# Transport equation for weakly localized electrons

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The weak-localization regime is usually cited as an example of the breakdown of the Boltzmann equation. Using the techniques of quantum transport theory, we generalize the Boltzmann equation to include the coherent backscattering associated with weak localization. The new transport equation includes, in addition to the usual impurity scattering, a backscattering which occurs on the time scale of the phase-coherence lifetime. All the standard weak-localization magnetoresistance results can be reproduced by properly modifying this term. One effect which is nonlinear in the electric field is also calculated.

## I. INTRODUCTION

The Kubo formula is the usual starting point for calculations of the conductivity of weakly localized systems,[1-4] which are often cited as situations to which the standard Boltzmann transport theory does not apply. In this paper we show that the Boltzmann equation *can* be generalized to include the coherent backscattering that is known to be at the root of weak localization. This is important for two reasons. First, it is interesting that a transport equation still holds for coherent effects which involve the interference between two possible paths for an electron scattering. Second, a transport equation can more easily deal with nonlinear and nonequilibrium phenomena, which are beyond the scope of the Kubo formula.

If one thinks in too simple semiclassical terms, it is paradoxical that weak localization can be treated within the framework of a transport equation. In the usual Boltzmann equation, scattering events are independent. All that matters is the electron's position and velocity after its previous collision. It is not surprising then that transport properties are governed by a distribution function which keeps track of how many electrons are coming in and out of a given volume. With weak localization, though, it is not just the number of electrons coming in or out of a given volume which matters, but also the phase of these electrons. Since a classical distribution function does not contain information about phase interference, it might appear impossible to treat weak localization in a transport equation.

The apparent paradox is resolved by considering the transport equations that occur in the quasiclassical theory of superconductivity or superfluid $^3$He.[5,6] There the analog of the distribution function is a well-defined quantum-mechanical object, not to be thought of classically, but merely as the best one can do to store information about local-position and momentum densities in quantum mechanics. Once we start from quantum mechanics and no longer interpret the distribution function literally, it is possible, as we shall show, to include the coherent backscattering in the transport equation. As in all quasiclassical equations, the reason the left-hand side of the resulting equation resembles the classical Boltzmann equation is that the distribution function is taken to be slowly varying in space and time, and the part of the Hamiltonian not contained in the scattering term consists of the kinetic energy and the potential energy due to an external field. The physics of what scattering mechanisms are included, which distinguishes the classical from the quantum-mechanical equation, is contained on the right-hand side of the transport equation.

The inclusion of coherent backscattering leads to a novel collision integral that is nonlocal in time. [See Eq. (22).] In the resulting transport equation the only restriction is that the external fields be slowly varying in space and time. One result of our approach which cannot be obtained via the Kubo formalism concerns electron heating, a nonequilibrium effect. Generalizing a recent treatment of electron heating using the Boltzmann equation,[7] we solve for the effective temperature of an electron gas. We find that, as in the case of computing the conductivity, the effect of weak localization is to increase the elastic impurity scattering rate by a frequency-dependent factor $\alpha(\nu)$ given in Eq. (21).

## II. DISTRIBUTION FUNCTION

Implicit in deriving a transport equation is the choice of a distribution function, $f(\mathbf{p},\mathbf{R},T)$. In quantum mechanics, unlike classical mechanics, there is no *a priori* well-defined distribution function because of the uncertainty principle. Nonetheless, as first pointed out by Wigner,[8] one can still define a distribution function in quantum mechanics from which the density and current can be obtained in the usual way,

$$n(\mathbf{R},T)=\int \frac{d^3p}{(2\pi)^3} f(\mathbf{p},\mathbf{R},T) , \tag{1}$$

$$\mathbf{j}(\mathbf{R},T)=\int \frac{d^3p}{(2\pi)^3} \frac{\mathbf{p}}{m} f(\mathbf{p},\mathbf{R},T) . \tag{2}$$

The quantities which can be computed easily from nonequilibrium quantum statistical mechanics are the Green's functions. In particular, the Green's function $g^<$ in a mixed representation analogous to Wigner's is simply related to the electron density and current,

 

$$g^<(\mathbf{p},\omega,\mathbf{R},T)=\int d^3r \int dt\, e^{-i\mathbf{p}\cdot\mathbf{r}}e^{i\omega t}\langle\psi^\dagger(\mathbf{R}-\mathbf{r}/2,T-t/2)\psi(\mathbf{R}+\mathbf{r}/2,T+t/2)\rangle \tag{3}$$

Here, $\psi^\dagger$ and $\psi$ are creation and destruction operators for single electrons, and the brackets denote the thermal average.

A natural definition for the distribution function is $g^<$ integrated with respect to $\omega/2\pi$. The resulting distribution function is the Wigner distribution function and satisfies Eqs. (1) and (2). Even for the weakly-disordered metals considered here, the elastic-impurity scattering rate $\Gamma$ is much larger than $k_BT$. Since specifying the momentum of an electron only specifies its energy to within $\Gamma$, this means that the Wigner distribution function changes from zero to one over a region of width in energy $\Gamma \gg k_BT$, bearing little resemblance to the conventional distribution function.

An alternative to the Wigner function, which also satisfies Eqs. (1) and (2), was introduced by Prange and Kadanoff,[9] following ideas due to Migdal.[10] They integrated $g^<$ with respect to $\varepsilon_p/2\pi$ instead of $\omega/2\pi$, where $\varepsilon_p=p^2/2m$ for the free-electron model considered here. A new momentum vector $\mathbf{k}$ is then introduced which is in the same direction as the original momentum vector, but whose magnitude is $\{2m[\omega-U(\mathbf{R},T)]\}^{1/2}$. $U(\mathbf{R},T)$ is the potential energy due to an external field. Since $g^<$ as a function of $\omega$ decays within $k_BT$ of the Fermi surface, the resulting distribution function,

$$f(\mathbf{k},\mathbf{R},T)=\int \frac{d\varepsilon_p}{2\pi} g^<(p\hat{\mathbf{k}},\omega=\varepsilon_k+U(\mathbf{R},T),\mathbf{R},T) \tag{4}$$

looks more like the Fermi distribution function.

We can see this more explicitly by calculating $g^<$ for some simple cases using the standard weak-localization model. This model consists of a noninteracting free-electron gas scattering from a dilute but random distribution of impurities, so that $k_Fl \gg 1$. (The Fermi momentum is $k_F$ and $l$ is the mean-free path.) We set $\hbar=1$ throughout. Using only the self-energy diagram depicted in Fig. 1(a), the elastic impurity scattering rate $\Gamma$ equals $2\pi n_i |V|^2 N(0)$, where $n_i$ is the number of impurities per unit volume, $V$ is the matrix element for scattering from one momentum state to another, which is taken to be constant, and $N(0)$ is the density of states per spin at the Fermi surface. For zero field the Green's functions are given by

$$g^<(\mathbf{p},\omega,\mathbf{R},T)=i[g_r(\mathbf{p},\omega)-g_a(\mathbf{p},\omega)]f_{\rm eq}(\omega)\ , \tag{5}$$

$$\left.\begin{matrix} g_r(\mathbf{p},\omega) \\ g_a(\mathbf{p},\omega) \end{matrix}\right\} = [\omega-\varepsilon_p \pm i\Gamma/2]^{-1}\ . \tag{6}$$

For this $g^<$, the Prange-Kadanoff distribution function is exactly the Fermi distribution function $f_{\rm eq}(\varepsilon_k)$. As we turn on the electric field the structure of these Green's functions does not change very much. For example, assuming that the external electric field is slowly varying in space and time, the retarded and advanced Green's functions are the following:

$$\left.\begin{matrix} g_r(\mathbf{p},\omega,\mathbf{R},T) \\ g_a(\mathbf{p},\omega,\mathbf{R},T) \end{matrix}\right\} = [\omega-\varepsilon_p-U(\mathbf{R},T)\pm i\Gamma/2]^{-1}\ . \tag{7}$$

Also, the change in $g^<$ to linear order in a uniform electric field within the same self-energy approximation is

$$\delta g^<(\mathbf{p},\omega,\mathbf{R},\nu)=\frac{f_{\rm eq}(\omega-\nu/2)-f_{\rm eq}(\omega+\nu/2)}{\nu} \times \frac{-e\mathbf{E}(\nu)\cdot\mathbf{p}/m}{(\omega-\varepsilon_p)^2+(\Gamma-i\nu)^2/4}\ . \tag{8}$$

We have Fourier transformed in $T$ to get the $\nu$ variable. The Prange-Kadanoff distribution function is still strongly peaked at the Fermi surface, whereas the Wigner distribution function is not. Also, the denominator of $g^<$ remains unchanged from equilibrium provided that $\nu \ll \Gamma$. This will be important latter in deriving the transport equation, because there will be integrals involving $\varepsilon_p$ which may be done if we can neglect the corrections of order $\nu/\Gamma$.

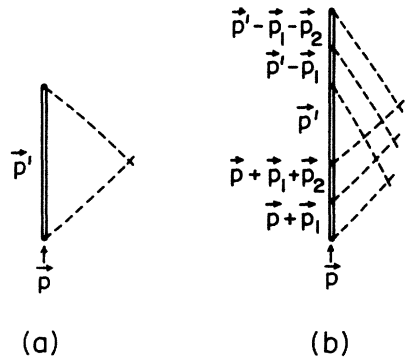


FIG. 1. (a) Feynman graph leading to the ordinary collision integral, (b) graph corresponding to a typical term in the series that leads to the coherent backscattering collision integral.

## III. BOLTZMANN EQUATION

In this section we outline a derivation of the Boltzmann equation for elastic impurity scattering following closely the derivation of Prange and Kadanoff for phonon scattering. The only change will be the addition of another self-energy term, describing coherent backscattering from the impurities. At the temperatures of weak-localization experiments, phonon scattering is not important for the conductivity and can be ignored. Phonons do play an important role in maintaining thermal equilibrium between the lattice and the electrons. Within the transport equation this equilibrium is maintained by taking the spherical average of the distribution function to be the Fermi distribution function corresponding to the temperature of the lattice. This is valid so long as there is no heating of the electron gas.

The Green's functions used here are defined following the conventions of Langreth:[11]

$$g^{>}(1,1')=\langle\psi(1)\psi^{\dagger}(1')\rangle\ , \tag{9}$$

$$g^{<}(1,1')=\langle\psi^{\dagger}(1')\psi(1)\rangle\ , \tag{10}$$

$$g_a(1,1')=i[g^{>}(1,1')+g^{<}(1,1')]\Theta(t_{1'}-t_1)\ , \tag{11}$$

$$g_r(1,1')=-i[g^{>}(1,1')+g^{<}(1,1')]\Theta(t_1-t_{1'})\ . \tag{12}$$

The discontinuous behavior of the self-energy operator $\sigma$ is treated analogously. Following Langreth's formalism the equations of motion for the Green's functions are the following:

$$\left[i\frac{\partial}{\partial t_1}+\frac{\nabla_1^2}{2m}+U(1)\right]g^{<}(1,1') =\int d2[\sigma^{<}(1,2)g_a(2,1')+\sigma_r(1,2)g^{<}(2,1')]\ , \tag{13}$$

$$\left[-i\frac{\partial}{\partial t_1'}+\frac{\nabla_{1'}^2}{2m}+U(1')\right]g^{<}(1,1) =\int d2[g^{<}(1,2)\sigma_a(2,1')+g_r(1,2)\sigma^{<}(2,1')]\ . \tag{14}$$

Although our conventions are those of Langreth, the formalism due to Kadanoff and Baym[12] and to Keldysh[13] yield exactly the same result. By taking the potential $U$ due to the external field to be slowly varying in space and time, we can now perform a gradient expansion[12,11] on the difference between Eqs. (13) and (14):

$$\left[\frac{\partial}{\partial T}+\frac{\mathbf{p}}{m}\cdot\nabla_R-\nabla_R U\cdot\nabla_p-\frac{\partial U}{\partial T}\frac{\partial}{\partial\omega}\right]g^{<}(\mathbf{p},\omega,\mathbf{R},T) =-i(\sigma_r-\sigma_a)g^{<}+i(g_r-g_a)\sigma^{<}\ . \tag{15}$$

The terms on the right-hand side now have the same arguments and are being multiplied.

In order to make this into an equation for the distribution function we must integrate both sides with respect to $\varepsilon_p/2\pi$ and use Eq. (4). This yields the usual left-hand side of the Boltzmann equation. To get the right-hand side we must also make assumptions about the self-energy. The standard Boltzmann equation follows from the choice of a self-energy term which corresponds to independent Born-approximation scattering from impurities,

$$\sigma^{<}(\mathbf{p},\omega,\mathbf{R},T)=n_i\,|\,V\,|^2\int\frac{d^3p'}{(2\pi)^3}g^{<}(\mathbf{p}',\omega,\mathbf{R},T)\ . \tag{16}$$

Analogous expressions hold for the other Green's functions and self-energies. Diagrammatically, this term can be represented in the impurity-averaged scheme as shown in Fig. 1(a). In order to get the final result we must also use Eq. (8) for the retarded and advanced Green's functions when integrating with respect to $\varepsilon_p/2\pi$. As our final result for the usual Boltzmann equation we now get

$$\left[\frac{\partial}{\partial T}+v_F\hat{\mathbf{p}}\cdot\nabla_R-\nabla_R U\cdot\nabla_p\right]f(\mathbf{p},\mathbf{R},T) =-\Gamma[f(\mathbf{p},\mathbf{R},T)-\bar{f}(p,\mathbf{R},T)]\ , \tag{17}$$

where $\bar{f}$ denotes the spherical average of $f$.

## IV. GENERALIZED BOLTZMANN EQUATION

In this section we generalize the Boltzmann equation to include the coherent backscattering. As mentioned previously this involves adding a new self-energy term to the right-hand side of Eq. (15). The self-energy terms corresponding to the coherent backscattering are the familiar maximally crossed graphs from linear-response theory. A typical term is shown in Fig. 1(b).

The contribution to $\sigma^{<}$ from this graph contains integrals involving all five combinations of the Green's functions from $g^{<}g_ag_ag_ag_a$ to $g_rg_rg_rg_rg^{<}$. These Green's functions are listed from left to right as they occur[11] from top to bottom in Fig. 1(b). One can estimate them by substituting in the Green's functions of Eqs. (5) and (6). As in linear response[14] the momentum integrals reduce to integrals over pairs of Green's functions of the form

$$n_i\,|\,V\,|^2\int\frac{d^3k}{(2\pi)^3}g_{r(a)}(\mathbf{k},\mu)g_{r(a)}(\mathbf{k}+\mathbf{q},\mu)\ , \tag{18}$$

where $\mathbf{q}=\mathbf{p}+\mathbf{p}'$ and $\mu$ is the Fermi energy. For small $\mathbf{q}$ integrals of the form (18) with one retarded and one advanced Green's function are of order one, whereas those with two Green's functions of the same kind are of order $(k_Fl)^{-1}\ll 1$. Thus the terms for which $g^{<}$ occupies the three center-most momentum positions are larger than the other terms by a factor of order $k_Fl$. We will always be keeping only these three terms, since this is a general property which holds true for all maximally crossed graphs.

To sum all the self-energy terms exactly we first consider the momentum integrals involving only $g_r$ and $g_a$, not $g^{<}$. The retarded and advanced Green's functions of Eq. (7) change very little upon including the maximally crossed graphs. The reason for this is that the self-energies for $g_r$ and $g_a$ involve only retarded and only advanced Green's functions, respectively, not combinations of both as with $g^{<}$.[11] Thus for essentially the same reason that Eq. (18) can be neglected when both Green's functions are the same, we now neglect the correction to $\Gamma$ which is of order $\Gamma/k_Fl$. This is also the reason we are only looking at the change in $\sigma^{<}$ and not in $\sigma_r$ and $\sigma_a$. The integrals involving $g_r$ and $g_a$ are now the same as in linear response except for the inclusion of the electric field. Altshuler, Aronov, and Khmel'nitskii[15] have evaluated these using the Keldysh formalism for nonequilibrium quantum statistical mechanics. Essentially, what is done is to look at integrals of the form (18) in real space and see how they change upon including a finite electric field. They find that a static electric field has no effect on the evaluation of these integrals, whereas a time-dependent electric field does change the integrals and can result in the destruction of the weak-localization coherent backscattering. This destruction only occurs for

sufficiently large and high-frequency fields. For simplicity we shall take the electric field to be weak and slowly varying, so this effect can be neglected. We are also not including magnetic field and spin-flip scattering effects for simplicity. As with the electric field, these may be included by appropriately modifying these integrals.

Within the above approximations the momentum integrals not involving $g^<$ are the same as in linear response. Upon summing their contribution for all the maximally crossed graphs to $\sigma^<$ we again find that the integral is strongly peaked for $\mathbf{q}=\mathbf{p}+\mathbf{p}'\approx 0$. The remaining momentum integrals become particularly simple if we set $\mathbf{q}=0$ elsewhere. For the two terms in which $g^<$ is on either side of the central momentum, marked $\mathbf{p}'$ in Fig. 1(b), the integral over $g^<$ samples the Fermi surface, taking the spherical average of $g^<$, which we denote as $\bar{g}^<$. This still leaves an integral over energy. In order to do this integral we make an ansatz for the structure of $g^<$:

$$g^<(\mathbf{p},\omega,\mathbf{R},\nu)=\frac{\Gamma f(\hat{p},\omega,\mathbf{R},\nu)}{(\omega-\varepsilon_p)^2+\Gamma^2/4} \tag{19}$$

and set $\nu=0$ everywhere except in the denominator of $\alpha(\nu)$ defined in Eq. (21) and in $g^<$. Both of these approximations will be justified later. For the term in which $g^<$ occupies the central momentum we merely replace $\mathbf{p}'$ by $-\mathbf{p}$. The additional contribution to $\sigma^<$ is the following:

$$\delta\sigma^<(\mathbf{p},\omega,\mathbf{R},\nu)=\alpha(\nu)\frac{\Gamma}{2}[g^<(-\mathbf{p},\omega,\mathbf{R},\nu) -\bar{g}^<(p,\omega,\mathbf{R},\nu)] , \tag{20}$$

$$\alpha(\nu)=\int' \frac{d^3q}{(2\pi)^3}\frac{2n_i\,|\,V\,|^2}{Dq^2-i\nu+\tau_\phi^{-1}} . \tag{21}$$

In Eq. (21) we have included the upper and lower cutoffs to the $\mathbf{q}$ integral from linear-response theory. The upper cutoff, denoted by the prime over the integral, requires $|\,\mathbf{q}\,|$ to be less than the reciprocal of the mean free path $\Gamma/v_F$. Our model breaks down for distances smaller than the mean free path. The lower cutoff is put in by the phase-coherence lifetime $\tau_\phi$ in the denominator of $\alpha(\nu)$. Within the transport equation the phase-coherence lifetime will turn out to be the time during which the electron distribution retains memory of its previous value. This is in agreement with the standard interpretation in which two alternative paths for electrons scattering become out of phase after $\tau_\phi$.[14]

In order to find the contribution to the right-hand side of our transport equation from the new self-energy term we must multiply by $i(g_r-g_a)$ and integrate with respect to $\varepsilon_p/2\pi$ [see Eqs. (4) and (15)]. The integral may be done by again using the ansatz about the structure of the distribution function given in Eq. (19). Using Eq. (4) for the definition of the distribution function and neglecting $U(\mathbf{R},T)-U(\mathbf{R},T')$ in comparison to the Fermi energy, we get as our final result for the generalized transport equation

$$\left[\frac{\partial}{\partial T}+v_F\hat{\mathbf{p}}\cdot\nabla_R-\nabla_R U\cdot\nabla_p\right]f(\mathbf{p},\mathbf{R},T) =-\Gamma[f(\mathbf{p},\mathbf{R},T)-\bar{f}(p,\mathbf{R},T)] +\int_{-\infty}^{T}dT'\alpha(T-T') \times[f(-\mathbf{p},\mathbf{R},T')-\bar{f}(p,\mathbf{R},T')] , \tag{22}$$

$$\alpha(T-T')=2n_i\,|\,V\,|^2 \times\int' \frac{d^3q}{(2\pi)^3}\exp[-(Dq^2+\tau_\phi^{-1})(T-T')]. \tag{23}$$

This is the central result of the paper. The new backscattering term is nonlocal in time since the electron undergoes many elastic collisions in one phase-coherence lifetime. There is no width to this backscattering because we have taken $\mathbf{q}=0$ in one of the integrals involving $g^<$. Neglecting the width of the backscattering cone is reasonable because it is narrow compared to the angular variation of the distribution function in the weak-localization regime.

At this point we can justify the ansatz of Eq. (19). From Eq. (22) we can see that $\alpha(\nu)$ is essentially the weak-localization correction to $\Gamma$. Thus in the denominator of Eq. (8) when weak localization is taken into account there should be a $\Gamma+\alpha$ instead of $\Gamma$. In making the ansatz we have made errors of order $\alpha/\Gamma$ in computing $\alpha$. Since $\alpha$ is already much less than $\Gamma$, we can neglect this correction. Similarly, we can neglect the corrections of order $\nu/\Gamma$ to $\alpha$ made by setting $\nu=0$ outside of $\alpha(\nu)$ and $g^<$.

We can solve the generalized transport equation of Eq. (22) for the conductivity in a uniform electric field by multiplying by $\mathbf{p}$ on both sides and integrating with respect to $\mathbf{p}$. The result is

$$\sigma(\nu)=\frac{ne^2}{m}\frac{1}{\Gamma-i\nu+\alpha(\nu)}\approx\frac{ne^2}{m}\frac{1}{\Gamma-i\nu}-\frac{ne^2}{m\Gamma^2}\alpha(\nu) . \tag{24}$$

The main effect of the weak-localization correction is to increase the elastic-impurity scattering rate. The correction comes in the denominator because we have solved self-consistently for the distribution function. Indeed if we use the Einstein relation, $\sigma(0)=2N(0)e^2D$, and identify this diffusion constant with $D$ in Eq. (23), we reproduce the self-consistent calculation of Vollhardt and Wölfle.[16]

We can also solve for the effective temperature in the case of electron heating. To treat electron heating in a Boltzmann equation we no longer take the spherical average of the distribution function in Eq. (22) to be the equilibrium distribution function.[7] Instead we include an additional scattering term on the right-hand side,

$$-\Gamma_i[f(\mathbf{p},\mathbf{R},T)-f_{\rm eq}(p,\mathbf{R},T)] ,$$

which relaxes the distribution function to thermal equilibrium. The inelastic scattering lifetime $\Gamma_i^{-1}$ is not neces-

sarily the same as the phase-coherence lifetime $\tau_\phi$. The effective temperature of the electron gas $T^*$ satisfies

$$(k_B T^*)^2=(k_B T)^2+\frac{6}{\pi^2}(eEl_i)^2 \tag{25}$$

except that the inelastic mean-free path $l_i$ has changed from $v_F/(3\Gamma\Gamma_i)^{1/2}$ to $v_F/[3(\Gamma+\alpha)\Gamma_i]^{1/2}$. Thus as with the conductivity, the effect of weak localization is to increase the elastic scattering rate by $\alpha$.

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