are given by vector potential \( A \in \mathbb{R}^3 \) and scalar potential \( \varphi \in \mathbb{R} \) as

\[
E = -\nabla \varphi - \frac{\partial}{\partial t} A, \quad B = \nabla \times A.
\]  

The state \( \psi(t,x) \in \mathbb{R} \) \((t \in \mathbb{R}, x \in \mathbb{R}^3)\) of this system evolves according to the Schrödinger equation

\[
i\hbar \frac{\partial}{\partial t} \psi(t,x) = \mathcal{H} \psi(t,x).
\]  

The Hamiltonian \( \mathcal{H} \) is given as

\[
\mathcal{H} = \frac{1}{2m_e} (p + eA)^2 + e\varphi + U_{\text{tot}}(x),
\]  

where \( p = -i\hbar \nabla, -e \) and \( m_e \) are the charge and mass of an electron, and \( U_{\text{tot}}(x) = U(x) + V(x) \). Here \( U(x) \) is a \( d \)-dimensional \((d \leq 3)\) periodic potential and \( V(x) \) is a random potential. The periodic potential satisfies

\[
U(z + \nu) = U(z),
\]  

where \( \nu \) belongs to the lattice \( L \):

\[
L = \left\{ \sum_{j=1}^{d} n_j e_j \mid n_j \in \mathbb{Z} \right\}.
\]  

and \( e_1, \ldots, e_d \) form a basis of \( \mathbb{R}^d \) with the dual basis \( e_1^*, \ldots, e_d^* \) defined by \( e_j \cdot e_k = 2\pi \delta_{jk} \). The dual lattice \( L^* \) is spanned by \( \{e^k\} \). We let \( C \) denote the basic period cell of \( L \) and \( \Omega_{\text{BZ}} \) denote the Brillouin zone. Note that

\[
|C|\Omega_{\text{BZ}} = (2\pi)^d.
\]  

The random potential has the following properties.

\[
\langle V(y)V(y+x) \rangle = R(x), \quad \langle \tilde{V}(q)\tilde{V}(q') \rangle = (2\pi)^d \tilde{R}(q') \delta(q + q').
\]  

Here \( \langle \cdot \rangle \) denotes ensemble average and the Fourier transform is defined as

\[
\tilde{V}(q) = \int_{\mathbb{R}^d} dx e^{-iq \cdot x} V(x).
\]  

Because of the \( U(1) \) gauge symmetry, we can set

\[
\varphi = 0.
\]
We scale the variables as
\[
t → \frac{l}{\varepsilon}, \quad x → \frac{x}{\varepsilon},
\] where \(\varepsilon (>0)\) is small. We assume weak electromagnetic fields:
\[
E → \varepsilon E, \quad B → \varepsilon B.
\] Equation (1) implies that \(A\) is independent of \(\varepsilon\). Since the cyclotron radius \(\ell\) is inversely proportional to \(|B|\), we have \(\ell → \ell/\varepsilon\) and \(\ell\) gets much larger than the cell size of the lattice \(L\). Furthermore, we assume that the random potential is weak. We obtain
\[
\frac{\partial}{\partial t} \psi_\varepsilon(t,x) = \frac{i\hbar e}{2m_e} \left[ \nabla_x + \frac{i e}{\hbar E} A(t,x) \right]^2 \psi_\varepsilon(t,x) + \frac{1}{i\hbar \varepsilon} U \left( \frac{x}{\varepsilon} \right) \psi_\varepsilon(t,x)
+ \frac{1}{i\hbar \sqrt{\varepsilon}} V \left( \frac{x}{\varepsilon} \right) \psi_\varepsilon(t,x),
\] where the initial wave function \(\psi_\varepsilon(0,x) ∈ L^2(\mathbb{R}^d)\) is \(\varepsilon\)-oscillatory. In [12], the RTE is derived from this equation in the absence of the vector potential \(A(t,x)\). Let us consider the Wigner distribution function associated with \(\psi_\varepsilon\).
\[
W_\varepsilon(t,x,\mu) = \int_{\mathbb{R}^d} \frac{dy}{(2\pi)^d} e^{ik·y} \psi_\varepsilon(t,x - \varepsilon y) \psi_\varepsilon(t,x).\]
Whenever necessary, we use the fact that \(k ∈ \mathbb{R}^d\) is uniquely decomposed as \(k = q + \mu, \quad q ∈ Ω_{BZ}, \quad \mu ∈ L^*\). Note that \(W_\varepsilon(t,x,\mu)\) and its symmetric version
\[
\int_{\mathbb{R}^d} \frac{dy}{(2\pi)^d} e^{ik·y} \psi_\varepsilon(t,x - \varepsilon y) \psi_\varepsilon(t,x + \varepsilon y)
\] have the same weak limit as \(\varepsilon → 0\) [20]. We obtain the time evolution of \(W_\varepsilon\) as
\[
\frac{\partial}{\partial t} W_\varepsilon(t,x,\mu) + \left[ \frac{\hbar k}{m_e} \cdot \nabla_x + \frac{i\hbar e}{2m_e} \Delta_x + \frac{e}{m_e} (A(t,x) \cdot \nabla_x - k \cdot A(t,\nabla_\mu)) \right]
\frac{\varepsilon^2}{m_e \hbar} \left( A(t,x) + \frac{i e}{2} A(t,\nabla_\mu) \cdot A(t,\nabla_\mu) \right) W_\varepsilon(t,x,k)
+ \frac{1}{i\hbar \varepsilon} \sum_{\mu' ∈ L^*} e^{i\mu' \cdot x/\varepsilon} \hat{U}(\mu') \left[ W_\varepsilon(t,x,k - \mu') - W_\varepsilon(t,x,k) \right]
+ \frac{1}{i\hbar \sqrt{\varepsilon}} \int_{\mathbb{R}^d} \frac{dk'}{(2\pi)^d} e^{ik' \cdot x/\varepsilon} \hat{V}(k') \left[ W_\varepsilon(t,x,k - k') - W_\varepsilon(t,x,k) \right],
\] where we used
\[
\psi_\varepsilon(t,x) \frac{\partial}{\partial x_j} \psi_\varepsilon(t,x) \xrightarrow{\varepsilon → 0} 0, \quad (j = 1, \ldots, d),
\]
and introduced
\[ U(y) = \sum_{\mu \in L} e^{i\mu \cdot y} \tilde{U}(\mu), \quad \tilde{U}(\mu) = \frac{1}{|C|} \int_C dy e^{-i\mu \cdot y} U(y). \] (18)

Note that we have
\[ 1 \left| C \right| \sum_{\mu \in L} e^{i\mu \cdot z} = \sum_{\nu \in L} \delta(z - \nu). \] (19)

Let us define
\[ H(x, \mu, q) = \frac{\hbar}{2m_e} \left[ k + \frac{e}{\hbar} A(t, x) \right]^2. \] (20)

Noting that
\[ \frac{\partial A(x)}{\partial x_i} \frac{\partial}{\partial \mu_i} = A(t, 0, \ldots, 0, \frac{\partial}{\partial \mu_i}, 0, \ldots, 0), \] (21)

we obtain
\[
\frac{\partial}{\partial t} W_\epsilon + \left[ \nabla \mu H(x, \mu, q) \cdot \nabla_x - \nabla_x H(x, \mu, q) \cdot \nabla_\mu \right] W_\epsilon(t, x, k) =
\left[ \frac{i\hbar e^2}{2m_e^2} \Delta_x + \frac{i\hbar e^2}{2m_e \hbar} A(t, \mu) \cdot A(t, \nabla_\mu) \right] W_\epsilon(t, x, k)
+ \frac{1}{i\hbar} \sum_{\mu \in L} e^{i\mu \cdot x/k} \tilde{U}(\mu') \left[ W_\epsilon(t, x, k - \mu') - W_\epsilon(t, x, k) \right]
+ \frac{1}{i\hbar \sqrt{\epsilon}} \int_{R^3} \frac{dk'}{(2\pi)^3} e^{i\mu \cdot x/k} \nabla(k') \left[ W_\epsilon(t, x, k - k') - W_\epsilon(t, x, k) \right]. \tag{22}
\]

We note that the term \(-\nabla_x H\) is responsible for the Lorentz force:
\[
-\nabla_x H = -\frac{e}{m_e} \nabla_x (k \cdot A) + O(|A|^2),
-\frac{e}{m_e} \nabla_x (k \cdot A) = -\frac{e}{m_e} \left( (k \cdot \nabla_x)A + k \times (\nabla_x \times A) \right)
= -\frac{e}{\hbar} \left(-E + v \times B\right), \tag{23}
\]

where \(\hbar k = m_e v + eA\) and \(v = dx / dr\). The left-hand side of Eq. (22) can be expressed as
\[
\frac{\partial}{\partial t} W_\epsilon + \left[ H \left( x - \frac{1}{2} \nabla_\mu, \mu + \frac{1}{2} \nabla_x, q \right) - H \left( x + \frac{1}{2} \nabla_\mu, \mu - \frac{1}{2} \nabla_x, q \right) \right] W_\epsilon(t, x, k). \tag{24}
\]

This expression was first obtained by Kubo [21].

We introduce a two-scale expansion for \(W_\epsilon\):
\[
W_\epsilon(t, x, k) = W_0(t, x, z, k) + \sqrt{\epsilon} W_1(t, x, z, k) + \epsilon W_2(t, x, z, k) + \cdots. \tag{25}
\]

We assume that \(W_0\) is deterministic and periodic with respect to \(z = x/\epsilon\). We replace
\[
\nabla_x \rightarrow \nabla_x + \frac{1}{\epsilon} \nabla_z. \tag{26}
\]
By collecting terms of $O(\varepsilon^{-1})$, we have
\[ \mathcal{L} W_0 = 0, \] (27)
where the skew symmetric operator $\mathcal{L}$ is given by
\[
\mathcal{L} f(z,k) = \nabla_x H(x,\mu,q) \cdot \nabla_z f(z,k) + \frac{i\hbar}{2m_e} \Delta_x f(z,k) - \frac{1}{i\hbar} \sum_{\mu \in L^*} e^{i\mu \cdot z} \mathcal{U}(\mu') \left[ f(z,k-\mu') - f(z,k) \right] = \left[ \frac{\hbar k}{m_e} + \frac{e}{m_e} A(t,x) \right] \cdot \nabla_z f(z,k) + \frac{i\hbar}{2m_e} \Delta_x f(z,k) - \frac{1}{i\hbar} \sum_{\mu \in L^*} e^{i\mu \cdot z} \mathcal{U}(\mu') \left[ f(z,k-\mu') - f(z,k) \right]. \] (28)

By collecting terms of $O(\varepsilon^{-1/2})$, we have
\[
\mathcal{L} W_1 = \frac{1}{i\hbar} \int_{R^d} \frac{dk'}{(2\pi)^d} e^{ik' \cdot z} \tilde{V}(k') \left[ W_0(t,x,k-k') - W_0(t,x,k) \right]. \] (29)

By collecting terms of $O(1)$, we have
\[
\frac{\partial}{\partial t} W_0 + (\nabla_\mu H \cdot \nabla_x - \nabla_x H \cdot \nabla_\mu) W_0 = -\mathcal{L} W_2 - \frac{i\hbar}{m_e} \nabla_x \cdot \nabla_z W_0(t,x,k) + \frac{1}{i\hbar} \int_{R^d} \frac{dk'}{(2\pi)^d} e^{ik' \cdot z} \tilde{V}(k') \left[ W_1(t,x,k-k') - W_1(t,x,k) \right]. \] (30)

3 The Bloch Functions

To obtain the eigenvalues and eigenfunctions of the operator $\mathcal{L}$, we consider the following eigenproblem.
\[
\left[ \frac{1}{2m_e} \left( \frac{\hbar}{i} \nabla_z + eA(t,x) \right)^2 + U(z) \right] \Phi_{ma}(z,q) = E_m(q) \Phi_{ma}(z,q). \] (31)

Here, $\alpha$ labels degenerate energy levels of $E_m$ with multiplicity $r_m$: $\alpha = 1, \ldots, r_m$. We assume that there is no level crossing and
\[
E_1(q) \leq E_2(q) \leq \cdots. \] (32)

The parameter $q \in \mathbb{R}^d$ labels eigenvalues of the translational operator $T (= e^{\nu \cdot \nabla_z}, \nu \in L)$:
\[
T \Phi(z,q) = \Phi(z+\nu,q) = e^{iq \cdot \nu} \Phi(z,q). \] (33)

Note that $q$ moves inside the Brillouin zone $(\Omega_{BZ})$. It is, however, convenient to extend $\Phi(z,q)$ to $\mathbb{R}^d$ in $q$ with $L^*$-periodic. The eigenfunctions $\Phi_{ma}(z,q)$ form a complete orthonormal basis in $L^2(C)$:
\[
(\Phi_{ma}, \Phi_{\beta}) = \int_C \frac{dz}{|C|} \Phi_{ma}(z,q) \Phi_{\beta}(z,q) = \delta_{ma} \delta_{\alpha \beta}. \] (34)
Similarly, we also have

Thus we have

The Bloch functions satisfy the following orthogonality relations

They are eigenfunctions of

\[
\mathcal{L} Q_{mn}^{\alpha \beta}(z, \mu, q) = \frac{i}{\hbar} [E_m(q) - E_n(q)] Q_{mn}^{\alpha \beta}(z, \mu, q),
\]

We rewrite the eigenproblem using the periodic function

\[
\phi(z, q) = e^{-iqz} \Phi(z, q).
\]

We obtain

\[
\left[ \frac{1}{2m_c} \left( \frac{\hbar^2}{i} \nabla_z + \hbar q + eA(t, x) \right) + U(z) \right] \phi_{ma}(z, q) = E_m(q) \phi_{ma}(z, q).
\]

By differentiating the equation with respect to \( q_j \), we obtain

\[
\frac{\partial E_m}{\partial q_j} \delta_{mn} \delta_{\alpha \beta} = -i \frac{\hbar^2}{m_c} \left( \frac{\partial \phi_{ma}}{\partial z_j} \phi_{n\beta} \right) + \frac{\hbar^2}{m_c} \left( q_j + \frac{e}{\hbar} A_j \right) \delta_{mn} \delta_{\alpha \beta}.
\]

Thus we have

\[
\frac{\partial E_m}{\partial q_j} \delta_{mn} \delta_{\alpha \beta} = -i \frac{\hbar^2}{m_c} \left( \frac{\partial \phi_{ma}}{\partial z_j} \phi_{n\beta} \right) + \frac{e \hbar}{m_c} A_j(t, x) \delta_{mn} \delta_{\alpha \beta}.
\]

Similarly, we also have

\[
\left( A_l \frac{\partial \Phi_{ma}}{\partial z_j}, \Phi_{n\beta} \right) = \frac{i m_e}{\hbar^2} \frac{\partial E_m}{\partial q_j} \left( A_l \Phi_{ma}, \Phi_{n\beta} \right) - \frac{i e}{\hbar} A_j(t, x) \left( A_l \Phi_{ma}, \Phi_{n\beta} \right),
\]

where

\[
\left( A_l \Phi_{ma}, \Phi_{n\beta} \right) = \int_C \frac{dz}{|\mathcal{C}|} A_l(t, z) \Phi_{ma}(z, q) \Phi_{n\beta}(z, q).
\]

The Bloch functions satisfy the following orthogonality relations [12].

\[
\frac{1}{\Omega_{\text{BZ}}} \sum_{m, \alpha} \int_{\Omega_{\text{BZ}}} dq \, \Phi_{ma}(x, q) \Phi_{ma}(y, q) = \delta(y - x),
\]

\[
\frac{1}{\Omega_{\text{BZ}}} \int_{\Omega_{\text{BZ}}} dx \, \Phi_{j\alpha}(x, q) \Phi_{n\beta}(x, q') = \delta_{jm} \delta_{\alpha \beta} \delta(q - q').
\]

4 Decomposition of \( W_0 \)

Let us define the \( z \)-periodic functions \( Q_{mn}^{\alpha \beta}(z, \mu, q) \), \( \mu \in L^*, q \in \Omega_{\text{BZ}} \) by

\[
Q_{mn}^{\alpha \beta}(z, \mu, q) = \int_C \frac{dy}{|\mathcal{C}|} e^{i(q+\mu)z} \Phi_{ma}(z - y, q) \Phi_{n\beta}(z, q).
\]

These functions satisfy the following orthogonality relation.

\[
\sum_{\mu \in L^*} \int_C \frac{dz}{|\mathcal{C}|} \tilde{Q}_{j\alpha}^{\alpha \beta}(z, \mu, q) \tilde{Q}_{m\beta}^{\alpha \beta}(z, \mu, q) = \delta_{jm} \delta_{\alpha \alpha'} \delta_{\beta \beta'}.
\]

They are eigenfunctions of \( \mathcal{L} \):

\[
\mathcal{L} Q_{mn}^{\alpha \beta}(z, \mu, q) = \frac{i}{\hbar} [E_m(q) - E_n(q)] Q_{mn}^{\alpha \beta}(z, \mu, q).
\]
with \( k = q + \mu \).

Let us write \( \Phi_{mn}^{\alpha \beta} \) as \( \Phi_m^{\alpha \beta} \). Equation (45) implies that \( \text{ker} \, L \) is spanned by \( \Phi_m^{\alpha \beta} \). By Eq. (27), \( W_0(t, x, z, k) \) may be decomposed as

\[
W_0(t, x, z, k) = W_0(t, x, z, q + \mu) = \sum_{m, \alpha, \beta} (u_m(t, x, q) \Phi_m^{\alpha \beta}(z, \mu, q),
\]

(46)

where \( u_m(t, x, q) \) is a \( r_m \times r_m \) matrix.

5 Decomposition of \( W_1 \)

Let us look at Eq. (29). In general, \( W_1 \) is not periodic in the fast variable \( z \). Hence, instead of \( \Phi_{mn}^{\alpha \beta} \), we use the basis functions

\[
P_{mn}^\alpha(z, \mu, q, q_0) = \int_C \frac{d\eta}{|C|} e^{i(\eta+\mu)z} \Phi_{mn}^\alpha(z, \mu, q) \Phi_{n\beta}(z, q + q_0),
\]

(47)

where \( z \in \mathbb{R}^d \) and \( q, q_0 \in \Omega_{BZ} \). The functions \( P_{mn}^{\alpha \beta} \) are quasi-periodic in \( z \):

\[
P_{mn}^{\alpha \beta}(z + \nu, \mu, q, q_0) = P_{mn}^{\alpha \beta}(z, \mu, q, q_0) e^{-i\nu q_0},
\]

(48)

where \( \nu \in L \). Using Eq. (19), Eq. (34), and Eq. (42), we obtain the following orthogonality relation.

\[
\sum_{\mu \in L^*} \int_{\Omega_{BZ}} \frac{dz}{\Omega_{BZ}} P_{mn}^{\alpha \beta}(z, \mu, q, q_0) P_{mn}^{\alpha' \beta'}(z, \mu, q, q_0') = \delta_{\alpha \alpha'} \delta_{\beta \beta'} \delta(q' - q'').
\]

(49)

The functions \( P_{mn}^{\alpha \beta} \) are also eigenfunctions of \( L \).

\[
L \Phi_{mn}^{\alpha \beta}(z, \mu, q, q_0) = \frac{i}{\hbar} [E_m(q) - E_n(q + q_0)] P_{mn}^{\alpha \beta}(z, \mu, q, q_0).
\]

(50)

We write \( W_1 \) in this basis as

\[
W_1(t, x, z, q + \mu) = \sum_{mn, \alpha, \beta} \int_{\Omega_{BZ}} \frac{d\eta}{\Omega_{BZ}} \eta_{mn}^{\alpha \beta}(t, x, q, q') P_{mn}^{\alpha \beta}(z, \mu, q, q'),
\]

(51)

where \( z \in \mathbb{R}^d, q \in \Omega_{BZ}, \) and \( \mu \in L^* \). We plug this into Eq. (29), multiply \( P_{mn}^{\alpha \beta}(z, \mu, q, q_0) \), sum over \( \mu \in L^* \), and integrate over \( z \in \mathbb{R}^d \). The lhs becomes

\[
\sum_{\mu \in L^*} \int_{\mathbb{R}^d} dz \tilde{P}_{mn}^{\alpha \beta}(z, \mu, q, q_0) \mathcal{L} \sum_{mn, \alpha, \beta} \int_{\Omega_{BZ}} \frac{d\eta}{\Omega_{BZ}} \eta_{mn}^{\alpha \beta}(t, x, q, q') P_{mn}^{\alpha \beta}(z, \mu, q, q')
\]

\[
= \frac{i}{\hbar} [E_j(q) - E_l(q + q_0)] \eta_{jl}^{\alpha \beta}(t, x, q, q_0).
\]

(52)

We define

\[
T_{jm}^{\alpha \beta}(q', q) = \int_C \frac{dy}{(2\pi)^{d-1/2}|C|} e^{i(q'-q)z} \Phi_{jm}^{\alpha \beta}(y, q) \Phi_{j\alpha}(y, q').
\]

(53)
By taking the sum over $\mu$, the rhs becomes

$$
\frac{1}{\hbar} \sum_{\mu' \in L^*} \int_{B_\mathbb{Z}} \sum_{\alpha' \beta'} \frac{d\alpha'}{(2\pi)^d} \frac{d\beta'}{(2\pi)^d} \bar{V}(q' + \mu') \sum_{\alpha \beta} \frac{d\alpha}{(2\pi)^d} \frac{d\beta}{(2\pi)^d} \left[ (2\pi)^{(d-1)/2} T^\alpha_{\mu'}( q', q' - q') \{ u_m(t, x, q - q') \} \alpha' \beta' \Phi_m^\alpha(z, q - q') \\
- \delta_m \delta_{\alpha' \alpha} \{ u_m(t, x, q) \} \alpha' \beta' e^{i(q' + \mu')} \phi_m^\alpha(z, q) \right] \Phi^\beta_{\mu'}(z, q + q_0) \\
- \frac{1}{\hbar} \sum_{\mu' \in L^*} \frac{\Omega_{B_\mathbb{Z}}}{(2\pi)^{(d+1)/2}} \bar{V}(-q_0 - \mu) \sum_{\alpha' \beta'} T^\alpha_{\mu'}( q, q + q_0 + \mu) \{ u_l(t, x, q + q_0) \} \alpha' \beta' \\
- \frac{1}{\hbar} \int_{B_\mathbb{Z}} \sum_{\beta'} \left[ u_j(t, x, q) \right] \alpha' \beta' \frac{d\alpha'}{(2\pi)^d} \frac{d\beta'}{(2\pi)^d} \bar{V}(k') \sum_{\gamma} \{ u_j(t, x, q) \} \alpha' \beta' \Phi_j^\beta(z, q + q_0) \Phi_j^\gamma(z, q). \right]
$$

Therefore we obtain

$$
\eta^\alpha_{jl}(t, x, q, q_0) = \frac{\Omega_{B_\mathbb{Z}}}{(2\pi)^{(d+1)/2}} \sum_{\mu' \in L^*} \frac{\bar{V}(-q_0 - \mu)}{E_l(q + q_0) - E_j(q) + i\xi} \\
\times \sum_{\alpha'} \left[ u_l(t, x, q + q_0) \right] \alpha' \beta' T^\alpha_{\mu'}( q, q + q_0 + \mu) \\
- \int_{B_\mathbb{Z}} \frac{d\alpha'}{(2\pi)^d} \frac{d\beta'}{(2\pi)^d} \frac{\bar{V}(k')}{(2\pi)^d} \sum_{\gamma} \{ u_j(t, x, q) \} \alpha' \beta' \Phi_j^\beta(z, q + q_0) \Phi_j^\gamma(z, q), \quad (55)
$$

where $\xi (> 0)$ is infinitesimally small.

6 Time Evolution of $W_0$

Next let us look at Eq. (50). We multiply $Q_j^\alpha(z, \mu, q)$, integrate both sides over $z$, and sum over $\mu$.

$$
\sum_{\mu \in L^*} \int_{C \setminus \Gamma} \frac{dz}{|z|} Q_j^\alpha(z, \mu, q) \\
\times \left[ \frac{\partial}{\partial t} W_0 + \frac{\hbar}{m_e} \left( k + \frac{e}{\hbar} A_l(t, x) \right) \cdot \nabla_x W_0 - \frac{e}{m_e} \sum_{\alpha} \left( k_l + \frac{e}{\hbar} A_l(t, x) \right) \frac{\partial A_l(t, x)}{\partial x_\alpha} \right] \\
= \sum_{\mu \in L^*} \int_{C \setminus \Gamma} \frac{dz}{|z|} Q_j^\alpha(z, \mu, q) \\
\times \left[ \frac{\partial}{\partial t} W_0 + \sum_\gamma \left( k_l + \frac{e}{\hbar} A_l(t, x) \right) \left( \frac{\hbar}{m_e} \frac{\partial}{\partial x_l} - \frac{e}{m_e} A_l(t, \nabla_\mu) \right) \right] \\
= - \sum_{\mu \in L^*} \int_{C \setminus \Gamma} \frac{dz}{|z|} Q_j^\alpha(z, \mu, q) \left[ \mathcal{L} W_0 + \frac{i\hbar}{m_e} \nabla_x \cdot \nabla_\mu W_0 \right]
$$
\[ + \sum_{\mu, \alpha} \int \frac{dz}{|C|} Q_{\alpha}^\mu (z, \mu, q) \]
\[ \times \frac{1}{\hbar} \int_{\mathbb{R}^3} \frac{dk'}{(2\pi)^3} e^{i k' \cdot \bar{z}} [W_1(t, x, z, k') - W_1(t, x, z, k)] . \]

(56)

The first integral on the rhs vanishes (\( \mathcal{L} \) is skew symmetric and \( Q_{\alpha}^\mu \in \ker \mathcal{L} \)).

6.1 LHS

The lhs of Eq. (56) is calculated as follows. The first term is easy.
\[
\sum_{\mu, \alpha} \int \frac{dz}{|C|} Q_{\alpha}^\mu (z, \mu, q) \frac{\partial}{\partial t} W_0
\]
\[ = \sum_{\mu, \alpha, \beta} \frac{\partial}{\partial t} \{u_{m}(t, x, q)\} a'_{\alpha} b'_{\beta} \sum_{\mu, \alpha} \int \frac{dz}{|C|} Q_{\alpha}^\mu (z, \mu, q) Q_{\beta}^{a'} (z, \mu, q)
\]
\[ - \frac{\partial}{\partial t} \{u_j(t, x, q)\} a_{\beta} . \]  
(57)

The second term is calculated as follows.
\[
\sum_{\mu, \alpha} \int \frac{dz}{|C|} Q_{\alpha}^\mu (z, \mu, q) \left[ k_l + \frac{e}{\hbar} A_l(x) \right] \left( \frac{\partial}{\partial x_l} - \frac{e}{\hbar} A_l(\nabla_{\mu}) \right)
\]
\[ \times \{u_{m}(t, x, q)\} a'_{\alpha} b'_{\beta} Q_{m}^{a'} (z, \mu, q)
\]
\[ = \sum_{\mu, \alpha, \beta} \frac{\partial}{\partial x_l} \left[ u_{m}(t, x, q) \right] a'_{\alpha} b'_{\beta} \sum_{\alpha} \int \frac{dz}{|C|} \frac{d\gamma'}{|C|} \left[ -i \frac{\partial}{\partial y'_l} + \frac{e}{\hbar} A_l(\gamma') \right] e^{i(q+\mu)\gamma'}
\]
\[ \times \left\{ \frac{\partial u_m}{\partial x_l} - \frac{ie}{\hbar} u_m A_l(y') \right\} a'_{\alpha} b'_{\beta} \Phi_{m \alpha'} (z - y', q) \Phi_{m \beta'} (z, q).
\]
\[ = \frac{\partial}{\partial x_l} \left[ u_{m}(t, x, q) \right] a'_{\alpha} b'_{\beta} \left[ -i \left( \frac{\partial \Phi_{m \alpha'}}{\partial z_l}, \Phi_{j \alpha} \right) + \frac{e}{\hbar} A_l(x) \delta_{\alpha \alpha'} \right]
\]
\[ - \frac{ie}{\hbar} \left[ u_{m}(t, x, q) \right] a'_{\alpha} b'_{\beta} \left[ -i \left( \frac{\partial \Phi_{m \alpha'}}{\partial z_l}, \Phi_{j \alpha} \right) \left( A_l \Phi_{j \beta}, \Phi_{m \beta'} \right) + \frac{e}{\hbar} A_l(x) \delta_{j m} \delta_{\alpha \alpha'} \left( A_l \Phi_{j \beta}, \Phi_{m \beta'} \right) \right]
\]
\[ + i \delta_{j m} \delta_{\beta \beta'} \left( A_l \frac{\partial \Phi_{m \alpha'}}{\partial z_l}, \Phi_{j \alpha} \right) - \delta_{j m} \delta_{\beta \beta'} \frac{e}{\hbar} A_l(x) \left( A_l \Phi_{m \alpha'}, \Phi_{j \alpha} \right). \]  
(58)

Therefore, the lhs of Eq. (56) is written as
\[
\frac{\partial}{\partial t} \{u_j(t, x, q)\} a_{\beta} + \frac{1}{\hbar} \nabla_q E_j(q) \cdot \nabla_z \{u_j(t, x, q)\} a_{\beta} + \frac{e}{\hbar}
\]
\[ \times \sum_{\alpha} \left( \frac{i}{\hbar} \nabla_q E_j(z) \Phi_{j \alpha}(z), \Phi_{j \alpha}(z) \right) \{u_j(t, x, q)\} a_{\beta}
\]
\[ - \sum_{\beta'} \{u_j(t, x, q)\} a_{\beta'} \left( \frac{i}{\hbar} \nabla_q E_j(z) \Phi_{j \beta'}(z), \Phi_{j \beta'}(z) \right) . \]  
(59)
6.2 RHS

Let us calculate the rhs of Eq. (56). After taking ensemble average, the rhs is given by the sum of two matrices $I_1$ and $I_2$ where

\[ {I}_1 = I_{11} - I_{12}, \]  

\[ \{I_{11}\}_{\alpha\beta} = \frac{1}{i\hbar} \sum_{\mu \in L} \int_C \frac{dz}{|C|} \bar{Q}_j^{\alpha\beta} (z, \mu, q) \int_{R^d} \frac{dk'}{(2\pi)^d} e^{ik'z} \]  

\[ \times \left< \check{V}(k') W_1 (t, x, z, k' - k) \right>, \]  

\[ \{I_{12}\}_{\alpha\beta} = \frac{1}{i\hbar} \sum_{\mu \in L} \int_C \frac{dz}{|C|} Q_j^{\alpha\beta} (z, \mu, q) \int_{R^d} \frac{dk'}{(2\pi)^d} e^{ik'z} \]  

\[ \times \left< \check{V}(k') W_1 (t, x, z, k) \right>. \]  

Using Eq. (51) and Eq. (55), $I_1$ is written as

\[ I_1 = I_{11} - I_{12}, \]  

where

\[ \{I_{11}\}_{\alpha\beta} = \frac{1}{i\hbar} \sum_{\mu \in L} \int_C \frac{dz}{|C|} \bar{Q}_j^{\alpha\beta} (z, \mu, q) \int_{R^d} \frac{dk'}{(2\pi)^d} e^{ik'z} \sum_{nn'\beta'} \int_{BZ} \frac{d\Omega_{BZ}}{(2\pi)^{d+1}/2} \sum_{\mu' \in L} \frac{\langle \check{V}(k') \check{V}(q' - q'' - \mu') \rangle}{E_n (q - q' + q'') - E_m (q - q') + i\xi} \]  

\[ \times \sum_{\alpha''} \{ u_m (t, x, q - q' + q'') \} \alpha''_{\alpha''} \phi_{mn}^{\alpha''} (q - q', q - q' + q'' + \mu'') \]  

\[ \times \left< \check{V}(k') W_1 (t, x, q - q' + q'' + \mu'') \right>, \]  

and

\[ \{I_{12}\}_{\alpha\beta} = \frac{1}{i\hbar} \sum_{\mu \in L} \int_C \frac{dz}{|C|} Q_j^{\alpha\beta} (z, \mu, q) \int_{R^d} \frac{dk'}{(2\pi)^d} e^{ik'z} \sum_{nn'\beta'} \int_{BZ} \frac{d\Omega_{BZ}}{(2\pi)^{d+1}/2} \sum_{\mu' \in L} \frac{\langle \check{V}(k') \check{V}(q') \rangle}{E_n (q - q' + q'') - E_m (q - q') + i\xi} \]  

\[ \times \sum_{\beta''} \{ u_m (t, x, q - q') \} \beta''_{\beta''} \phi_{mn}^{\beta''} (q' - q' + q'' - \mu'') \]  

\[ \times \left< \check{V}(k') W_1 (t, x, q' - q' + q'') \right>. \]  

\[ \{I_{11}\}_{\alpha\beta} = \frac{1}{i\hbar} \sum_{m} \sum_{\mu \in L} \int_{BZ} \frac{d\Omega_{BZ}}{2\pi} \frac{\check{R} (-q'' - \mu'')}{E_j (q) - E_m (q - q'') + i\xi} \sum_{\alpha'\alpha''} \{ u_j (t, x, q) \} \alpha''_{\alpha''} \]  

\[ \times T_{mn}^{\alpha'' \alpha''} (q - q'', q + \mu'') T_{jm}^{\alpha' \alpha'} (q + \mu'', q - q'). \]
Similarly we also obtain \( I_{12} \).

\[
\{ I_{12} \}_{\alpha\beta} = \frac{1}{i \hbar} \int_{\text{Re} \zeta} \frac{dk'}{2\pi} \sum_{m} E_j(q) - E_m(q - q') + i\tilde{\varepsilon} \left\{ u_n(t, x, q - q') \delta_{\alpha\beta} T_{jm}^{\alpha\beta}(q, q - q') \right\}
\]

where we used

\[
\int_{\text{Re} \zeta} dq' = \sum_{\gamma L} \int_C dq, \quad \frac{1}{\Omega_{\text{BZ}}} \sum_{\mu L^*} e^{i q \cdot \mu} = \sum_{\mu L^*} \delta(q + \mu).
\]

We have

\[
\{ I_1 \}_{\alpha\beta} = \frac{1}{i \hbar} \sum_{n \mu \nu L^*} \int_{\text{BZ}} \frac{d\gamma'}{2\pi} \frac{\tilde{R}(-q' - \mu')}{E_n(q + q') - E_j(q) + i\tilde{\varepsilon}} \left[ \sum_{\alpha' \alpha''} T_{jm}^{\alpha'\alpha''}(q, q + q' + \mu') \delta_{\alpha'\beta} \delta_{\alpha''\gamma} T_{nj}^{\beta\gamma}(q + q' + \mu', q) \right] \]

In the same way, we have

\[
\{ I_2 \}_{\alpha\beta} = -\frac{1}{i \hbar} \sum_{n \mu \nu L^*} \int_{\text{BZ}} \frac{d\gamma'}{2\pi} \frac{\tilde{R}(-q' - \mu')}{E_n(q + q') - E_j(q) + i\tilde{\varepsilon}} \left[ \sum_{\alpha' \alpha''} T_{jm}^{\alpha'\alpha''}(q, q + q' + \mu') \delta_{\alpha'\beta} \delta_{\alpha''\gamma} T_{nj}^{\beta\gamma}(q + q' + \mu', q) \right] \]

Thus we see the relation

\[
I_2 = I_1^*,
\]

where * denotes the Hermitian conjugate. By summing \( I_1 \) and \( I_2 \), and using the relation

\[
\tilde{T}_{jm}^{\beta\alpha}(q, q') = T_{jm}^{\alpha\beta}(q', q),
\]

the rhs of Eq. (66) becomes

\[
I_1 + I_2 = \frac{1}{i \hbar} \sum_{n \mu \nu L^*} \int_{\text{BZ}} \frac{d\gamma'}{2\pi} \tilde{R}(-q' - \mu') T_{jm}(q, q + q' - \mu') u_n(t, x, q - q') T_{mj}(q + q' - \mu', q).
\]
Furthermore let us define the following superoperators.

We change the variable as $q' \rightarrow q - q'$ and obtain

$$I_1 + R_1 = \frac{1}{i\hbar} \sum_m \sum_{\mu \in L^*} \int_{\text{BZ}} \frac{dq'}{2\pi} \tilde{R}(-q' - \mu')$$

$$2\pi i T_{jm}(q, q' - \mu') u_m(t, x, q') T_{mj}(q' - \mu', q) \delta(E_j(q) - E_m(q'))$$

$$+ \left( \frac{1}{E_j(q) - E_m(q') + i\xi} \right)$$

$$\frac{u_j(t, x, q) T_{jm}(q, q' - \mu') T_{mj}^*(q, q' - \mu') u_j(t, x, q)}{E_j(q) - E_m(q') - i\xi} \right].$$

$$I_1 + \hat{R} = \frac{1}{i\hbar} \sum_m \sum_{\mu \in L^*} \int_{\text{BZ}} \frac{dq'}{2\pi} \tilde{R}(-q' - \mu')$$

$$2\pi i T_{jm}(q, q' - \mu') u_m(q_0) T_{mj}(q' - \mu', q)$$

$$+ \frac{1}{E_j(q) - E_m(q') + i\xi}$$

$$\left[ \frac{u_j(q_0) T_{jm}(q, q' - \mu') T_{mj}^*(q, q' - \mu') u_j(q)}{E_j(q) - E_m(q') + i\xi} \right].$$

6.3 Radiative Transport Equation

We define a vector $v_j(q)$, a matrix $M_j(q)$, and a superoperator $\hat{\mu}_L$ as

$$v_j(q) = \frac{1}{\hbar} \nabla_q E_j(q),$$

$$\{M_j(q)\}_{\alpha\beta} = \left( \frac{i e}{\hbar} v_j(q) \cdot A \Phi_{\beta}, \Phi_{\alpha} \right),$$

$$\hat{\mu}_L : u_j(q) \mapsto [M_j(q), u_j(q)] = M_j(q) u_j(q) - u_j(q) M_j(q).$$

Furthermore let us define the following superoperators.

$$\hat{A}(q, q') : u_j(q_0) \mapsto \frac{1}{\hbar} \sum_m \sum_{\mu \in L^*} \tilde{R}(-q' - \mu') \delta(E_j(q) - E_m(q'))$$

$$T_{jm}(q, q' - \mu') u_m(q_0) T_{mj}(q' - \mu', q),$$

$$\hat{\mu}_s : u_j(q) \mapsto -\frac{1}{i\hbar} \sum_m \sum_{\mu \in L^*} \int_{\text{BZ}} \frac{dq'}{2\pi} \tilde{R}(-q' - \mu')$$

$$\left[ \frac{T_{jm}(q, q' - \mu') T_{mj}^*(q, q' - \mu') u_j(q)}{E_j(q) - E_m(q') + i\xi} \right].$$
Finally, by Eqs. (30), (56), (59), and (73), we obtain the RTE as

\[
\frac{\partial}{\partial t} u_j(t, x, q) + v_j(q) \cdot \nabla_x u_j(t, x, q) + (\hat{\mu}_L + \hat{\mu}_s) u_j(t, x, q) = \int_{BZ} dq' \hat{A}(q, q') u_j(t, x, q'). \quad (79)
\]

Note that the term for $\hat{\mu}_L$ stems from the Lorentz force. The terms for $\hat{\mu}_s$ and $\hat{A}$ stem from the random potential.

References

1. Chandrasekhar, S.: Radiative Transfer. Dover, New York (1960).
2. Case, K. M., Zweifel, P. F.: Linear Transport Theory. Addison-Wesley, Massachusetts (1967).
3. Martin, P., Emch, G. G.: A rigorous model sustaining van Hove’s phenomenon. Helv. Phys. Acta 48 59–78 (1975)
4. Spohn, H.: Derivation of the transport equation for electrons moving through random impurities. J. Stat. Phys. 17 385–412 (1977)
5. Dell’Antonio, G.: Large time, small coupling behaviour of a quantum particle in a random field. Ann. Inst. H. Poincaré Sect. A 39 339–384 (1983)
6. Ho, T. G., Landau, L. J., Wilkins, A. J.: On th weak coupling limit for a Fermi gas in a random potential. Rev. Math. Phys. 5 209–298 (1993)
7. Markowich, P. A., Mauser, N. J., Poupaud, F.: A Wigner-function approach to (semi)classical limits: electrons in a periodic potential. J. Math. Phys. 35 1066–1094 (1994)
8. Gérard, P., Markowich, P. A., Mauser, N. J., Poupaud, F.: Homogenization limits and Wigner transforms. Comm. Pure Appl. Math. 50 323–379 (1997)
9. Erdős, L., Yau, H.-T.: Linear Boltzmann equation as the weak coupling limit of a random Schrödinger equation. Comm. Pure Appl. Math. 53 667–735 (2000)
10. Ryzhik, L., Papanicolaou, G., Keller, J. B.: Transport equations for elastic and other waves in random media. Wave Motion 24, 327–370 (1996)
11. Bal, G., Papanicolaou, G., Ryzhik, L.: Radiative transport limit for the random Schrödinger equation Nonlinearity 15, 513–529 (2002)
12. Bal, G., Fannjiang, A., Papanicolaou, G., Ryzhik, L.: Radiative transport in a periodic structure. J. Stat. Phys. 95, 479–494 (1999)
13. Bal, G., Komorowski, T., Ryzhik, L.: Kinetic limits for waves in a random medium. Kinetic and Related Models 3 529–644 (2010)
14. Guillot, J. C., Raolon, J., Trubowitz, E.: Semi-classical asymptotics in solid state physics. Commun. Math. Phys. 116 401–415 (1988)
15. Chang, M.-C., Niu, Q.: Berry phase, hyperorbits, and the Hofstadter spectrum: Semi-classical dynamics in magnetic Bloch bands. Phys. Rev. B 53 7010–7023 (1996)
16. Sundaram, G., Niu, Q.: Wave-packet dynamics in slowly perturbed crystals: Gradient corrections and Berry-phase effects. Phys. Rev. B 59 14915–14925 (1999)
17. Hövermann, F., Spohn, H., Teufel, S.: Semi-classical limit for the Schrödinger equation with a short scale periodic potential. Commun. Math. Phys. 215 609–629 (2001)
18. Dimassi, M., Guillot, J. C., Raolon, J.: Semi-classical asymptotics in magnetic Bloch bands. J. Phys. A: Math. Gen. 35 7597–7605 (2002)
19. Panati, G., Spohn, H., Teufel, S.: Effective dynamics for Bloch electrons: Peierls substitution and beyond. Commun. Math. Phys. 242 547–578 (2003)
20. P. Gérard and E. Leichtnam, Ergodic properties of eigenfunctions for the Dirichlet problem, Duke Math. J. 71: 559–607 (1993).
21. R. Kubo, Wigner representation of quantum operators and its applications to electrons in a magnetic Field, J. Phys. Soc. Japan 19: 2127–2139 (1964).