Radiative Transport in a Periodic Structure

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Abstract

We derive radiative transport equations for solutions of a Schrödinger equation in a periodic structure with small random inhomogeneities. We use systematically the Wigner transform and the Bloch wave expansion. The streaming part of the radiative transport equations is determined entirely by the Bloch spectrum, while the scattering part by the random fluctuations.

Keywords. Radiative transport, waves in random media, Wigner distribution, semiclassical limits, Bloch waves.

1 Introduction

Radiative transport equations describe propagation of the phase space energy density of high frequency waves in a medium with weak random impurities whose correlation length is comparable to the wave length $\lambda$. The background medium may vary but only on scales that are much larger than $\lambda$. The phase space energy density has also been studied for a periodic potential when the period is comparable to the wave length $\lambda$. It is then found that the limiting phase space energy density satisfies a system of decoupled Liouville equations with Hamiltonians given by the Bloch eigenvalues. Thus, we expect that the addition of small random fluctuations to the periodic structure will give rise to a system of coupled radiative transport equations. This is what we show in this paper formally, using asymptotic expansions. The rigorous proof of our final result remains an open problem. Our main result is the system of the radiative transport equations

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that describes the propagation of phase space energy densities \( \sigma_m(t,x,p) \) corresponding to various Bloch eigenvalues \( E_m(p) \). We derive here the transport equations only for the Schrödinger equation. However, the generalization to more general types of waves in a periodic and random medium, like those described by hyperbolic systems considered in [19], is straightforward. This results in the replacement of the eigenvalues \( E_m(p) \) in (40) by the corresponding Bloch eigenvalues for the hyperbolic system under consideration. The paper is organized as follows. First, we recall in Section 2 some properties of the Bloch eigenfunctions and also give a formal derivation of the Liouville transport equations in the absence of random inhomogeneities. These results were previously derived rigorously in [15] and [10], and we show the connection between our formalism and their results in Section 2.4. Section 3 is the main part of the paper, where we derive the radiative transport equations in the presence of a random potential.

2 Waves in a periodic structure

2.1 The Schrödinger equation

We give here a derivation of the Liouville equation for the phase space energy density like the one in [19]. A different analysis is given in [10, 15]. We then adapt the analysis of [19] to the periodic-random case.

There is not a lot of mathematical work on the transport limit for the Schrödinger equation with random potential. We cite here the work of Martin and Emch [16], of Spohn [20], of Dell’Antonio [3] and the recent extensive study of Ho, Landau and Wilkins [11]. These papers established the validity of the kinetic linear transport equation for a small time \( T > 0 \). The global validity of this limit was proved recently by Erdős and Yau in [4]. They treat only spatially homogeneous problems but it is known how to extend the analysis to the spatially inhomogeneous case (slow \( x \)-dependent initial data and potential) [5]. A really satisfactory mathematical treatment of radiative transport asymptotics from random wave equations is lacking at present.

It is convenient for us to use the usual Wigner distribution and not the Wigner band-series as in [10, 13]. The two formulations are, however, equivalent [13]. Let \( \phi_\varepsilon(t,x) \) be the solution of the initial value problem

\[
\begin{align*}
  i\varepsilon \frac{\partial \phi_\varepsilon}{\partial t} + \frac{\varepsilon^2}{2} \Delta \phi_\varepsilon - V(\frac{x}{\varepsilon}) &= 0 \\
  \phi_\varepsilon(0,x) &= \phi_\varepsilon^0(x).
\end{align*}
\]
The initial data \( \phi^0_\varepsilon(x) \) is uniformly bounded in \( L^2(\mathbb{R}^d) \): \( \| \phi^0_\varepsilon \|_{L^2} \leq C \). We also assume that it is \( \varepsilon \)-oscillatory, that is, for any test function \( \psi \in C_c(\mathbb{R}^d) \):

\[
\limsup_{\varepsilon \to 0} \int_{|k| \geq R/\varepsilon} |\hat{\psi} \phi^0_\varepsilon(k)|^2 dk \to 0 \quad \text{as} \quad R \to +\infty. \tag{2}
\]

Finally we assume that the family \( \phi^0_\varepsilon \) is compact at infinity:

\[
\limsup_{\varepsilon \to 0} \int_{|x| \geq R} |\phi^0_\varepsilon(x)|^2 dx \to 0 \quad \text{as} \quad R \to +\infty. \tag{3}
\]

A sufficient condition for (2) is \( \| \nabla \phi^0_\varepsilon \| \leq C/\varepsilon \). The case of \( \varepsilon \)-independent initial data was studied in [2], where the Liouville equation for the wave amplitudes (not energies) was derived.

The potential \( V(z) \) is periodic:

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

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

\[
L = \left\{ \sum_{j=1}^d n_j e_j \mid n_j \in \mathbb{Z} \right\}, \tag{4}
\]

and \( e_1, \ldots, e_d \) form a basis of \( \mathbb{R}^d \) with the dual basis \( e^j \) defined by

\[
(e_j \cdot e^k) = 2\pi \delta_{jk}
\]

and the dual lattice \( L^* \) defined by \( (4) \) with \( e_j \) replaced by \( e^j \). We denote by \( C \) the basic period cell of \( L \) and by \( B \) the Brillouin zone:

\[
B = \left\{ k \in \mathbb{R}^d \mid k \text{ is closer to } \mu=0 \text{ than any other point } \mu \in L^* \right\}.
\]

We define the Wigner distribution by

\[
W_\varepsilon(t, x, k) = \int_{\mathbb{R}^d} \frac{dy}{(2\pi)^d} e^{ik \cdot y} \phi_\varepsilon(t, x - \varepsilon y) \overline{\phi_\varepsilon(t, x)}.
\tag{5}
\]

This definition is equivalent to its symmetric version

\[
\tilde{W}_\varepsilon(t, x, k) = \int_{\mathbb{R}^d} \frac{dy}{(2\pi)^d} e^{ik \cdot y} \phi_\varepsilon(t, x - \varepsilon y) \overline{\phi_\varepsilon(t, x + \varepsilon y / 2)},
\]

in the sense that \( W_\varepsilon \) and \( \tilde{W}_\varepsilon(x, k) \) have the same weak limit as \( \varepsilon \to 0 \). We also have that

\[
\mathcal{E}_\varepsilon(t, x) = |\phi_\varepsilon(t, x)|^2 = \int_{\mathbb{R}^d} dk W_\varepsilon(t, x, k) = \int_{\mathbb{R}^d} dk \tilde{W}_\varepsilon(t, x, k).
\]
The basic properties of the Wigner distributions are reviewed in detail in [10, 18]. In particular the weak limit \( W_\varepsilon(t, x, k) \) of \( \mathcal{W}_\varepsilon(t, x, k) \) exists in \( \mathcal{S}'(\mathbb{R}^d \times \mathbb{R}^d) \) and under assumptions (2) and (3) it captures correctly the behavior of the energy \( E_\varepsilon \):

\[
\lim_{\varepsilon \to 0} \int dxdk W_\varepsilon(t, x, k) = \int dxdk W(t, x, k).
\]

We deduce from (1) and (5) the following evolution equation for \( W_\varepsilon(t, x, k) \):

\[
\frac{\partial W_\varepsilon}{\partial t} + \mathbf{k} \cdot \nabla_x W_\varepsilon + \frac{i\varepsilon}{2} \Delta_x W_\varepsilon = \frac{1}{i\varepsilon} \sum_{\mu \in \mathbb{L}} e^{i\mu \cdot x/\varepsilon} \hat{V}(\mu) \left[ W_\varepsilon(x, k - \mu) - W_\varepsilon(x, k) \right].
\]

Here \( \hat{V}(\mu) \) are the periodic Fourier coefficients of \( V(y) \):

\[
\hat{V}(\mu) = \frac{1}{|C|} \int_C dy e^{-i\mu \cdot y} V(y),
\]

so that if \( V(y) \) is smooth we have

\[
V(y) = \sum_{\mu \in \mathbb{L}} e^{i\mu \cdot y} \hat{V}(\mu)
\]

and

\[
\frac{1}{|C|} \sum_{\mu \in \mathbb{L}} e^{i\mu \cdot z} = \sum_{\nu \in \mathbb{L}} \delta(z - \nu).
\]

We introduce a multiple scales expansion for \( W_\varepsilon \):

\[
W_\varepsilon(t, x, k) = W_0(t, x, \frac{x}{\varepsilon}, k) + \varepsilon W_1(t, x, \frac{x}{\varepsilon}, k) + \ldots
\]

and assume that the leading term \( W_0(t, x, z, k) \) is periodic in the fast variable \( z = \frac{x}{\varepsilon} \). As usual, we replace then

\[
\nabla_x \to \nabla_x + \frac{1}{\varepsilon} \nabla_z
\]

in (3) and rewrite it as

\[
\frac{\partial W_\varepsilon}{\partial t} + \mathbf{k} \cdot \left[ \nabla_x + \frac{1}{\varepsilon} \nabla_z \right] W_\varepsilon + \frac{i\varepsilon}{2} \left( \nabla_x + \frac{1}{\varepsilon} \nabla_z \right) \cdot \left( \nabla_x + \frac{1}{\varepsilon} \nabla_z \right) W_\varepsilon
\]

\[
= \frac{1}{i\varepsilon} \sum_{\mu \in \mathbb{L}} e^{i\mu \cdot z} \hat{V}(\mu) \left[ W_\varepsilon(k - \mu) - W_\varepsilon(k) \right].
\]

We insert the perturbation expansion (3) into (11) and get at the order \( \varepsilon^{-1} \):

\[
\mathcal{L} W_0 = 0,
\]

where the skew symmetric operator \( \mathcal{L} \) is given by

\[
\mathcal{L} f(z, k) = \mathbf{k} \cdot \nabla_z f + \frac{i}{2} \Delta_z f - \frac{1}{i} \sum_{\mu \in \mathbb{L}} e^{i\mu \cdot z} \hat{V}(\mu) \left[ f(z, k - \mu) - f(z, k) \right].
\]
2.2 The Bloch functions

The eigenfunctions of $\mathcal{L}$ are constructed as follows. Given $p \in \mathbb{R}^d$ consider the eigenvalue problem

\[ -\frac{1}{2} \Delta z \Psi(z, p) + V(z) \Psi(z, p) = E(p) \Psi(z, p) \quad (12) \]

\[ \Psi(z + \nu, p) = e^{ip \cdot \nu} \Psi(z, p), \text{ for all } \nu \in L \]

\[ \frac{\partial \Psi}{\partial z_j}(z + \nu, p) = e^{ip \cdot \nu} \frac{\partial \Psi}{\partial z_j}(z), \text{ for all } \nu \in L. \]

This problem has a complete orthonormal basis of eigenfunctions $\Psi^\alpha_m(z, p)$ in $L^2(C)$:

\[ (\Psi^\alpha_m, \Psi^\beta_j) = \int_C \frac{dz}{|C|} \Psi^\alpha_m(z, p) \bar{\Psi}^\beta_j(z, p) = \delta_{mj} \delta_{\alpha\beta}. \quad (13) \]

They are called the Bloch eigenfunctions, corresponding to the real eigenvalues $E_m(p)$ of multiplicity $r_m$. Here $\alpha = 1, \ldots, r_m$ labels eigenfunctions inside the eigenspace. The eigenvalues $E_m(p)$ are $L^*$-periodic in $p$ and have constant finite multiplicity outside a closed subset $F_m$ of $p \in \mathbb{R}^d$ of measure zero. They may be arranged $E_1(p) < E_2(p) < \ldots < E_j(p) < \ldots$ with $E_j(p) \to \infty$ as $j \to \infty$, uniformly in $p$. We consider momenta $p$ outside the set $F_m$.

The problem (12) may be rewritten in terms of periodic functions $\Phi(z, p) = e^{-ip \cdot z} \Psi(z, p)$:

\[ -\frac{1}{2} \Delta z \Phi^\alpha_m + V(z) \Phi^\alpha_m - ip \cdot \nabla_z \Phi^\alpha_m + \frac{|p|^2}{2} \Phi^\alpha_m = E_m(p) \Phi^\alpha_m(z, p). \quad (14) \]

We differentiate (14) with respect to $p_j$ and take the scalar product of the resulting equation and $\Phi^\beta_m$ to get

\[ \frac{\partial E_m}{\partial p_j} \delta_{\alpha\beta} = p_j \delta_{\alpha\beta} - i(\frac{\partial \Phi^\alpha_m}{\partial z_j}, \Phi^\beta_m), \]

which may be rewritten as

\[ \frac{\partial E_m}{\partial p_j} \delta_{\alpha\beta} = i(\Psi^\alpha_m, \frac{\partial \Psi^\beta_m}{\partial z_j}). \quad (15) \]

There is no summation over $m$ in (15).

Recall the Bloch transform of a function $\phi(x) \in L^2(\mathbb{R}^d)$

\[ \tilde{\phi}^\alpha_m(p) = \int_{\mathbb{R}^d} dz \phi(z) \Psi^\alpha_m(z, p). \]

It has the following properties:

(i) $\phi(x) = \frac{1}{|B|} \sum_{m=1}^{\infty} \sum_{\alpha=1}^{r_m} \int_B dp \tilde{\phi}^\alpha_m(p) \Psi^\alpha_m(x, p), \quad x \in \mathbb{R}^d.$

(ii) Let $\phi(x), \eta(x) \in L^2(\mathbb{R}^d)$, then the Plancherel formula holds:

\[ \int_{\mathbb{R}^d} dx \phi(x) \bar{\eta}(x) = \frac{1}{|B|} \sum_{m,\alpha} \int_B dp \tilde{\phi}^\alpha_m(p) \bar{\tilde{\eta}}^\alpha_m(p). \]
(iii) The mapping $\phi \rightarrow \tilde{\phi}$ is one-to-one and onto, from $L^2(R^d) \rightarrow \oplus_m L^2(B)$.

We deduce from these properties the orthogonality relations:

$$\delta(y - x) = \frac{1}{|B|} \sum_{m,\alpha} \int_B dp \Psi_m^\alpha(x, p) \bar{\Psi}_m^\alpha(y, p)$$

and

$$\delta_m \delta_{\alpha \beta} \delta_{\text{per}}(p - q) = \frac{1}{|B|} \int_{R^d} dx \Psi_j^\alpha(x, p) \bar{\Psi}_m^\beta(x, q).$$  \hspace{1cm} (16)

The periodic delta function $\delta_{\text{per}}$ in (14) is understood as follows: for any function $\phi(p) \in C^\infty(B)$

$$\phi(p) = \int_B dq \phi(q) \delta_{\text{per}}(p - q).$$

Given any vector $k \in R^d$ we may decompose it uniquely as

$$k = p_k + \mu_k$$  \hspace{1cm} (17)

with $p_k \in B$ and $\mu_k \in L^*$. We then define the $z$-periodic functions $Q_{mn}^{\alpha \beta}(z, \mu, p), \mu \in L^*, p \in B$ by

$$Q_{mn}^{\alpha \beta}(z, \mu, p) = \int_C dy \frac{1}{|C|} e^{i(p + \mu) \cdot y} \Psi_m^\alpha(z - y, p) \bar{\Psi}_n^\beta(z, p).$$  \hspace{1cm} (18)

Then a direct computation shows that

$$\mathbb{L} Q_{mn}^{\alpha \beta}(z, \mu, p) = i(E_m(p) - E_n(p))Q_{mn}^{\alpha \beta}(z, \mu, p)$$  \hspace{1cm} (19)

with $\mu = \mu_k, p = p_k$, so $Q_{mn}^{\alpha \beta}$ are eigenfunctions of $\mathbb{L}$.

### 2.3 The Liouville equations

Now (19) implies that, for any $p$, $\ker \mathbb{L}$ is spanned by the functions $Q_{mn}^{\alpha \beta}$, which we denote by $Q_{m}^{\alpha \beta}$ (to indicate that there is no summation over $m$). Then (11) implies that $W_0(t, x, z, k)$ may be written as

$$W_0(t, x, z, k) = W_0(t, x, z, p + \mu) = \sum_{m,\alpha,\beta} \sigma_{m}^{\alpha \beta}(t, x, p) Q_{mn}^{\alpha \beta}(z, \mu, p), \ p \in B, \ \mu \in L^*$$  \hspace{1cm} (20)

with $\mu = \mu_k, p = p_k$. This defines $\sigma_m$, which is scalar if the eigenvalue $E_m(p)$ is simple, and is a matrix of size $r_m \times r_m$ if $E_m(p)$ has multiplicity $r_m > 1$. We call $\sigma_m$ the coherence matrices in analogy to the non-periodic case [19]. They are defined inside the Brillouin zone $p \in B$ but it is convenient to extend them as functions in $R^d, L^*$-periodic in $p$. 

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Next we look at $\varepsilon^0$ terms in (10). We get

$$\frac{\partial W_0}{\partial t} + k \cdot \nabla_x W_0 + i \nabla_x \cdot \nabla_z W_0 = -\mathcal{L} W_1.$$  \hspace{1cm} (21)$$

We now integrate both sides of (21) against $\check{Q}_j^{\alpha\beta}(z, \mu, p)$ over $z$ in $C$ and sum over $\mu$. To evaluate the left side we note that we have after summing over $\mu$ using (8), and using (13) and a change of variables $y \rightarrow z - y$:

$$\sum_{\mu \in L^*} \int_C |C| \check{Q}_m^{\alpha\beta \prime}(z, \mu, p) \check{Q}_j^{\alpha\beta}(z, \mu, p) = \int_{C \times C} |C|^2 \check{\Psi}_m^{\alpha\beta}(z, p) \check{\Psi}_m^{\beta\prime}(y, p) \check{\Psi}_j^{\alpha\beta}(z, p) \check{\Psi}_j^{\beta\prime}(y, p) = \delta_{mj} \delta_{\alpha\alpha} \delta_{\beta\beta}.$$  \hspace{1cm} (22)$$

Further, using the change of variables and equations above and also (15), we get

$$\sum_{\mu \in L^*} (\mu \mu) \check{Q}_m^{\alpha\beta \prime}, Q_j^{\alpha\beta}) = \sum_{\mu \in L^*} \int_C |C^3| \check{\Psi}_m^{\alpha\beta}(z - y \mu) \check{\Psi}_m^{\beta\prime}(y, p) \check{\Psi}_j^{\alpha\beta}(z, p) \check{\Psi}_j^{\beta\prime}(y, p) = \frac{1}{i} \int_{C \times C} |C|^2 \psi_m^{\alpha\beta}(y, p) \psi_j^{\alpha\beta}(z, p) \psi_j^{\alpha\beta}(y, p) = \frac{1}{i} \delta_{mj} \delta_{\alpha\alpha} \delta_{\beta\beta}.$$  \hspace{1cm} (23)$$

A similar calculation shows that the third term on the left vanishes:

$$\sum_{\mu \in L^*} \frac{\partial Q_m^{\alpha\beta \prime}}{\partial z l}, Q_j^{\alpha\beta}) = \int_{C \times C} |C|^2 \check{\Psi}_m^{\alpha\beta}(z - y \mu) \check{\Psi}_m^{\beta\prime}(z - y, p) \check{\Psi}_j^{\alpha\beta}(z, p) \check{\Psi}_j^{\beta\prime}(y, p) \psi_j^{\alpha\beta}(z, p) \psi_j^{\beta\prime}(y, p) = -\frac{1}{i} \delta_{\alpha\alpha} \delta_{\beta\beta} \delta_{mj} \frac{\partial E_m}{\partial p_l} + \frac{1}{i} \delta_{\alpha\alpha} \delta_{\beta\beta} \delta_{mj} \frac{\partial E_m}{\partial p_l} = 0.$$  

The right side of (21) integrated against $\check{Q}_j^{\alpha\beta}$ vanishes since $\mathcal{L}$ is skew symmetric, and $Q_j^{\alpha\beta} \in \ker \mathcal{L}$.

Putting together (21), (22) and (23) we obtain the Liouville equations for the coherence matrices $\sigma_m$:

$$\frac{\partial \sigma_m}{\partial t} + \nabla_p E_m \cdot \nabla_x \sigma_m = 0.$$  \hspace{1cm} (24)$$

The initial data for equations (24) is constructed as follows. Let $W_0^\varepsilon(x, k)$ be the Wigner transform of the initial data $\phi_0^\varepsilon(x)$. Then $\sigma_m(0, x, p)$ is given by

$$\sigma_m^{\alpha\beta}(0, x, p) = \lim_{\varepsilon \rightarrow 0} \sum_{\mu \in L^*} W_0^\varepsilon(x, p + \mu \mu) \check{Q}_j^{\alpha\beta}(x, \mu, p)$$

with the limit understood in the weak sense.
2.4 The Wigner band series

The Liouville equations (24) were previously derived in [15, 10] in terms of the Wigner series defined by

\[ w_\varepsilon(t, x, k) = \frac{|C|}{(2\pi)^d} \sum_{\nu \in L} e^{ik\nu} \phi_\varepsilon(x - \varepsilon\nu) \tilde{\phi}_\varepsilon(x) = \sum_{\mu \in L^*} W_\varepsilon(x, k + \mu). \]

It was shown that the weak limit \( w(t, x, k) \) of \( w_\varepsilon(t, x, k) \) has the form

\[ w(t, x, k) = \sum_j w_j(t, x, k). \]

Here \( w_j \) is the limit Wigner series of the projection \( \phi_\varepsilon^j \) of the solution \( \phi_\varepsilon \) of the Schrödinger equation on the Bloch spaces \( S_\varepsilon^j \):

\[ S_\varepsilon^j = \left\{ f \in L^2(R^d) : f(x) = \sum_\alpha \frac{1}{|B|} \int_B \frac{d\nu}{2} f_\varepsilon^\alpha(p) \Psi_\varepsilon^\alpha(x, p) \right\}. \]

Each projection \( w_j \) evolves according to the Liouville equation (24). This result may be related to our approach as follows. The Wigner distribution \( W_\varepsilon(t, x, k) \) has the asymptotics

\[ W_\varepsilon(t, x, p + \mu) \approx \sum_{m,\alpha,\beta} \sigma_m^{\alpha\beta}(t, x, p) Q_m^{\alpha\beta} \left( \frac{x}{\varepsilon}, \mu, p \right). \]  

(25)

Then the weak limit of \( w_\varepsilon \) is given by

\[ w(t, x, p) = \sum_{m,\alpha,\beta} \sigma_m^{\alpha\beta}(t, x, p) \sum_{\mu \in L^*} \int_C \frac{dz}{|C|} Q_m^{\alpha\beta}(z, \mu, p) = \sum_m \text{Tr} \sigma_m(t, x, p). \]

If we take the trace of (24) we get the transport equations for \( w_m(t, x, p) = \text{Tr} \sigma_m(t, x, p) \) obtained in [15] and [10]. However, the representation (25) captures not only the weak limit of \( w_\varepsilon \) but also the oscillations of \( W_\varepsilon \) on the fine scale. Moreover, the cross-polarization of various modes corresponding to the same eigenvalue is also taken into account by the off-diagonal terms in the coherence matrices. The oscillations of the spatial energy density, which is the physically interesting quantity, are given by

\[ E_\varepsilon(t, x, p) \approx \sum_{m,\alpha,\beta} \int_B dp \sigma_m^{\alpha\beta}(t, x, p) \Psi_m^{\alpha}(\frac{x}{\varepsilon}, p) \bar{\Psi}_m^{\beta}(\frac{x}{\varepsilon}, p) \to \sum_m \int_B dp \text{Tr} \sigma_m(t, x, p) \quad \text{as} \quad \varepsilon \to 0. \]

This information on the energy oscillations may be useful in numerical simulations. We see that \( \sigma_m^{\alpha\alpha} \) are phase space resolved energy densities of different modes inside the Brillouin zone.
3 The random perturbation

3.1 Simple eigenvalues

We assume first that the Bloch eigenvalues $E_m(p)$ have multiplicity one for all $p \in B$. This assumption is known to be true for the leading eigenvalue when the Fourier transform of the periodic potential $V(y)$ is negative. In many physical problems the absence of level crossings restricts our results to the lower part of the spectrum. We consider now small random perturbations of the periodic problem with randomness being on the same scale as the periodic potential but weak:

$$i\varepsilon \frac{\partial \phi_\varepsilon}{\partial t} + \frac{\varepsilon^2}{2} \Delta \phi_\varepsilon - V(\frac{x}{\varepsilon}) - \sqrt{\varepsilon} N(\frac{x}{\varepsilon}) = 0$$

$$\phi_\varepsilon(0, x) = \phi_\varepsilon^0(x).$$

Here $N(y)$ is a time independent mean zero spatially homogeneous random process with covariance tensor $R(x)$ defined by:

$$\langle N(y)N(y + x) \rangle = R(x), \quad \langle \hat{N}(p)\hat{N}(q) \rangle = (2\pi)^d \hat{R}(q)\delta(p + q). \quad (26)$$

Here $\langle \cdot \rangle$ denotes the ensemble average and the Fourier transform $\hat{N}(q)$ is

$$\hat{N}(q) = \int_{\mathbb{R}^d} dx e^{-i q \cdot x} N(x). \quad (27)$$

The Wigner distribution $W_\varepsilon(t, x, k)$ satisfies the evolution equation

$$\frac{\partial W_\varepsilon}{\partial t} + k \cdot \nabla_x W_\varepsilon + i\varepsilon^2 \Delta_x W_\varepsilon = \frac{1}{i\varepsilon} \sum_{\mu \in L^*} e^{i \mu \cdot x/\varepsilon} \hat{V}(\mu) [W_\varepsilon(k - \mu) - W_\varepsilon(k)]$$

$$+ \frac{1}{i\sqrt{\varepsilon}} \int_{\mathbb{R}^d} \frac{dq}{(2\pi)^d} e^{iq \cdot x/\varepsilon} \hat{N}(q) [W_\varepsilon(k - q) - W_\varepsilon(k)].$$

Here $\hat{V}(\mu)$ is the periodic Fourier transform and $\hat{N}(q)$ is the Fourier transform over $\mathbb{R}^d$. We consider the asymptotic expansion

$$W_\varepsilon(t, x, k) = W_0(t, x, \frac{x}{\varepsilon}, k) + \sqrt{\varepsilon} W_1(t, x, \frac{x}{\varepsilon}, k) + \varepsilon W_2(t, x, \frac{x}{\varepsilon}, k) + \ldots,$$

with the leading order term $W_0$ being deterministic. We introduce as before the fast variable $z = \frac{x}{\varepsilon}$, replace $\nabla_x \rightarrow \nabla_x + \frac{1}{\varepsilon} \nabla_z$ and collect the powers of $\varepsilon$. The order $\varepsilon^{-1}$ gives as before

$$\mathcal{L}W_0 = 0.$$
Thus we still have the decomposition (20):

$$W_0(t, x, z, p + \mu) = \sum_m \sigma_m(t, x, p)Q_m(z, \mu, p)$$

(28)

with $\sigma_m$ being scalar because the spectrum is simple. Recall that the functions $\sigma_m(t, x, p)$ are $L^*$-periodic in $p$ and the $z$-periodic functions $Q_m$ are given by (18) with $m = n$. The order $\epsilon^{-1/2}$ terms give

$$\mathcal{L} W_1 = \frac{1}{i} \int_{R^d} \frac{dq}{(2\pi)^d} e^{iq \cdot z}[W_0(z, k - q) - W_0(z, k)].$$

(29)

The distribution $W_1$ need not be periodic in the fast variable $z$. Therefore it may not be expanded in $Q_{mn}$ and we use the the basis functions

$$P_{mn}(z, \mu, p, q) = \int_{C} \frac{d\nu}{|C|} e^{i(p+\mu)\cdot \nu} \psi_m(z - y, p)\bar{\psi}_m(z, p + q),$$

(30)

defined for $z \in R^d$ and $p, q \in B$, in place of the periodic functions $Q_{mn}(z, \mu, p)$. The functions $P_{mn}$ are quasi-periodic in $z:

$$P_{mn}(z + \nu, \mu, p, q) = P_{mn}(z, \mu, p, q)e^{-i\nu \cdot q}.$$

We use (16) and (8) to obtain the orthogonality relation for the functions $P_{mn}:

$$\sum_{\mu \in L^*} \int_{R^d} \frac{dz}{|B|} P_{mn}(z, \mu, p, q)\bar{P}_{jl}(z, \mu, p, q_0) = \delta_{mj}\delta_{nl}\delta_{\text{per}}(q - q_0).$$

(31)

The operator $\mathcal{L}$ acts on these functions as

$$\mathcal{L} P_{mn} = i(E_m(p) - E_n(p + q))P_{mn}(z, \mu, p, q),$$

which is the analog of (19) for the functions $Q_{mn}$. Note that the integrand in (30) is periodic in $y$ so no boundary terms are produced by integration by parts.

We decompose $W_1$ in this basis as

$$W_1(t, x, z, p + \mu) = \sum_{mn} \int_{R^d} \frac{dz}{|B|} \eta_{mn}(t, x, p, q)P_{mn}(z, \mu, p, q),$$

(32)

with $z \in R^d$, $p \in B$ and $\mu \in L^*$. We insert (32) into (29), multiply (29) by $\bar{P}_{jl}(z, \mu, p, q_0)$, sum over $\mu \in L^*$ and integrate over $z \in R^d$. Then we get using (19) on the left side

$$\eta_{jl}(t, x, p, q_0) = \sum_{\mu \in L^*} \int_{R^{2d}} \frac{dz dq e^{i q \cdot z} N(q)}{(2\pi)^d} \frac{[W_0(z, p + \mu - q) - W_0(z, p + \mu)]}{E_j(p + q_0) - E_j(p) + i\theta} \bar{P}_{jl}(z, \mu, p, q_0).$$

(33)
where $\theta$ is the regularization parameter. We let $\theta \to 0$ at the end. We insert expression (28) for $W_0$ and the definition (18) of $Q_m$ into (32). The resulting expression may be simplified using (17) and (8):

$$
\eta_{ij}(t, \mathbf{x}, \mathbf{p}, \mathbf{q}_0) = \frac{1}{(2\pi)^d} \sum_{\mathbf{p} \in L^*} \frac{\tilde{N}(\mathbf{p} - \mathbf{q}_0)\sigma_i(\mathbf{p} + \mathbf{q}_0)}{E_i(\mathbf{p} + \mathbf{q}_0) - E_j(\mathbf{p}) + i\theta} A_{ij}(\mathbf{p} + \mathbf{q}_0 + \mu, \mathbf{p}) - \int_{R^d \times R^d} \frac{d\mathbf{q}d\mathbf{p}}{(2\pi)^d} e^{i\mathbf{q} \cdot \mathbf{z}} \frac{\tilde{N}(\mathbf{q})\sigma_j(\mathbf{p})\Psi_j(\mathbf{p} + \mathbf{q}_0)}{E_i(\mathbf{p} + \mathbf{q}_0) - E_j(\mathbf{p}) + i\theta}. \tag{34}
$$

Here the amplitude $A_{ij}(\mathbf{q}, \mathbf{p})$ is given by

$$
A_{ij}(\mathbf{q}, \mathbf{p}) = \int_C \frac{d\mathbf{y}}{|C|} e^{-i(\mathbf{q} \cdot \mathbf{y})} \Psi_j(\mathbf{y}, \mathbf{q})\tilde{\Psi}_j(\mathbf{y}, \mathbf{p}). \tag{35}
$$

The next order equation is

$$
\frac{\partial W_0}{\partial t} + \mathbf{k} \cdot \nabla_x W_0 + i\nabla_x \cdot \nabla_x W_0 + \mathcal{L} W_2 = \frac{1}{i} \int_{R^d} \frac{d\mathbf{q}}{(2\pi)^d} e^{i\mathbf{q} \cdot \mathbf{z}} \tilde{N}(\mathbf{q}) [W_1(\mathbf{z}, \mathbf{k} - \mathbf{q}) - W_1(\mathbf{z}, \mathbf{k})].
$$

We multiply this equation by $\tilde{Q}_j(\mathbf{z}, \mu, \mathbf{p})$, integrate over $\mathbf{z}$ and sum over $\mu \in L^*$, and take average. Then as before the left side is

$$
\text{LHS} = \frac{\partial \sigma_j}{\partial t} + \nabla_p E_j \cdot \nabla_x \sigma_j. \tag{36}
$$

The right side is

$$
\text{RHS} = I_1 + I_2, \tag{37}
$$

where

$$
I_1 = \frac{1}{i} \sum_{\mu \in L^*} \int_C \frac{d\mathbf{z}}{|C|} \int_{R^d} \frac{d\mathbf{q}e^{i\mathbf{q} \cdot \mathbf{z}}}{(2\pi)^d} \langle \tilde{N}(\mathbf{q})W_1(\mathbf{p} + \mu - \mathbf{q})\tilde{Q}_j(\mathbf{z}, \mu, \mathbf{p}) \rangle \tag{38}
$$

and

$$
I_2 = -\frac{1}{i} \sum_{\mu \in L^*} \int_C \frac{d\mathbf{z}}{|C|} \int_{R^d} \frac{d\mathbf{q}e^{i\mathbf{q} \cdot \mathbf{z}}}{(2\pi)^d} \langle \tilde{N}(\mathbf{q})W_1(\mathbf{p} + \mu)\tilde{Q}_j(\mathbf{z}, \mu, \mathbf{p}) \rangle.
$$

We insert expression (32) for $W_1$ into (38) to get

$$
I_1 = \frac{1}{i} \sum_{\mu \in L^*} \int_C \frac{d\mathbf{z}}{|C|} \int_{R^d} \frac{d\mathbf{q}}{(2\pi)^d} \int_{B} \frac{d\mathbf{q}_0}{|B|} \langle \tilde{N}(\mathbf{q})\tilde{Q}_j(\mathbf{z}, \mu, \mathbf{p}) \rangle \sum_{m,n} \eta_{m\mu}(\mathbf{p} + \mu - \mathbf{q}, \mathbf{q}_0)P_{mn}(\mathbf{z}, \mu, \mathbf{p} - \mathbf{q}, \mathbf{q}_0). \tag{34}
$$

We may split $I_1 = I_{11} - I_{12}$ according to the two terms in (34). We insert the first term in (34) into the expression for $I_{11}$ and average using spatial homogeneity (26) of the random process $N(\mathbf{z})$,
orthogonality (13) of the Bloch functions $\Psi_m(z, p)$, and also sum over $\mu \in L^*$ using (8). Then we get

$$I_{11} = \frac{1}{i} \sum_{\mu \in L^*} \sum_m \int_B \frac{d\hat{R}(q + \mu) |A_{jm}(p, p - q - \mu)|^2 \sigma_j(p)}{E_j(p) - E_m(p - q) + i\theta}.$$ 

Here we have replaced integration over $q \in \mathbb{R}^d$ by integration over $B$ and sum over $\mu \in L^*$. The second term $I_{12}$ is evaluated similarly:

$$I_{12} = \frac{1}{i} \sum_{\mu \in L^*} \sum_m \int_B \frac{d\hat{R}(q + \mu) |A_{jm}(p, p - q - \mu)|^2 \sigma_m(p - q)}{E_j(p) - E_m(p - q) + i\theta}.$$ 

Thus we have

$$I_1 = \frac{1}{i} \sum_{\mu \in L^*} \sum_m \int_B \frac{d\hat{R}(q + \mu) |A_{jm}(p, p - q - \mu)|^2 |\sigma_j(p) - \sigma_m(p - q)|}{E_j(p) - E_m(p - q) + i\theta}. \hspace{1cm} (39)$$ 

One may verify that $I_2 = \bar{I}_1$ in (37). We insert then (39) into (37), take the limit $\theta \to 0$, make a change of variables $q \to p - q$, and combine it with (38) to get the system of radiative transport equations:

$$\frac{\partial \sigma_j}{\partial t} + \nabla_p E_j \cdot \nabla x \sigma_j = \sum_m \int_B \frac{d\hat{R}(p - q) |A_{jm}(p, q)|^2 |\sigma_m(q) - \sigma_j(p)|}{|E_j(p) - E_m(q)|}.$$ 

The differential scattering cross-sections $Q_{jm}(p, q)$ are given by

$$Q_{jm}(p, q) = \frac{1}{(2\pi)^d - 1} \frac{1}{\hat{R}(p - q + \mu) |A_{jm}(p + \mu, q)|^2}.$$ 

This is the main result of this paper: we have derived a system of coupled radiative transport equations for the phase space energy densities of the Bloch modes. The transition probabilities $Q_{jm}(p, q)$ are real and symmetric: $Q_{jm}(p, q) = Q_{mj}(q, p)$ as seen from the definition (35) of $A_{ij}(p, q)$. Therefore the total energy is conserved:

$$\mathcal{E}(t) = \sum_m \int_{\mathbb{R}} dx \int_B dp \sigma_m(t, x, p) = \text{const.}$$ 

Transport equations like (40) are well known in the theory of resistance of metals and alloys [17]. Their systematic derivation from the Schrödinger equation with a periodic and random potential (26) is new.

A Appendix. Multiple eigenvalues

When eigenvalues $E_j(p)$ are not simple, but their multiplicity is independent of $p$, so that there are still no level crossings, the analysis in the previous section can be extended to this case. This
case is probably very rare for the Schrödinger equation but is important for other types of waves, for instance, in symmetric hyperbolic systems. We present it here for the sake of completeness. The result is as follows. Let the matrices $T_{jm}^{\alpha\beta}(p, q)$, $\alpha = 1, \ldots, r_j$, $\beta = 1, \ldots, r_m$, where $r_j$ and $r_m$ are the multiplicities of $E_j$ and $E_m$, be defined by

$$T_{jm}^{\alpha\beta}(p, q) = \int_C \frac{dz}{(2\pi)^{\frac{d-1}{2}}} e^{i(p-q) \cdot z} \psi_m^\beta(z, q) \bar{\psi}_j^\alpha(z, p).$$

Then the coherence matrices $\sigma_j(p)$ satisfy the system of radiative transport equations

$$\frac{d\sigma_j}{dt} + \nabla_p E_j \cdot \nabla_x \sigma_j = \sum_{\mu \in \mathbb{L}, m \in \mathbb{N}} \int_B \frac{d|B|}{|B|} \hat{R}(p - q + \mu) T_{jm}^*(p, q - \mu) \sigma_m(q) T_{jm}^*(p, q - \mu) \delta(E_j(p) - E_m(q))$$

$$- \frac{i}{2\pi} \int_B \frac{d|B|}{|B|} \left[ \frac{T_{jm}(p, q - \mu) T_{jm}^*(p, q - \mu) \sigma_j(p)}{E_j(p) - E_m(q) + i0} - \frac{\sigma_j(p) T_{jm}(p, q - \mu) T_{jm}^*(p, q - \mu)}{E_j(p) - E_m(q) - i0} \right].$$

These equations have the same structure as the radiative transport equations for polarized waves derived in [19]. The expression of the total scattering cross-section as a principal value integral and not as a familiar integral against $\delta[E_m(q) - E_j(p)]$ is known in transport theory for polarized waves [12, 6, 19]. They reduce typically to the form common in scalar transport equations under additional symmetries, like rotational invariance of the original wave equations and the power spectrum tensor.

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