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Theories of impurity resistivity

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Abstract. For most theories of impurity resistivity the lowest-order results are the same for zero temperature, but for finite temperatures there are two different results. The fact that the Boltzmann results and the results from force-balance type theories disagree for finite temperatures has recently led to increased theoretical activity. In the present work we study how the newly proposed generalized Drude approach of Sernelius and the dynamical theory of Farvacque compare with other theories. We use the full temperature-dependent random-phase approximation screening in our numerical calculations, but also present results with the generalized temperature-dependent Thomas–Ferni screening. We furthermore give some analytical results where this is possible. We show that inclusion of electron–electron scattering in the solution to the Boltzmann equation brings the result closer to that from the force-balance type theories; very strong electron–electron scattering results in perfect agreement. Numerical results are presented for doped GaAs.

1. Introduction

In the present work we discuss transport in the case of impurity scattering, which in being elastic is the simplest scattering mechanism to treat theoretically. We neglect corrections from multiple scattering and non-linear screening.

Maybe the most strict formulation of transport theory in solids is the Kubo formula for the current-current correlation function. This formulation is, however, best suited for the high-frequency conductivity, which is important for the optical properties of solids. At zero frequency, which is the limit of interest here, the conductivity is inversely proportional to the scattering strength. As a consequence, the conductivity diverges in the weak scattering limit and one is bound to sum an infinite series of contributions or diagrams if one uses a diagrammatic perturbation expansion. This necessarily means that one cannot be fully confident in the results obtained.

Another method traditionally very much used is to solve the Boltzmann equation. The weaknesses with this approach is that the Boltzmann equation is semiclassical and that matrix elements for the scattering processes and the screening are introduced in an *ad hoc* manner, i.e. they do not fall into place automatically. However one can show [1] that, in the very dilute limit, when electron-electron interaction can be neglected, the

Boltzmann equation can be obtained from the equation of motion of the density matrix. The solution to the Boltzmann equation can be expressed as

$$\sigma = (ne^2/m^*)\langle \tau(k)\rangle \tag{1}$$

where the angle bracket stands for the following averaging procedure:

$$\langle A(k)\rangle = -\frac{4}{3n} \int \frac{\mathrm{d}^3 k}{(2\pi)^3} \frac{\mathrm{d} f^0(k)}{\partial \varepsilon_k} \varepsilon_k A(k). \tag{2}$$

The time $\tau(k)$ in (1) is the transport time, which differs from the lifetime for an electron in state k in that the matrix element for the scattering giving rise to τ contains a factor $1 - \cos \theta$, where θ is the scattering angle. This factor favours large-angle scattering. The Boltzmann equation can alternatively be solved with a variational technique [2].

In using the Kubo formula with diagrammatic perturbation theory and keeping only the lowest-order diagram but using dressed Green functions, one quickly and easily obtains (1) but with the lifetime instead of the transport time. Using dressed Green functions actually means that one sums an infinite series of diagrams. In order to obtain the same expression but with the correct transport time, one has to sum all ladder diagrams [3]. This is very complicated. The Boltzmann equation (BE) approach and the Kubo (K) formula give the same result when the Peierls criterion is satisfied, i.e. when $E_F \tau/\hbar \ge 1$.

Thus two quite different approaches give the same result: one method (K) with a strict foundation, but which leads to a very cumbersome derivation involving insecure approximations; one method (BE) with a somewhat weaker foundation, which is very simple to solve and in which the physics is much more transparent. The fact that the methods give the same result (especially since the derivations are so different) means a strong support for their validity. The belief in the validity of the results from these methods is so strong that the results are commonly used to test the outcome from other approaches.

Since the conductivity diverges in the weak scattering limit, people have developed theories in which the resistivity is determined directly [4–8]. This is to avoid the need for infinite summations. In the conductivity derivations discussed above, one starts from an applied electric field and calculates the current density. The current density j and the electric field E are in the linear reponse regime related according to

 $j = \sigma E \tag{3}$

which defines the conductivity σ . In the resistivity derivations one starts with the current and calculates the electric field. The electric field E and the current density j are in the linear response regime related according to

$$\boldsymbol{E} = \boldsymbol{\rho} \boldsymbol{j} \tag{4}$$

which defines the resistivity ρ , which is the inverse of σ . The resistivity from this derivation vanishes in the weak scattering limit and the first-order contribution is finite and can be written as

$$\rho = (m^*/ne^2)\langle 1/\tau(k)\rangle \tag{5}$$

where τ is the same as in (1). For T = 0 K the results from the conductivity and resistivity formulae agree, but for finite temperatures they do not. The deviation increases with temperature and is close to a factor of 3 in the high-temperature limit; equation (5) gives a higher resistivity. The reason the results agree at T = 0 K is that in this case the weight in the averaging is a delta function at the Fermi momentum. Another situation in which the results would agree is if τ were a constant.

Thus, since both the conductivity and the resistivity formulations can be shown to be exact for finite scattering strength, the deviation between their results in the weak scattering limit leads to a conflict. This conflict was solved by Huberman and Chester [9], who showed that if the proper limits are taken in the derivation of the resistivity formula higher-order terms diverge. If all diverging terms are summed the result agrees with that from the conductivity formula. One should first assure that the stationary state has occurred before the limit of weak scattering is taken. One has to take the limits in this order because if the weak scattering limit is taken first the stationary state will never be reached. If Huberman and Chester are correct, one did not gain anything in going from the conductivity derivation to the resistivity derivation. Also here a sum of infinite terms has to be taken.

Recently a new formulation [10–16] has been proposed, for both the linear response regime and for higher field strengths, the so-called force-balance (FB) method. In FB the Hamiltonian for the electronic system is separated into one part describing the centre-of-mass (CM) motion and one describing the relative motions. It is further assumed that the system is in contact with a heat bath that absorbs all excess energy given to the electrons through the scattering against the impurities; in the CM system the scattering processes are inelastic and the impurities are moving. The electronic system can be regarded as a heavy CM particle with internal degrees of freedom represented by the relative motion of the electrons. The electric field exerts a force on this particle, which is balanced by the frictional force due to the electron–ion scattering within the particle.

In the linear regime FB reproduces equation (5). In analogy with the resistivity formulations its higher-order contributions can be shown [17-19] to diverge if the proper order of the limits is taken; also here the summation of the diverging terms leads to a finite result [19] that agrees with (1). These results are found in the absence of a heat bath or processes like electron-electron (e-e) scattering that can bring the electrons into thermodynamic equilibrium in the CM system. Chen *et al* [20] have shown that the divergences disappear when e-e scattering is included and the result lies in between those of (1) and (5). For very strong e-e scattering, equation (5) is regained. The FB method has been very successful in providing results that compare quantitatively well with experimental results [21-24] for a wide range of electric field strengths. Furthermore the results reproduce successfully the results from Monte Carlo simulations [23, 24].

All theories of impurity resistivity discussed above have one of the two results presented in (1) and (5). These results are the same for zero temperature but differ for finite temperatures. In the present work we study how the newly proposed generalized Drude approach (GDA) [25] and the dynamical theory of Farvacque [26] compare with other theories. The numerical results are presented in section 2 and in section 3 a simplified treatment with the generalized Thomas-Fermi screening is reported. Section 4 is devoted to a derivation showing that the Boltzmann equation with the assumption of very strong electron-electron scattering reproduces a force-balance type of equation with (5) as solution. We also show that in the presence of e-e scattering a result in between those of (1) and (5) is obtained. Finally, in section 5 we give a summary and conclusions.

2. Impurity resistivity in GaAs

For the calculations in this work we assume that the donors are randomly distributed and that the impurity potential can be approximated by a pure Coulomb potential. We use the values 13.0 and $0.06m_e$ for the dielectric constant κ and effective mass m^* , respectively. The calculations are performed for a donor density n of 1.0×10^{18} cm⁻³. All equations are given in CGS units.

With these assumptions the transport time for an electron in state k is

$$\tau^{-1}(k) = \frac{4\pi n m^* e^4}{\hbar^3 \kappa^2 k^3} \int_0^{2k} \mathrm{d}q \, \frac{1}{q \varepsilon^2(q, 0)} \tag{6}$$

where $\varepsilon(q, 0)$ is the static temperature-dependent random-phase approximation (RPA) dielectric function for the donor electrons in the conduction band. Putting this result into (1) and (5) leads to the two different results discussed in the introduction. The lifetime τ_{life} from impurity scattering is

$$\tau_{\rm life}^{-1}(k) = \frac{8\pi nm^* e^4}{\hbar^3 \kappa^2 k} \int_0^{2k} \mathrm{d}q \, \frac{1}{q^3 \varepsilon^2(q,0)}.$$
(7)

In the dynamical theory of Farvacque [26] a third relaxation time appears, viz.

$$\tau_{\rm Farv}^{-1}(k) = -\frac{\pi n e^4}{\hbar \kappa^2 k^3} \frac{\partial f(k)}{\partial \varepsilon_k} \frac{1}{f(k)} \int_0^{2k} \mathrm{d}q \, q \, \frac{1}{\varepsilon^2(q,0)} \tag{8}$$

where f(k) is the distribution function and ε_k the kinetic energy for state k. This should be inserted into (1).

In GDA [25] one starts from a generalized Drude expression for the dynamical conductivity

$$\sigma(\omega) = \frac{ne^2}{m^*} \frac{1}{1/\tau(\omega) - i\omega}$$
(9)

with a complex-valued and frequency-dependent relaxation time. The high-frequency expansion of this formula is compared to a rigorous high-frequency result [27] based on the Kubo formalism and the expression for the relaxation time is identified. Under the assumption that this expression is generally valid, one obtains a formula for the conductivity that is presumably valid for the full frequency range. The resistivity is then obtained as $1/\sigma$ and is found to be

$$\rho(\omega) = -i \frac{m^* \omega}{n e^2} + i \frac{2}{3 \pi n \kappa \omega} \int_0^\infty dq \, q^2 \left(\frac{1}{\varepsilon(q, \omega)} - \frac{1}{\varepsilon(q, 0)} \right). \tag{10}$$

This result is actually identical to the result obtained from the so-called energy-loss (EL) method [28]. For a polar semiconductor at non-zero frequency the expression is slightly more complicated [29].

We are here interested in the static result, which can be written as

$$\rho = \frac{2}{3\pi n\kappa} \int_0^\infty \mathrm{d}q \, q^2 \frac{[\partial \varepsilon_2(q,\,\omega)/\partial \omega]_{\omega=0}}{\varepsilon^2(q,\,0)} \tag{11}$$

where $\varepsilon_2(q, \omega)$ is the imaginary part of $\varepsilon(q, \omega)$. This imaginary part can be obtained analytically in RPA [30] and can be written as

$$\varepsilon_{2}(Q, W) = -\frac{m^{*}e^{2}}{\hbar^{2}\kappa 2\pi k_{\rm F}} \frac{1}{Q^{3}} \left(\frac{\pi}{4B}\right) \\ \times \left[\ln \left(\frac{\cosh\{B[W + (Q^{2} + W^{2}/Q^{2} - M)/2]\}}{\cosh\{B[W - (Q^{2} + W^{2}/Q^{2} - M)/2]\}} \right) - 2BW \right]$$
(12)

where we have introduced the dimensionless variables

$$Q = q/2k_{\rm F} \qquad W = \hbar\omega/4E_{\rm F} \qquad M = \mu_{\rm c}/E_{\rm F} \qquad B = \beta E_{\rm F}.$$
(13)

The dielectric function entering the expressions is the retarded version and the real part can be obtained numerically from the imaginary part through the Kramers-Kronig dispersion relations.

The derivative in the numerator of (11) is given by

$$\left[\frac{\partial\varepsilon_2(q,\omega)}{\partial\omega}\right]_{\omega=0} = \frac{(m^*e)^2}{\hbar^3\kappa q^3} \left\{ 1 - \tanh\left[\frac{1}{2}\beta\left(\frac{\hbar^2 q^2}{8m^*} - \mu_c\right)\right] \right\}$$
(14)

where μ_c is the chemical potential and $\beta = 1/k_B T$. Thus, the resistivity is reduced to

$$\rho = \frac{2(m^*e)^2}{3\pi\hbar^3 n\kappa^2} \int_0^\infty \mathrm{d}q \, \frac{1 - \tanh[\frac{1}{2}\beta(\hbar^2 q^2/8m^* - \mu_c)]}{q\varepsilon^2(q,0)}.$$
 (15)

The temperature dependence enters through β and μ_c . The temperature variation of μ_c is obtained from the following implicit relation [31]:

$$B^{3/2} = \int_0^U \mathrm{d}x \, \frac{3x}{1-x^2} \left[A + \ln\left(\frac{1-x^2}{x^2}\right) \right]^{1/2} \tag{16}$$

where the upper limit is $U = (1 + e^{-A})^{-1/2}$ and $A = BM = \beta \mu_c$. For a given A one obtains B. Then M is obtained as A divided by B.

Combescot and Combescot [32] used the Boltzmann approach to determine the conductivity relaxation time for an electron-hole plasma in silicon in the quantum and classical limits. Their result in the classical limit, which was obtained with the variational Boltzmann equation technique (BEV), can be used here if properly modified to suit GaAs and by letting the mass of the holes go to infinity. In our notation the result is

$$1/\mu = ne\rho = \frac{8(m^*)^2 e^3}{9\pi^{3/2}\hbar^3 \kappa^2} B^{3/2} \ln\left(\frac{\hbar^2 k_{\rm F}\kappa}{m^* e^2 B^2}\right).$$
(17)

-

Now we have all relations needed for a numerical comparison between the results from the different theories. We present the results in the form of the reciprocal mobility $1/\mu = ne\rho = ne/\sigma$. In figure 1 the long broken curve A is the BE result, i.e. the result obtained from putting the transport time of (6) into (1). The full curve B is the result if instead of (1) one uses (5), i.e. this is the result from the resistivity derivations and from FB. This result turns out to be numerical identical to the GDA and EL results of (15). This identity can also be shown analytically through an integration by parts of (5) after the expression for the transport time has been inserted. The dotted curve C is the result from (17), i.e. a BEV result which is valid in the high-temperature limit only and where we find it approaches the full curve. Finally, the short broken curve D is the Farvacque (F) result. This result behaves differently from the others for both high and low temperatures.

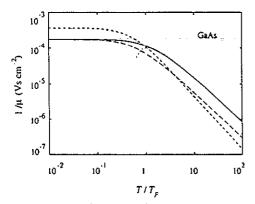


Figure 1. The reciprocal mobility as a function of T/T_F for various theories applied to doped GaAs. The long broken curve (———) is the Boltzmann result in the absence of e-e scattering. The full curve (———) is the result from force-balance type theories, resistivity formulations, the generalized Drude approach, the energy-loss method and the Boltzmann approach with very strong e-e scattering. The dotted curve (....) represents the high-temperature limit of a simple variational solution to the Boltzmann equation. The short broken curve (----) is the result from the dynamical theory of Farvacque.

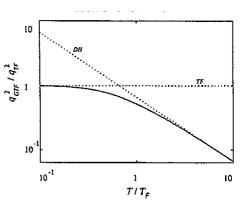


Figure 2. The square of the inverse generalized Thomas-Fermi screening length as a function of $T/T_{\rm F}$ (full curve). The dotted curves are the corresponding high- and low-temperature limits. All curves are normalized to the ordinary Thomas-Fermi result.

In the next section we repeat the calculations with a simplified screening, the generalized Thomas-Fermi screening, which leads to analytical results for the relaxation times.

3. The generalized Thomas–Fermi screening

The generalized Thomas–Fermi (GTF) screening gives rather accurate results especially in the high-temperature region. It has the advantage over the full RPA screening in that the relaxation times can be found analytically, which reduces the computation time. The dielectric function in GTF screening is

$$\varepsilon(q,0,T) = 1 + \frac{q_{GTF}^2(T)}{q^2} = 1 + \frac{4\pi e^2}{q^2 \kappa} \frac{\partial n}{\partial \mu_c}$$
(18)

which can be rewritten as

$$\varepsilon(q,0,T) = 1 + \frac{m^* e^2}{\pi \hbar^2 \kappa k_{\rm F}} \frac{1}{Q^2} \frac{\mathrm{d}B}{\mathrm{d}A}$$
(19)

where the variables Q and B were defined in (13) and A in connection with (16). This dielectric function has the following limiting forms:

$$\varepsilon(q,0,T) = 1 + \frac{2m^{*}e^{2}}{3\pi\hbar^{2}\kappa k_{F}Q^{2}}B \qquad T \to \infty \qquad \text{Debye-Hückel(DH)}$$

$$\varepsilon(q,0) = 1 + \frac{m^{*}e^{2}}{\pi\hbar^{2}\kappa k_{F}Q^{2}} \qquad T \to 0 \qquad \text{Thomas-Fermi(TF)}.$$
(20)

In figure 2 the temperature dependence of q_{GTF}^2 normalized to its zero-temperature

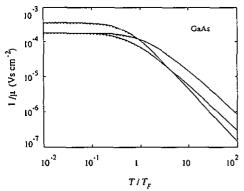


Figure 3. The three main curves of figure 1 (full curves) together with the corresponding results (dotted curves) when the screening has been treated in the simplified generalized Thomas-Fermi approximation.

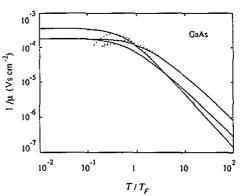


Figure 4. The three main curves of figure 1 (full curves) together with their corresponding high-temperature limits (dotted curves).

value q_{TF}^2 is shown together with the corresponding high- and low-temperature limits. With this normalization the results are universal for bands with parabolic energy dispersion.

The transport time (6) is in GTF screening reduced to

$$\tau^{-1}(k) = \frac{2\pi nm^* e^4}{\hbar^3 \kappa^2 k^3} \left[\ln\left(1 + \frac{4k^2}{q_{\rm GTF}^2}\right) - \frac{4k^2/q_{\rm GTF}^2}{1 + 4k^2/q_{\rm GTF}^2} \right].$$
 (21)

Similarly, the relaxation time (8) in the theory of Farvacque is reduced to

$$\tau_{\rm Farv}^{-1}(k) = -\frac{2\pi n e^4}{\hbar \kappa^2 k} \frac{\partial f(k)}{\partial \varepsilon_k} \frac{1}{f(k)} \left[1 + \frac{1}{1 + 4k^2/q_{\rm GTF}^2} - \frac{2\ln(1 + 4k^2/q_{\rm GTF}^2)}{4k^2/q_{\rm GTF}^2} \right].$$
(22)

The results for the reciprocal mobility when using GTF screening is shown in figure 3 as dotted curves. The full curves are the corresponding full RPA results. Obviously GTF is very good for high temperatures and acceptable for low temperatures, at least for the doping density considered here.

For zero temperature all theories treated here except that of Farvacque give one and the same result. When using the GTF screening this result can be found in the following analytical form:

$$\frac{1}{\mu} = \frac{(m^*)^2 e^3}{3\pi\hbar^3 \kappa^2} \left[\ln\left(1 + \frac{4k_{\rm F}^2}{q_{\rm TF}^2}\right) - \frac{4k_{\rm F}^2/q_{\rm TF}^2}{1 + 4k_{\rm F}^2/q_{\rm TF}^2} \right].$$
(23)

The high-temperature limit of the reciprocal mobility for GDA, EL and FB is given by

$$\frac{1}{\mu} = \frac{4(2\pi m^*)^{1/2} n\beta^{3/2} e^3}{3\kappa^2} \int_0^\infty dq \, \frac{\exp(-\beta\hbar^2 q^2/8m^*)}{q(1+q_{\rm DH}^2/q^2)^2}.$$
(24)

For BE and F the result is of the following form:

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$$\frac{1}{\mu} = \frac{3(2\pi m^*)^{1/2}(m^*)^3}{2e\hbar^5\beta^{5/2}} \frac{1}{\int_0^\infty dk \, k^4\tau(k) \exp(-\beta\hbar^2 k^2/2m^*)}.$$
(25)

In the BE case the relaxation time is the one in (21) with q_{GTF} replaced by q_{DH} . For F the relaxation time of (22) reduces to

$$\tau_{\rm Farv}^{-1}(k) = \frac{2\pi n e^4 \beta}{\hbar \kappa^2 k} \left(1 + \frac{1}{1 + 4k^2/q_{\rm DH}^2} - \frac{2\ln(1 + 4k^2/q_{\rm DH}^2)}{4k^2/q_{\rm DH}^2} \right).$$
(26)

The results with this high-temperature approximation are displayed in figure 4 as the dotted curves in comparison with the full curves, which are the corresponding full RPA results of figure 1.

4. Boltzmann equation with electron-electron scattering

In this section we first study the Boltzmann equation under the assumption of very strong e-e scattering and then we solve it in the presence of e-e scattering of general strength.

The Boltzmann equation says that for the steady-state condition the occupation number for a state k is unchanged with time, i.e.

$$\left[\frac{\partial f(\mathbf{k})}{\partial t}\right]_{\text{scatt}} + \left[\frac{\partial f(\mathbf{k})}{\partial t}\right]_{\text{field}} = 0$$
(27)

or in words, the filling of a state by the field is exactly balanced by the net scattering out of the state. If the only scattering process is impurity scattering, equation (27) results in

$$\frac{eE}{\hbar}\frac{\partial f(k)}{\partial k} = \frac{8e^4m^*n}{\hbar^3\kappa^2} \int d^3q \, \frac{[f(k) - f(k+q)]\delta[q^2 + 2kq\cos(k,q)]}{q^4\varepsilon^2(q,0)} \tag{28}$$

where the left-hand side is the filling rate of state k by the field and the right-hand side is the net scattering out of the state. The right-hand side consists of two terms where the first gives the scattering out of state k and the second the scattering in. In the derivation of the lifetime only the first term is present. Linearizing the equation and keeping only the lowest-order terms gives

$$\frac{eE}{\hbar} \frac{\partial f^{0}(k)}{\partial \varepsilon_{k}} \frac{\partial \varepsilon_{k}}{\partial k} = \frac{8e^{4}m^{*}n}{\hbar^{3}\kappa^{2}} \frac{eE}{\hbar} \tau(k) \frac{\partial f^{0}(k)}{\partial \varepsilon_{k}} \frac{\partial \varepsilon_{k}}{\partial k} \times \int d^{3}q \frac{[1 - \cos(k, k+q)]\delta[q^{2} + 2kq\cos(k, q)]}{q^{4}\varepsilon^{2}(q, 0)}$$
(29)

and

$$\frac{1}{\tau(k)} = \frac{8e^4m^*n}{\hbar^3\kappa^2} \int d^3q \, \frac{[1 - \cos(k, k+q)]\delta[q^2 + 2kq\cos(k, q)]}{q^4\varepsilon^2(q, 0)}.$$
 (30)

To obtain (29) we used the relation

$$f(\mathbf{k}) = f^0[\mathbf{k} + e\tau(\mathbf{k})E/\hbar]$$
(31)

which can be viewed as the definition of $\tau(k)$. After integration over angles in (30), equation (6) is obtained.

For pure impurity scattering there is a complete balance between the filling of a state by the field and the net scattering out by impurity scattering. When e-e scattering is

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present the net scattering out is shared between the two scattering processes. The two processes are quite different. Only the impurity scattering contributes directly to the resistivity. If the field is turned off, the impurity scattering slows down the centre-of-mass (CM) velocity while the e-e scattering has no direct effect on the CM. The e-e scattering thermalizes the electrons in the CM system. This thermalization, however, has an effect on the impurity scattering, which means that e-e scattering indirectly influences the CM motion.

In the case of very strong e-e scattering the Boltzmann equation is easily solved. The thermalization in this case is complete, which means that the distribution function is a Fermi-Dirac distribution function rigidly shifted in momentum space. Thus, the τ defined in (31) is now k-independent. The total momentum change per unit time produced by the field (i.e. the force) is balanced by the total momentum change due to the impurity scattering. The total momentum reduction due to impurity scattering is obtained by multiplying the right-hand-side of (28) by $\hbar k$ and summing over all momenta k. Thus,

$$F = -eEN = \frac{2V}{(2\pi)^3} \int d^3k \, \frac{8e^4 m^* n}{\hbar^3 \kappa^2} \int d^3q \\ \times \frac{\hbar k [f(k) - f(k+q)] \delta[q^2 + 2kq \cos(k,q)]}{q^4 \varepsilon^2(q,0)}$$
(32)

where N and V are the total number of electrons and the volume of the system, respectively. Using (31), linearized and with a constant τ gives

$$-eEn = \frac{2}{(2\pi)^3} \int d^3k \,\hbar k \,\frac{8e^4 m^* n}{\hbar^3 \kappa^2} \left(\frac{eE}{\hbar} \frac{\partial \varepsilon_k}{\partial k}\right) \tau \,\frac{\partial f^0(k)}{\partial \varepsilon_k} \\ \times \int d^3q \,\frac{[1 - \cos(k, k+q)] \delta[q^2 + 2kq \cos(k, q)]}{q^4 \varepsilon^2(q, 0)}.$$
(33)

Part of the expression on the right-hand side can be identified as $1/\tau(k)$, which leads to

$$-eEn = \frac{2}{(2\pi)^3} \int d^3k \, \hbar k \left(\frac{eE}{\hbar} \frac{\partial \varepsilon_k}{\partial k}\right) \tau \frac{\partial f^0(k)}{\partial \varepsilon_k} \frac{1}{\tau(k)}.$$
(34)

This gives

$$\frac{1}{\tau} = -\frac{2}{n} \int \frac{\mathrm{d}^3 k}{(2\pi)^3} \cos^2(k, E) \hbar k \frac{\hbar k}{m^*} \frac{\partial f^0(k)}{\partial \varepsilon_k} \frac{1}{\tau(k)} = -\frac{4}{3n} \int \frac{\mathrm{d}^3 k}{(2\pi)^3} \frac{\partial f^0(k)}{\partial \varepsilon_k} \varepsilon_k \frac{1}{\tau(k)} = \left\langle \frac{1}{\tau(k)} \right\rangle.$$
(35)

Thus (5) is valid in the case of very strong e-e scattering.

For general strength of the e-e scattering we have

$$\left[\frac{\partial f(k)}{\partial t}\right]_{\text{scatt}}^{\text{imp}} + \left[\frac{\partial f(k)}{\partial t}\right]_{\text{scatt}}^{e-e} + \left[\frac{\partial f(k)}{\partial t}\right]_{\text{field}} = 0.$$
(36)

The first term, which comes from impurity scattering, is given by the right-hand side of (27) with reversed sign. Defining $\tau(k)$ according to (31) the term can be transformed into the right-hand side of (29) with reversed sign. Part of this expression is identified as

the inverse transport time from impurity scattering $1/\tau_{imp}(k)$ given in (30). Thus we can write

$$\left[\frac{\partial f(k)}{\partial t}\right]_{\text{scatt}}^{\text{imp}} = -\frac{eE}{\hbar} \frac{\partial f^{0}(k)}{\partial \varepsilon_{k}} \frac{\partial \varepsilon_{k}}{\partial k} \frac{\tau(k)}{\tau_{\text{imp}}(k)}.$$
(37)

Up till now we have not used the relaxation-time approximation. We do this for the e-e scattering and find

$$\left[\frac{\partial f(k)}{\partial t}\right]_{\text{scatt}}^{\text{e-e}} = -\frac{f(k) - f^0(k + eE\langle \tau(k) \rangle/\hbar)}{\tau_{\text{e-e}}} = -\frac{\tau(k) - \langle \tau(k) \rangle}{\tau_{\text{e-e}}} \frac{eE}{\hbar} \frac{\partial f^0(k)}{\partial \varepsilon_k} \frac{\partial \varepsilon_k}{\partial k}$$
(38)

where the numerator on the right-hand side of the first line is the difference between the distribution function and the Fermi-Dirac distribution function in the centre-of-mass system.

Now, (36) can be written as

$$-\frac{eE}{\hbar}\frac{\partial f^{0}(k)}{\partial \varepsilon_{k}}\frac{\partial \varepsilon_{k}}{\partial k}\frac{\tau(k)}{\tau_{imp}(k)}-\frac{eE}{\hbar}\frac{\partial f^{0}(k)}{\partial \varepsilon_{k}}\frac{\partial \varepsilon_{k}}{\partial k}\frac{\tau(k)-\langle \tau(k)\rangle}{\tau_{e-e}}+\frac{eE}{\hbar}\frac{\partial f^{0}(k)}{\partial \varepsilon_{k}}\frac{\partial \varepsilon_{k}}{\partial k}=0.$$
(39)

After reduction and rearrangement we get

$$\tau(k) = \frac{\tau_{\rm imp}(k)\tau_{\rm e-e}}{\tau_{\rm e-e} + \tau_{\rm imp}(k)} + \frac{\langle \tau(k) \rangle \tau_{\rm imp}(k)}{\tau_{\rm e-e} + \tau_{\rm imp}(k)}$$
(40)

and averaging both sides as prescribed in (2) results in

$$\langle \tau(k) \rangle = \left\langle \frac{\tau_{\rm imp}(k)\tau_{\rm e-e}}{\tau_{\rm e-e} + \tau_{\rm imp}(k)} \right\rangle / \left(1 - \left\langle \frac{\tau_{\rm imp}(k)}{\tau_{\rm e-e} + \tau_{\rm imp}(k)} \right\rangle \right)$$

$$= \left\langle \frac{\tau_{\rm e-e}}{\tau_{\rm e-e} / \tau_{\rm imp}(k) + 1} \right\rangle / \left\langle \frac{\tau_{\rm e-e} / \tau_{\rm imp}(k)}{\tau_{\rm e-e} / \tau_{\rm imp}(k) + 1} \right\rangle.$$

$$(41)$$

Here we see that for vanishing e-e scattering $\langle \tau(k) \rangle = \langle \tau_{imp}(k) \rangle$, i.e. equation (1) is obtained. On the other hand very strong e-e scattering gives $\langle \tau(k) \rangle = 1/\langle 1/\tau_{imp}(k) \rangle$ and equation (5) is regained.

In summary, we have in this section shown that the solution of the Boltzmann equation with inclusion of e-e scattering gives a result in between those of (1) and (5); the result (5) is obtained if the e-e scattering dominates over the e-i scattering. This is in complete agreement with the results from the force-balance method as shown in [20].

5. Summary and conclusions

We have studied how the results from the generalized Drude approach for impurity resistivity and the dynamical theory of Farvacque compare numerically with the two different results that are obtained from other theories: straightforward solution of the Boltzmann equation or summation of a selected infinite subclass of diagrams in a diagrammatic perturbation expansion based on the Kubo formalism give result number one; microscopic resistivity formulations, force-balance theories, the energy-loss method and a simple variational solution to the Boltzmann equation give result number two. Both results numbers one and two are identical for zero temperature but are

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different for finite temperatures. We found that the generalized Drude approach gave results identical to those from the energy-loss method and consequently gave the second result. The result from the dynamical theory of Farvacque turned out not to belong to any of the two groups of results mentioned above. The results deviated in both temperature limits. In an effort to explain this behaviour we have tried to follow the derivation of the theory as given in [26]. We cannot see the validity in the term-by-term identification in equation (22) of that reference. If we first rearrange the terms on the right-hand side of the equation by substituting k-q for k in the first term of the summand and then make a term-by-term identification we obtain for $1/\tau$ not our (8) but our (6), i.e. the usual result.

The Boltzmann derivation produce a deformed distribution function in the centreof-mass system. If the e-e scattering is strong enough to thermalize the electrons, i.e. to make the distribution function a pure Fermi-Dirac distribution function in the centreof-mass system, the Boltzmann derivation produces the second of the results mentioned above. Thermalized electrons are equivalent to a constant τ . In the variational solution to the Boltzmann equation one uses $\tau(k)$ as a variational function. In the simplest variational solution, i.e. keeping τ constant, the second result is once again obtained. Using a series of variational functions with increasing flexibility gradually moves the result towards result number one; we should add that this is in the absence of e-e scattering.

The correct result probably lies somewhere in between the results numbers one and two. Where exactly it lies depends on the degree of thermalization. Quantitative results for the degree of thermalization for strong electric fields and high temperatures have been obtained in [33].

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References

- [1] Kohn W and Luttinger J M 1957 Phys. Rev. 108 590
- [2] Ziman J M 1967 Electrons and Phonons (London: Oxford University Press)
- [3] Mahan G D 1981 Many-Particle Physics (New York: Plenum)
- [4] Edwards S F 1965 Proc. Phys. Soc. 86 977
- [5] Rousseau J S, Stoddart J C and March N H 1973 J. Phys. C: Solid State Phys. 5 L175
- [6] Ghassib H B, Gilbert R and Morgan G J 1973 J. Phys. C: Solid State Phys. 6 1841
- [7] Kenkre V M and Dresden M 1972 Phys. Rev. A 6 769
- [8] Kenkre V M 1973 Phys. Rev. A 7 772
- [9] Huberman M and Chester G V 1975 Adv. Phys. 24 489
- [10] Lei X L and Ting C S 1984 Phys. Rev. B 30 4809
- [11] Lei X L and Ting C S 1985 J. Phys. C: Solid State Phys. 1877
- [12] Lei X L and Ting C S 1985 Phys. Rev. B 32 1112
- [13] Horing N J M, Lei X L and Cui H L 1986 Phys. Rev. B 33 66929
- [14] Ting C S and Nee T W 1986 Phys. Rev. B 33 7056
- [15] Lei X L and Ting C S 1987 Phys. Rev. B 35 3971
- [16] Lei X L, Xing D Y, Lin M, Ting C S and Birman J L 1985 Phys. Rev. B 36 9134
- [17] Argyres P N 1989 Phys. Rev. B 39 2982
- [18] Fishman R S and Mahan G D 1989 Phys. Rev. B 39 2990

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- [19] Fishman R S 1989 Phys. Rev. B 39 2994
- [20] Chen L Y, Ting C S and Horing N J M 1989 Phys. Rev. B 40 3756
- [21] Hirakawa K and Sasaki H 1988 J. Appl. Phys. 63 803
- [22] Xing D Y, Hu P and Ting C S 1987 Phys. Rev. B 35 6379
- [23] Liu M, Xing D Y, Ting C S and Xu W T 1988 Phys. Rev. B 37 2997
- [24] Xing D Y, Liu M and Ting C S 1988 Phys. Rev. B 37 10283
- [25] Sernelius B E 1989 Phys. Rev. B 40 12438
- [26] Farvacque J L 1989 Phys. Rev. B 39 1682
- [27] Sernelius B E 1987 Phys. Rev. B 36 1080
- [28] Gerlach E 1986 J. Phys. C: Solid State Phys. 19 4585
- [29] Sernelius B E and Morling M 1989 Thin Solid Films 177 69
- [30] Sirko R and Mills D L 1978 Phys. Rev. B 18 4373
- [31] Sernelius B E 1989 Shallow Impurities in Semiconductors ed B Monemar (Bristol: Institute of Physics) p 137
- [32] Combescot M and Combescot R 1987 Phys. Rev. B 35 7986
- [33] Wingreen N S, Stanton C J and Wilkins J W 1986 Phys. Rev. Lett. 57 1084; 1987 Phys. Rev. Lett. 59 376