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Quantum-Transport Theories and Multiple Scattering in Doped Semiconductors. I. Formal Theory*†

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Previous quantum-transport theories relevant to the calculation of multiple-scattering contributions to the electron mobility of a doped semiconductor are re-examined. The Green's-function evaluations of the Kubo formula are extended to include contributions of second order in the impurity concentration in addition to the first-order terms included previously. The simple rigorous results obtained are used to justify and simplify the Kohn–Luttinger transport equations. Apparent difficulties with the impurity averaging are clarified, and the second-order Kohn-Luttinger equation is reduced to a Boltzmann form. For an isotropic solid a simple closed formula for the mobility is derived, which contains such quantum corrections to the Brooks-Herring formula as coherent scattering from pairs of impurities, higher Born approximations for the single scattering, and dressing effects of the impurities on the electron energy levels and wave functions. It is noted that a variational principle of the Kohler type exists, which should be of use in estimating multiple-scattering contributions in anisotropic solids.

I. INTRODUCTION

In the Brooks-Herring theory[1] of electron scattering by randomly distributed ionized impurities in semiconductors, the mobility of a system of quasifree conduction-band electrons is obtained by solving a Boltzmann equation. In setting up the Boltzmann equation, Brooks and Herring assume that the impurities scatter the electrons independently, that the transition probability may be evaluated in first Born approximation, and that the perturbing effects of the impurities on the electron energy levels and wave functions may be neglected. Although the Brooks-Herring theory provides a good description of the mobility in many cases, the contributions from coherent scattering from pairs of impurity centers, from higher Born approximations for the single scattering, and from the dressing effects of the impurities can be important in practice. In order to include these contributions consistently, it is necessary to develop a quantum-transport theory. Several such quantum approaches have been discussed in the literature.[2–11] These approaches may be grouped into two main classes, which may be termed transport-equation and Kubo approaches, respectively.

A typical transport-equation approach is that of Kohn and Luttinger,[2,3] in which a perturbation expansion in powers of the impurity potential,[2] or in powers of the impurity concentration,[3] is used to reduce the quantum Liouville equation to a series of "transport equations" involving only the diagonal elements of the density matrix. In these expansions the coherent-scattering terms first appear in the third lowest order in the potential expansion and in the second lowest order in the density expansion. Unfortunately, however, these higher-order equations are sufficiently complicated that it is not apparent how to obtain an explicit expression for the conductivity from them. Accordingly, no applications of these equations to experimental results have yet been made. In addition, the Kohn-Luttinger theory suffers from some apparent formal difficulties. Rickayzen,[4] for example, has objected that the impurity averaging procedure used to derive the macroscopic current from the microscopic current is introduced at the wrong stage of the calculations.

In the Kubo approach a general expression for the conductivity (the socalled Kubo formula) is obtained by a formal solution of the Liouville equation. The explicit evaluation of the conductivity from the Kubo formula is a long and difficult calculation which has been carried through in various ways. Abrikosov and Gor'kov,[5] Edwards,[6] Rickayzen,[4] Langer,[7] and Ambegaokar[8] have obtained explicit results using thermodynamic Green's-function techniques. However, these calculations are restricted to the lowest order in an impurity-concentration expansion, and hence the coherent scattering effects are not included. Chester and

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[1] H. Brooks, Phys. Rev. 83, 879 (1951); Advan. Electron. Electron Phys. 7, 128 (1955).

[2] W. Kohn and J. M. Luttinger, Phys. Rev. 108, 590 (1957).

[3] J. M. Luttinger and W. Kohn, Phys. Rev. 109, 1892 (1958).

[4] G. Rickayzen, in *Lecture Notes on the Many-Body Problem*, edited by C. Fronsdal (W. A. Benjamin, Inc., New York, 1961).

[5] A. A. Abrikosov and L. P. Gorkov, Zh. Eksperim. i Teor. Fiz. 35, 1558 (1958); 36, 319 (1959) [English transls.: Soviet Phys.—JETP 8, 1090 (1959); 9, 220 (1959)].

[6] S. F. Edwards, Phil. Mag. 3, 1020 (1958); 4, 1171 (1959).

[7] J. S. Langer, Phys. Rev. 120, 714 (1960); 124, 1003 (1961); 127, 5 (1962).

[8] V. Ambegaokar, in *Astrophysics and the Many-Body Problem, 1962 Brandeis Lectures* (W. A. Benjamin, Inc., New York, 1962).

[9] G. V. Chester and A. Thellung, Proc. Phys. Soc. (London) 73, 765 (1959); 77, 1005 (1961); G. V. Chester, *ibid.* 81, 938 (1963).

[10] E. Verboven, Physica 26, 1091 (1960).

[11] P. Berger, J. M. J. Van Leeuwen, and E. Verboven, Physica 29, 1409 (1963).

Thellung,[9] Verboven,[10] and Berger *et al.*[11] have used perturbation-expansion methods closely related to those of Van Hove.[12] These calculations have been carried through to the third lowest order in a potential expansion, and thus coherent-scattering effects are included. However, the results obtained by this method are extremely complicated and do not easily yield a useable formula for the conductivity.

Although a Green's-function evaluation of the Kubo formula is probably the most powerful and general method available for evaluating quantum conductivities, this approach suffers from certain practical disadvantages in connection with the impurity scattering problem. It is difficult, for example, to apply it to an anisotropic system, and it involves sophisticated mathematical techniques that are not always familiar to people in the semiconductor field. The transport-equation approach is a more practical method which has the advantages of familiarity, easy generalization to anisotropic systems, and ready adaptability to the evaluation of transport coefficients other than the conductivity. However, as mentioned previously, it is not entirely rigorous, and some difficulties of interpretation are encountered if the results of a Green's-function calculation are not known.

The present work has both formal and practical aspects. The formal part of the work, which is discussed in this paper, has three objectives: (1) to demonstrate the mutual consistency of the Green's-function and transport-equation results; (2) to derive far simpler, practical formulas for the conductivity of isotropic semiconductors in which such quantum effects as coherent scattering from pairs of impurities and the dressing of the electron energy levels and wave functions are important; and (3) to develop a practical quantum-variational principle for estimating the conductivity of anisotropic solids. The more practical aspects of the work, which will be discussed in a subsequent paper, are concerned with the estimation of the quantum effects in a typical *n*-type semiconductor (GaAs) and with a comparison of the quantum mobility of gallium arsenide with the Brooks-Herring mobility and with experimental data.

The general outline of the present paper is as follows. In Sec. II the system of interest is described and basic formulas required in the later sections are presented. In Sec. III the Green's-function evaluation of the Kubo formula is extended to include the coherent scattering terms. In this development the impurity potential expansions[13] are used, since these are much simpler than the concentration expansions and are more immediately useful for doped semiconductors. This calculation leads to a simple closed formula for the conductivity of an isotropic semiconductor and provides a framework for the subsequent discussion of the transport-equation approach. In IV we re-examine the first Kohn-Luttinger paper[2] (hereafter referred to as KL), in which potential expansions are used. A brief outline of a method, suggested by the physical interpretation of the Green's-function result, for reducing the second-order[14] KL transport equation to a Boltzmann form is given. For an isotropic solid this second-order Boltzmann equation may be solved to obtain the same conductivity formula resulting from the Green's-function method, thus verifying that the assumptions made in KL are valid for the system considered. Since the reasons for the validity of these assumptions are not entirely clear, we briefly outline a third method (based on a Van Hove $\lambda^2 t$ expansion) of deriving the conductivity which clarifies these reasons. Finally, we note that the existence of the second-order Boltzmann equation implies the existence of a Kohler-type variational principle,[15] which is useful for estimating the conductivity of anisotropic semiconductors.

II. DESCRIPTION OF SYSTEM

The system we shall examine is virtually identical with that considered by Brooks and Herring[1] and consists of a gas of independent conduction electrons, described in the effective mass approximation, interacting via a finite-range potential with N randomly distributed static impurities in a volume Ω. It is assumed that N and Ω are large, but that the impurity concentration $n_I = N/\Omega$ is finite. In this Brooks-Herring model the electron-electron interaction is not included explicitly, but the screening effects of this interaction are included self consistently, i.e., in the random-phase approximation. We are interested in obtaining the three lowest orders in an expansion of the dc conductivity in powers of the impurity potential.

The total Hamiltonian for the system is a sum of one-electron Hamiltonians, which will be taken to be of the form

$$H_T = H_0 + H' + H_F = H + H_F\,, \qquad (1)$$

where

$$H_0 = p_x^2/2m_x + p_y^2/2m_y + p_z^2/2m_z \qquad (2)$$

is the Hamiltonian for an electron in an ellipsoidal valley, and

$$H' = \lambda \textstyle\sum_{j=1}^{N} V(\mathbf{r} - \mathbf{R}_j)$$

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[12] L. Van Hove, Physica **21**, 517 (1955); **23**, 441 (1957); G. V. Chester, Rept. Progr. Phys. **26**, 411 (1963).

[13] Although it is questionable whether an expansion of the conductivity in powers of the potential is possible, the results presented here should be correct. Langer and Neal [J. S. Langer and T. Neal, Phys. Rev. Letters **16**, 984 (1966)] have shown that the series expansion of the conductivity in powers of the impurity concentration does not exist. However, the more correct calculation and the calculation based on concentration expansions agree to the order being considered in this paper (i.e., to second order in the concentration), with the differences appearing in the next highest order.

[14] The lowest-order terms in the transport equation are of zeroth order in the impurity potential.

[15] M. Kohler, Z. Physik **124**, 772 (1948); **125**, 679 (1949); **126**, 495 (1949); J. M. Ziman, *Electrons and Phonons* (Oxford University Press, New York, 1960), p. 275ff.

describes the electron-impurity interaction. The finite-range function $V(\mathbf{r}-\mathbf{R}_j)$ is the potential energy of an electron at $\mathbf{r}$ due to the jth impurity at $\mathbf{R}_j$, and λ is a dimensionless parameter characteristic of the strength of the impurity potential. Finally,

$$H_F=-e\mathbf{\mathcal{E}}\cdot\mathbf{r}e^{st} \tag{3}$$

contains the effect of the adiabatically switched-on electric field.

The experimentally measured conductivity relates the macroscopic current density to the total electric field. For the present model, the total electric field is identical with the electric field appearing explicitly in the Hamiltonian (3), since we are considering an effective single-electron problem. The macroscopic current density is the average of the microscopic current density over a macroscopic volume of the solid. Rickayzen[4] has given a physically plausible, although not completely rigorous, argument that this average over a macroscopic volume is equivalent, for spatially slowly varying applied fields, to an average over an ensemble of solids with random impurity distributions. Kohn and Luttinger[2] follow the slightly different procedure of obtaining the macroscopic current density directly by calculating the total current flowing in a large volume. This total current is a function of the impurity distribution in the solid. KL then use an "ensemble average theorem"[16] to argue that there is a vanishingly small probability (order $N^{-1/2}$) for the current corresponding to a particular impurity configuration to differ from the average value in an ensemble of solids with random-impurity distributions. Thus KL's argument also leads to the macroscopic current density's being the ensemble average of the microscopic current density. However, this KL argument is not completely rigorous, since the ensemble-average theorem cannot be rigorously applied if the current is calculated from the KL transport-equation approach.[17] The theorem is, however, applicable to the Green's function method, where it provides a proof for the plausibility argument of Rickayzen.[18] We shall assume at this point in the development that the macroscopic current density is the ensemble average of the microscopic density. The justification of this assumption by the ensemble average theorem is given in Sec. III.

In the Ohmic conduction region, the total density matrix may be conveniently written as the sum of the equilibrium density matrix $\rho=[\exp\beta(H-\mu)+1]^{-1}$ and a correction term f, which is linear in the applied electric field, i.e.,

$$\rho_T=\rho+f. \tag{4}$$

When the impurity potential is weak, it is convenient to work in a momentum representation, since the momentum wave functions (plane waves) are the eigenfunctions of the free-electron Hamiltonian H_0. The required matrix elements of the Hamiltonian, the current-density operator, and the equilibrium-density matrix are collected in the Appendix.

If intervalley scattering can be neglected, the macroscopic current density for an electron in one of the equivalent valleys may be written

$$\begin{aligned}\mathcal{J}(\mathbf{r},t)&=\int\frac{d\mathbf{R}_1}{\Omega}\cdots\frac{d\mathbf{R}_N}{\Omega}\,\mathrm{tr}\{\rho_T(t;\mathbf{R}_1,\mathbf{R}_2\cdots\mathbf{R}_N)\mathbf{J}(\mathbf{r})\}\\&=\sum_{\mathbf{kk}'}\langle\rho_T\rangle_{\mathbf{kk}'}\mathbf{J}_{\mathbf{k}'\mathbf{k}}(\mathbf{r})=\sum_{\mathbf{kk}'}\langle f\rangle_{\mathbf{kk}'}\mathbf{J}_{\mathbf{k}'\mathbf{k}}(\mathbf{r}),\end{aligned} \tag{5}$$

where ensemble averaging[19] is denoted by $\langle\ \rangle$, $\mathbf{J}(\mathbf{r})$ is the current-density operator, and we have used the fact that the equilibrium system carries no current. In order to calculate the current, it is necessary to obtain the density matrix f from the Liouville equation. The method of doing this distinguishes the Kubo and transport-equation approaches.

III. THE KUBO APPROACH

The method of constructing a Kubo formula for the dc conductivity and of evaluating this formula by means of thermodynamic Green's functions is well-known.[4–8,20] The extension of these Green's-function calculations to include the lowest-order coherent scattering terms involves comparatively minor modifications in the methods described by Rickayzen[4] and Langer.[7] Hence we shall only briefly outline the main results obtained, concentrating on those required for the justification and simplification of the KL equations. The discussion is restricted to isotropic systems for which $m_x=m_y=m_z=m$, where m is an effective mass.

In the present work the formalism of Kadanoff and Martin[20] is used to express the microscopic current density in terms of linear response functions which are grand canonical expectation values of current-current commutators. Using standard Green's-function techniques,[21] modified for a system not possessing translational invariance, we write the microscopic response functions in a spectral representation form involving a product of two one-electron spectral functions. After

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[16] Appendix B of Ref. 2.

[17] See discussion after Eq. (25).

[18] The ensemble averaging arguments break down if: (1) the impurities are not randomly distributed, e.g., if they form a regular lattice; or (2) if the charge carriers are bosons which have undergone a Bose-Einstein condensation [cf. J. M. Blatt, *Theory of Superconductivity* (Academic Press Inc., New York, 1962), Chap. 9].

[19] Identical results would be obtained if the impurities were restricted to lattice sites.

[20] L. P. Kadanoff and P. C. Martin, Phys. Rev. **124**, 670 (1961); H. Ehrenreich, in *Proceedings International School of Physics "Enrico Fermi," Course 34* (Academic Press Inc., New York, 1966).

[21] P. C. Martin and J. Schwinger, Phys. Rev. **115**, 1342 (1959); L. P. Kadanoff and G. Baym, *Quantum Statistical Mechanics* (W. A. Benjamin, Inc., New York, 1962); D. N. Zubarev, Usp. Fiz. Nauk **71**, 71 (1960) [English transl.: Soviet Phys.—Uspeki **3**, 320 (1960)].

ensemble averaging and some algebra, we finally obtain a result similar to one quoted by Langer[7] in his theory of the impurity resistance of an isotropic metal, namely,[22]

$$\sigma=-\frac{e^2}{6m^2}\frac{1}{2\pi\Omega}\sum_{\mathbf{k}\mathbf{k}'}(\mathbf{k}\cdot\mathbf{k}')\times\int_{-\infty}^{\infty}\frac{df_0(\omega)}{d\omega}\langle A(\mathbf{k},\mathbf{k}';\omega)A(-\mathbf{k},-\mathbf{k}';\omega)\rangle d\omega\,, \quad (6)$$

where $f_0(\omega)=[\exp\beta(\omega-\mu)+1]^{-1}$ is the Fermi distribution, and

$$A(\mathbf{k},\mathbf{k}';\omega)=\langle\mathbf{k}|A(\omega)|\mathbf{k}'\rangle = i\lim_{s\to 0}\langle\mathbf{k}|[G(\omega+is)-G(\omega-is)]|\mathbf{k}'\rangle\,, \quad (7)$$

with $G(z)=(z-H)^{-1}$, is the one-electron spectral function. $G(z)$ is the resolvent for a conduction-band electron in the presence of the impurities.

The conductivity (6) can be evaluated by following the method described by Rickayzen[4] and Langer,[7] among others, of first constructing a Dyson's equation relating the ensemble averaged resolvent (real propagator) to a self-energy function. A Bethe-Salpeter equation may then be set up to express the averaged spectral product appearing in (6) in terms of the propagators and thus of the self-energy function. For an isotropic system this equation may be solved, yielding a simple expression for the conductivity in terms of the physically meaningful real and imaginary parts of the self-energy function, i.e., in terms of quasiparticle energy levels and transition probabilities.

The standard method of evaluating the impurity averaged resolvent is to introduce the free-electron resolvent $G_0(z)=(z-H_0)^{-1}$ and to use the equation $G(z)=G_0(z)+G_0(z)H'G(z)$ to expand G in a perturbation expansion in powers of the strength parameter λ of the impurity potential. The averaging over the random impurity ensemble eliminates the microscopic or non-momentum-conserving terms in G, and only the macroscopic (momentum-conserving) terms remain. The expansion for $\langle G(\mathbf{k},\mathbf{k};z)\rangle$ so obtained cannot be used immediately in evaluating the dc conductivity, since it would yield an expansion in which each term is infinite.[4,22] However, a finite result for the conductivity will be obtained if an analytic continuation (renormalization) procedure involving the systematic replacement of bare propagators $(z-E_{\mathbf{k}})^{-1}$ by the real propagators $\langle G(\mathbf{k},\mathbf{k};z)\rangle$ is applied to the expansion for $\langle G\rangle$. The resulting expansion for $\langle G\rangle$ may be summed to yield the Dyson's equation

$$\langle G(\mathbf{k}',\mathbf{k}'';z)\rangle=\delta_{\mathbf{k}'\mathbf{k}''}\langle G(\mathbf{k}';z)\rangle = \delta_{\mathbf{k}'\mathbf{k}''}[z-E_{\mathbf{k}'}-\Sigma(\mathbf{k}';z)]^{-1}\,, \quad (8)$$

where $\Sigma(\mathbf{k}';z)$ is the self-energy. If we retain only the three lowest orders in λ in the self-energy, the expansion for it may be written in diagrammatic form as in Fig. 1 and in analytic form as in Eq. (9).[22]

$$\begin{aligned}\Sigma(\mathbf{k}')=N\frac{\lambda^2}{\Omega^2}\sum_{\mathbf{k}_1}|V_{\mathbf{k}'\mathbf{k}_1}|^2\langle G(\mathbf{k}_1)\rangle+N\frac{\lambda^3}{\Omega^3}\sum_{\mathbf{k}_1\mathbf{k}_2}V(\mathbf{k}'\mathbf{k}_1\mathbf{k}_2\mathbf{k}')\langle G(\mathbf{k}_1)\rangle\langle G(\mathbf{k}_2)\rangle \\ +N\frac{\lambda^4}{\Omega^4}\sum_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3}V(\mathbf{k}'\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}')\langle G(\mathbf{k}_1)\rangle\langle G(\mathbf{k}_2)\rangle\langle G(\mathbf{k}_3)\rangle \\ +N^2\frac{\lambda^4}{\Omega^4}\sum_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3}V(\mathbf{k}'\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}')\langle G(\mathbf{k}_1)\rangle\langle G(\mathbf{k}_2)\rangle\langle G(\mathbf{k}_3)\rangle\delta_{\mathbf{k}'-\mathbf{k}_1+\mathbf{k}_2-\mathbf{k}_3,0}+O(\lambda^5)\,, \quad (9)\end{aligned}$$

where

$$V_{\mathbf{k}\mathbf{k}'}=\int e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}}V(\mathbf{r})d\mathbf{r}$$

and

$$V(\mathbf{k}\mathbf{k}'\mathbf{k}''\cdots\mathbf{k}^{(n)})=V_{\mathbf{k}\mathbf{k}'}V_{\mathbf{k}'\mathbf{k}''}\cdots V_{\mathbf{k}^{(n-1)}\mathbf{k}^{(n)}}\,.$$

The first, second, and third terms in Fig. 1 and Eq. (9), which contain only a single impurity (represented by a cross), can be interpreted as the first, second, and third Born approximations, respectively, for the interaction between a quasiparticle (represented by a directed line or propagator $\langle G\rangle$) and a single impurity. The factor N arises from the fact that there are N impurities in the solid. These linear terms in N have been included in previous Green's-function calculations.[4-8] The fourth term in (9), which has not been included previously, involves two distinct impurities and can be interpreted as the lowest Born approximation for the interaction between a quasiparticle and a pair of impurities, there being $N(N-1)\approx N^2$ ordered pairs in the solid. The Kronecker delta arises from the requirement imposed by the ensemble averaging that momentum must be conserved individually at each impurity.

The physically significant values of the complex frequency z are given by $z=\omega\pm is$, where ω is a real

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[22] E. J. Moore, thesis, Harvard University, 1966 (unpublished); Division of Engineering and Applied Physics, Harvard University, Technical Report No. ARPA-24, 1966 (unpublished).

frequency and s is a positive infinitesimal. In the limit of $s\to 0$, $G(\mathbf{k},\omega+is)^*=G(\mathbf{k},\omega-is)$, and it is then customary to define a dressing function $\Delta_{\mathbf{k}}(\omega)=\mathrm{Re}\Sigma(\mathbf{k},\omega+is)=\mathrm{Re}\Sigma(\mathbf{k},\omega-is)$ and a width function $\Gamma_{\mathbf{k}}(\omega)=\mathrm{Im}\Sigma(\mathbf{k},\omega-is)=-\mathrm{Im}\Sigma(\mathbf{k},\omega+is)$. In the present calculations, it is possible to assume that $\Gamma_{\mathbf{k}}(\omega)$ is small[23] and that there is one and only one zero[24] of $\omega-E_{\mathbf{k}}-\Delta_{\mathbf{k}}(\omega)$, given by $\omega\approx E_{\mathbf{k}}+\Delta_{\mathbf{k}}(E_{\mathbf{k}})+O(\lambda^3)=\epsilon_{\mathbf{k}}+O(\lambda^3)$. The spectral function

$$\langle A(\mathbf{k},\mathbf{k};\omega)\rangle=\lim_{s\to 0} i[\langle G(\mathbf{k},\omega+is)\rangle-\langle G(\mathbf{k},\omega-is)\rangle]$$

is then sharply peaked at $\omega=\epsilon_{\mathbf{k}}$, and may generally be replaced in integrands by the equivalent δ function[23]

$$\begin{aligned}\langle A(\mathbf{k},\mathbf{k};\omega)\rangle&=\frac{2\Gamma_{\mathbf{k}}(\omega)}{[\omega-E_{\mathbf{k}}-\Delta_{\mathbf{k}}(\omega)]^2+\Gamma_{\mathbf{k}}(\omega)^2}\\&\approx\frac{2\Gamma_{\mathbf{k}}(\epsilon_{\mathbf{k}})}{[\omega-\epsilon_{\mathbf{k}}]^2[1-\Delta_{\mathbf{k}}'(E_{\mathbf{k}})]^2+\Gamma_{\mathbf{k}}(\epsilon_{\mathbf{k}})^2}\\&\approx 2\pi\delta(\omega-\epsilon_{\mathbf{k}})/[1-\Delta_{\mathbf{k}}'(E_{\mathbf{k}})],\end{aligned}\tag{10}$$

where

$$\Delta_{\mathbf{k}}'(E_{\mathbf{k}})=\left[\frac{\partial}{\partial\omega}\Delta_{\mathbf{k}}(\omega)\right]_{\omega=E_{\mathbf{k}}}.$$

The quantity $\langle A(\mathbf{k},\mathbf{k};\omega)\rangle$ may be interpreted as the spectral distribution for quasiparticles with energy levels $\epsilon_{\mathbf{k}}$ and with lifetimes related to the width functions $\Gamma_{\mathbf{k}}(\epsilon_{\mathbf{k}})$. The function $\Delta_{\mathbf{k}}'(E_{\mathbf{k}})$ represents a change in the normalization between the quasiparticle wave functions and the plane-wave free-electron wave functions.

In calculating the dc conductivity to a given order in λ, we require the same number of terms in the expansion for the energy as in the expansion for the scattering. To obtain the three lowest orders in the energy $(\lambda^0,\lambda,\lambda^2)$, $\Delta_{\mathbf{k}}(\omega)$ is required to order λ^2, whereas to obtain the three lowest orders in the scattering $(\lambda^2,\lambda^3,\lambda^4)$, we require $\Gamma_{\mathbf{k}}(\epsilon_{\mathbf{k}})$ to order λ^4. On taking the real and imaginary parts of the self-energy (9) and making use of (10), we obtain[22] (P denotes principal value)

$$\Delta_{\mathbf{k}}(\omega)=\tfrac{1}{2}N\frac{\lambda^2}{\Omega^2}\sum_{\mathbf{k}'}|V_{\mathbf{k}\mathbf{k}'}|^2\left[\frac{1}{\omega-E_{\mathbf{k}'}+is}+\frac{1}{\omega-E_{\mathbf{k}'}-is}\right]=N\frac{\lambda^2}{\Omega^2}\sum_{\mathbf{k}'}P\frac{|V_{\mathbf{k}\mathbf{k}'}|^2}{\omega-E_{\mathbf{k}'}}+O(\lambda^3)\tag{11}$$

and

$$\Gamma_{\mathbf{k}}(\epsilon_{\mathbf{k}})=\tfrac{1}{2}[1-\Delta_{\mathbf{k}}'(E_{\mathbf{k}})]\sum_{\mathbf{k}'}[W_1(\mathbf{k},\mathbf{k}')+W_2(\mathbf{k},\mathbf{k}')+W_3(\mathbf{k},\mathbf{k}')+U(\mathbf{k},\mathbf{k}')]+O(\lambda^5),\tag{12}$$

where the W's and U are transition probabilities per unit time defined by

$$W_1(\mathbf{k},\mathbf{k}')=2\pi N(\lambda^2/\Omega^2)|V_{\mathbf{k}\mathbf{k}'}|^2\delta(\epsilon_{\mathbf{k}}-\epsilon_{\mathbf{k}'})/\{[1-\Delta_{\mathbf{k}}'(E_{\mathbf{k}})][1-\Delta_{\mathbf{k}'}'(E_{\mathbf{k}'})]\}+O(\lambda^5),\tag{13}$$

$$W_2(\mathbf{k},\mathbf{k}')=2\pi N(\lambda^3/\Omega^3)\delta(\omega_{\mathbf{k}\mathbf{k}'})\sum_{\mathbf{k}_1}[V(\mathbf{k}\mathbf{k}_1\mathbf{k}'\mathbf{k})/d_{\mathbf{k}\mathbf{k}_1}{}^-+V(\mathbf{k}\mathbf{k}'\mathbf{k}_1\mathbf{k})/d_{\mathbf{k}\mathbf{k}_1}{}^+]+O(\lambda^5),\tag{14}$$

$$W_3(\mathbf{k},\mathbf{k}')=2\pi N\frac{\lambda^4}{\Omega^4}\delta(\omega_{\mathbf{k}\mathbf{k}'})\sum_{\mathbf{k}_1\mathbf{k}_2}\left[\frac{V(\mathbf{k}\mathbf{k}'\mathbf{k}_1\mathbf{k}_2\mathbf{k})}{d_{\mathbf{k}\mathbf{k}_1}{}^-d_{\mathbf{k}\mathbf{k}_2}{}^-}+\frac{V(\mathbf{k}\mathbf{k}_2\mathbf{k}_1\mathbf{k}'\mathbf{k})}{d_{\mathbf{k}\mathbf{k}_1}{}^+d_{\mathbf{k}\mathbf{k}_2}{}^+}+\frac{V(\mathbf{k}\mathbf{k}_2\mathbf{k}'\mathbf{k}_1\mathbf{k})}{d_{\mathbf{k}\mathbf{k}_1}{}^-d_{\mathbf{k}\mathbf{k}_2}{}^+}\right],\tag{15}$$

and

$$U(\mathbf{k},\mathbf{k}')=2\pi N^2\frac{\lambda^4}{\Omega^4}\delta(\omega_{\mathbf{k}\mathbf{k}'})\sum_{\mathbf{k}_1\mathbf{k}_2}\left\{\delta_{\mathbf{k}-\mathbf{k}'+\mathbf{k}_1-\mathbf{k}_2}\left[\frac{V(\mathbf{k}\mathbf{k}'\mathbf{k}_1\mathbf{k}_2\mathbf{k})}{d_{\mathbf{k}\mathbf{k}_1}{}^-d_{\mathbf{k}\mathbf{k}_2}{}^-}+\frac{V(\mathbf{k}\mathbf{k}_2\mathbf{k}_1\mathbf{k}'\mathbf{k})}{d_{\mathbf{k}\mathbf{k}_1}{}^+d_{\mathbf{k}\mathbf{k}_2}{}^+}\right]+\delta_{\mathbf{k}+\mathbf{k}'-\mathbf{k}_1-\mathbf{k}_2}\frac{V(\mathbf{k}\mathbf{k}_2\mathbf{k}'\mathbf{k}_1\mathbf{k})}{d_{\mathbf{k}\mathbf{k}_1}{}^-d_{\mathbf{k}\mathbf{k}_2}{}^+}\right\}.\tag{16}$$

In these equations $\omega_{\mathbf{k}\mathbf{k}'}=E_{\mathbf{k}}-E_{\mathbf{k}'}$ and $d_{\mathbf{k}\mathbf{k}'}{}^\pm=\omega_{\mathbf{k}\mathbf{k}'}\pm is$. W_1 is the term derived from Fig. 1(a), and hence it is the first-Born-approximation transition rate for processes in which the impurities scatter the quasiparticles incoherently. Similarly, W_2 and W_3, which come respectively from Figs. 1(b) and 1(c), are the second and third Born approximations for the incoherent scatter-

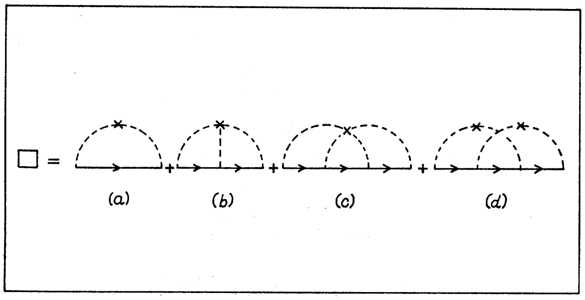

FIG. 1. The diagrammatic expansion for the self-energy function [Eq. (9)]. The first three diagrams represent scattering of quasiparticles by single impurities, while the fourth diagram is the lowest-order contribution to coherent scattering from pairs of impurities.

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[23] The restrictions which these assumptions impose on the region of validity of the final result (18) for the conductivity are discussed in Chap. 2 of Ref. 22. They are: (1) for Boltzmann statistics, $\tau\gg\hbar/\kappa T$, where τ is the relaxation time defined in (19); and (2) for a degenerate gas, $\tau\gg\hbar/E_F$, where E_F is the Fermi energy.

[24] For $\Delta_{\mathbf{k}}(\omega)$ given by (11) and for the special case of a screened Coulomb potential it may be proved explicitly that there is only one zero. These potential expansions are therefore obviously unsatisfactory if there is a significant contribution to the conductivity from an impurity band.

ing. U arises from Fig. 1(d) and is therefore the lowest approximation for coherent scattering from pairs of impurities.

The next stage in the derivation of the dc conductivity is to set up a Bethe-Salpeter integral equation relating a general pair of resolvents $G(\mathbf{k}',\mathbf{k}'';z)$ $G(\mathbf{k}''',\mathbf{k}^{\mathrm{IV}};z')$ to the $\langle G\rangle$, and hence to the quasiparticle energies and transition probabilities. Since the microscopic conductivity tensor is a sum of such resolvent products, it is possible to establish rigorously the equivalence of the macroscopic conductivity and the ensemble average of the microscopic conductivity by showing that the volume and the ensemble averages of the above products are identical.[18] To establish this result, we note that the equation $G=G_0+G_0H'G$ may be used to expand $G(\mathbf{k}',\mathbf{k}'';z)G(\mathbf{k}''',\mathbf{k}^{\mathrm{IV}};z')$ as a power series in H'. This expansion is a sum of impurity Hamiltonian products of the form

$$H'(\mathbf{k}\mathbf{k}_1\mathbf{k}_2\cdots\mathbf{k}_n)=(\lambda/\Omega)^n\sum_{j1\cdots jn}V(\mathbf{k}\mathbf{k}_1\cdots\mathbf{k}_n)\times\exp\{-i[(\mathbf{k}-\mathbf{k}_1)\cdot\mathbf{R}_{j1}+(\mathbf{k}_1-\mathbf{k}_2)\cdot\mathbf{R}_{j2}+\cdots+(\mathbf{k}_{n-1}-\mathbf{k}_n)\cdot\mathbf{R}_{jn}]\}\,, \quad (17)$$

in which all the dependence on the impurity positions appears explicitly in the rapidly varying exponential factors.[25] We note two points: (1) In a term in which momentum is not conserved the exponential factors fluctuate over regions of space of atomic dimensions, and hence the average value over a macroscopic volume is vanishingly small. Also it can easily be proved[22] that the ensemble averages of these terms vanish, and hence the ensemble and the volume averages yield the same (zero) result. (2) The terms in which momentum is conserved satisfy the conditions of the ensemble average theorem of KL.[16] Hence there is a vanishingly small probability that the values of these terms for a particular impurity configuration differ from the ensemble average values, which are independent of position. We therefore require only the ensemble-averaged GG.

The method of setting up and solving a Bethe-Salpeter equation for the $\langle GG\rangle$ has been described in detail by several authors.[4–8] The extension of these calculations, which are restricted to lowest order in the impurity density, to include the lowest-order coherent-scattering contribution is straightforward, and hence we shall only present the final results obtained for the conductivity. Details of the calculation are given in Ref. 22. After introducing an extra factor of 2 to allow for the two spin states of the electron, we find

$$\sigma=-(2e^2/3\Omega)\sum_{\mathbf{k}}(\nabla_{\mathbf{k}}\epsilon_{\mathbf{k}})^2f_0'(\epsilon_{\mathbf{k}})\tau(\mathbf{k})\,, \quad (18)$$

where we have formally introduced a relaxation time $\tau(\mathbf{k})$ defined by

$$1/\tau(\mathbf{k})=\sum_{\mathbf{k}'}[W_1(\mathbf{k},\mathbf{k}')+W_2(\mathbf{k},\mathbf{k}')+W_3(\mathbf{k},\mathbf{k}')+U(\mathbf{k},\mathbf{k}')](1-\cos\theta_{\mathbf{k}\mathbf{k}'})\,. \quad (19)$$

Formulas of the form (18) are very familiar from the Boltzmann-equation theory of conductivity. This is the result which would be obtained from a Boltzmann equation for particles of charge e and velocity $\nabla_{\mathbf{k}}\epsilon_{\mathbf{k}}$ whose interaction with an external scattering mechanism is given by the relaxation time (19). As mentioned previously, the W terms can be identified as the first, second, and third Born approximations, respectively, for the incoherent scattering of the quasiparticles from the N randomly distributed impurities, while the U term is due to coherent scattering from pairs of impurities.

IV. THE KL TRANSPORT-EQUATION APPROACH

The Green's function calculation of Sec. III has yielded a simple rigorous result for the conductivity of an isotropic semiconductor and a simple physical interpretation for the behavior of the electrons in the presence of the impurities. In the present section these results are used to justify and simplify the second-order Kohn and Luttinger equations. We shall first outline the KL procedure, briefly discussing some of the assumptions involved. Then, using the quasiparticle description as a guide, we reduce the second-order KL equation to a Boltzmann form. Since the restriction to isotropic systems, which was introduced in Sec. III to permit the solution of the Bethe-Salpeter equation, is no longer necessary, and since one of the main practical advantages of the transport equation approach is that it can easily be applied to anisotropic materials, we shall consider the anisotropic system described in Sec. II. Although KL originally discussed an isotropic model with a Boltzmann distribution for the electrons, their equations can be taken over virtually unchanged, the sole differences being a trivial redefinition of the free-electron energy and the use of the Fermi distribution.

KL examine the Liouville equation for the one-electron density matrix in the momentum representation. If only linear terms in the electric field are retained and it is assumed that f, which is defined in (4), has an e^{st} time dependence,[26] the matrix form of the Liouville equation may be written

$$d_{\mathbf{k}\mathbf{k}'}-f_{\mathbf{k}\mathbf{k}'}=[\rho,H_F]_{\mathbf{k}\mathbf{k}'}+\sum_{\mathbf{k}''}(f_{\mathbf{k}\mathbf{k}''}H'_{\mathbf{k}'\mathbf{k}''}-H'_{\mathbf{k}\mathbf{k}''}f_{\mathbf{k}''\mathbf{k}'})\,. \quad (20)$$

From the expansion (50) of the equilibrium density matrix it can be seen that the expansion for the diagonal elements begins with zeroth-order terms in the impurity

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[25] This situation contrasts with that in the KL transport-equation approach in which the dependence on the impurity configuration appears both implicitly (in $f_{\mathbf{k}}$ and $f_{\mathbf{k}\mathbf{k}'}$) and explicitly (in H' products).

[26] This assumption is discussed in KL, Appendix D.

potential strength parameter λ, whereas that for the off-diagonal elements starts with first-order terms. The inhomogeneous terms in the diagonal and the off-diagonal parts of the Liouville equation are therefore of different order in λ. The diagonal and the off-diagonal equations are, with superscripts indicating the orders of the inhomogeneous terms,

$$-isf_{\mathbf{k}}=[\rho,H_F]_{\mathbf{k}}^{(0)}+[\rho,H_F]_{\mathbf{k}}^{(2)} + \sum_{\mathbf{k}''(\neq\mathbf{k})}(f_{\mathbf{k}\mathbf{k}''}H'_{\mathbf{k}''\mathbf{k}}-H'_{\mathbf{k}\mathbf{k}''}f_{\mathbf{k}''\mathbf{k}}) \quad (21)$$

and

$$d_{\mathbf{k}\mathbf{k}'}^{-}f_{\mathbf{k}\mathbf{k}'}=[\rho,H_F]_{\mathbf{k}\mathbf{k}'}^{(1)}+[\rho,H_F]_{\mathbf{k}\mathbf{k}'}^{(2)}+(f_{\mathbf{k}}-f_{\mathbf{k}'})H'_{\mathbf{k}\mathbf{k}'} + \sum_{\mathbf{k}''(\neq\mathbf{k},\mathbf{k}')}(f_{\mathbf{k}\mathbf{k}''}H'_{\mathbf{k}''\mathbf{k}'}-H'_{\mathbf{k}\mathbf{k}''}f_{\mathbf{k}''\mathbf{k}'}). \quad (22)$$

In order to develop an iterative procedure for solving these equations, it is necessary to make an assumption about either the λ or the s dependence of f. One possibility is to assume that $sf_{\mathbf{k}}\to 0$ as $s\to 0$ ($sf_{\mathbf{k}}$ nonzero implies an infinite dc conductivity), or, equivalently, that the leading term in $f_{\mathbf{k}}$ is $0(\lambda^{-2})$. Either of these assumptions implies the other and leads to transport equations of the KL type. The other possibility is to consider finite s and arbitrary values of λ^2/s. Van Hove-type $\lambda^2 t(\equiv\lambda^2/s)$ expansions for $f_{\mathbf{k}}$ and $f_{\mathbf{k}\mathbf{k}'}$ are then obtained. This second method does not lead to transport equations but yields perturbation expansions for the conductivity which are essentially equivalent to those of III. In the following discussion we shall first examine the KL transport equation approach. Then, in Sec. V, we briefly examine the Van Hove expansions in order to clarify the assumptions of the KL method.

If $f_{\mathbf{k}}$ is of lowest-order λ^{-2}, Eq. (22) implies that $f_{\mathbf{k}\mathbf{k}'}$ is of lowest-order λ^{-1}. Iteration of this equation then gives a series of equations which express the off-diagonal elements of f in terms of the diagonal components. When these equations are substituted into (21), a series of transport equations in which only the diagonal elements of f appear is obtained. These equations are frequency-dependent microscopic equations. The required macroscopic dc transport equations are obtained from them by letting $s\to 0$ and by ensemble averaging.

To lowest order in λ, Eq. (22) becomes

$$d_{\mathbf{k}\mathbf{k}'}^{-}f_{\mathbf{k}\mathbf{k}'}=(f_{\mathbf{k}}-f_{\mathbf{k}'})H'_{\mathbf{k}\mathbf{k}'}+0(\lambda^0), \quad (23)$$

which on substitution into (21) yields

$$-isf_{\mathbf{k}}=[\rho,H_F]_{\mathbf{k}}^{(0)}+\sum_{\mathbf{k}'}{}'\,|H'_{\mathbf{k}\mathbf{k}'}|^2(f_{\mathbf{k}}-f_{\mathbf{k}'}) \times[1/d_{\mathbf{k}\mathbf{k}'}^{-}-1/d_{\mathbf{k}\mathbf{k}'}^{+}]. \quad (24)$$

The term on the left of (24) is of order s/λ^2, and hence may be neglected in the dc limit. As KL have pointed out, there is a large range of values of s for which (24) is practically independent of s, and for which the summation over $\mathbf{k}'$ may be replaced by an integration, and the factor $[1/d_{\mathbf{k}\mathbf{k}'}^{-}-1/d_{\mathbf{k}\mathbf{k}'}^{+}]$, by a δ function.

In order to compute the macroscopic current density (5) from a transport equation approach it is necessary to reduce (23) to an equation for $\langle f\rangle_{\mathbf{k}\mathbf{k}'}$ and (24) to one for $\langle f\rangle_{\mathbf{k}}$. On averaging (23) and (24), however, we obtain equations which contain quantities of the form $\langle f_{\mathbf{k}}H'_{\mathbf{k}\mathbf{k}'}\rangle$ and $\langle f_{\mathbf{k}}|H'_{\mathbf{k}\mathbf{k}'}|^2\rangle$, and hence $\langle f\rangle$ does not appear explicitly. To obtain equations for $\langle f\rangle_{\mathbf{k}}$ and $\langle f\rangle_{\mathbf{k}\mathbf{k}'}$ we introduce a "decoupling assumption" that

$$\langle f_{\mathbf{k}_i}H'(\mathbf{k}_1\mathbf{k}_2\cdots\mathbf{k}_i\cdots\mathbf{k}_n)\rangle =\langle f\rangle_{\mathbf{k}_i}\langle H'(\mathbf{k}_1\mathbf{k}_2\cdots\mathbf{k}_i\cdots\mathbf{k}_n)\rangle[1+O(\Omega^{-1})]. \quad (25)$$

It is worth pointing out here that $f_{\mathbf{k}}$ is a microscopic quantity and may easily be shown[22] to contain rapidly varying exponential factors of the form

$$\exp[i(\mathbf{k}_1-\mathbf{k}_2+\cdots)\cdot\mathbf{R}_j].$$

In applying their ensemble-average theorem to the microscopic Eq. (24), KL implicitly make the physically plausible assumption, which is completely equivalent to the decoupling assumption (25), that $f_{\mathbf{k}}$ does not contain any physically important, rapidly varying exponential factors.

An explicit proof of (25) and of the equivalent KL assumption can readily be given by developing λ^2/s expansions for f. These expansions, which are briefly discussed in Sec. V, also yield some insight into the physical significance of (25), particularly of the connection between it and the Van Hove conditions for irreversibility.[12]

On averaging (23) and (24) and making use of (25), we obtain $\langle f\rangle_{\mathbf{k}\mathbf{k}'}=0$ and the zeroth-order KL equation

$$0=e\boldsymbol{\mathcal{E}}\cdot\nabla_{\mathbf{k}}f_0(E_{\mathbf{k}}) +2\pi N(\lambda/\Omega)^2\sum_{\mathbf{k}'}|V_{\mathbf{k}\mathbf{k}'}|^2\delta(\omega_{\mathbf{k}\mathbf{k}'})(\langle f\rangle_{\mathbf{k}}-\langle f\rangle_{\mathbf{k}'}), \quad (26)$$

which is, of course, the Boltzmann equation used in the Brooks-Herring theory.[1]

The higher-order equations may be obtained by following the procedure of KL. We again find that $\langle f\rangle_{\mathbf{k}\mathbf{k}'}=0$, and that the decoupling assumption must be made in the derivation of the macroscopic transport equations from the microscopic equations. In first-order KL obtain a result analogous to the zeroth-order, the sole exception being that the transition probability also includes second-Born-approximation terms. The effects in which we are interested (the coherent scattering from pairs of impurities and the impurity dressing of the electron energy levels and wave functions) first appear in the second-order equations. In this order KL obtain a complicated equation which may be written in the form

$$0=\langle C_{\mathbf{k}}\rangle+\sum_{\mathbf{k}'(\neq\mathbf{k})}[\langle C_{\mathbf{k}\mathbf{k}'}H'_{\mathbf{k}'\mathbf{k}}\rangle/d_{\mathbf{k}\mathbf{k}'}{}^{-}-\text{c.c.}]+i\sum_{\mathbf{k}'}{}'\,[W_2(\mathbf{k},\mathbf{k}')+W_3(\mathbf{k},\mathbf{k}')+U(\mathbf{k},\mathbf{k}')][\langle f\rangle_{\mathbf{k}}-\langle f\rangle_{\mathbf{k}'}]$$
$$+\sum_{\mathbf{k}'}{}'\,(\langle f\rangle_{\mathbf{k}}-\langle f\rangle_{\mathbf{k}'})\left\{\frac{\langle|H'_{\mathbf{k}\mathbf{k}'}|^2\rangle}{d_{\mathbf{k}\mathbf{k}'}{}^{-}}\left[1+\frac{1}{d_{\mathbf{k}\mathbf{k}'}{}^{-}}\left(\sum_{\mathbf{k}''}{}'\,\frac{\langle|H'_{\mathbf{k}'\mathbf{k}''}|^2\rangle}{d_{\mathbf{k}\mathbf{k}''}{}^{-}}-\sum_{\mathbf{k}''}{}'\,\frac{\langle|H'_{\mathbf{k}\mathbf{k}''}|^2\rangle}{d_{\mathbf{k}\mathbf{k}''}{}^{+}}\right)\right]-\text{c.c.}\right\}$$
$$-\sum_{\mathbf{k}'\mathbf{k}''}{}'\,(\langle f\rangle_{\mathbf{k}'}-\langle f\rangle_{\mathbf{k}''})\langle|H'_{\mathbf{k}\mathbf{k}'}|^2\rangle\langle|H'_{\mathbf{k}'\mathbf{k}''}|^2\rangle[1/(d_{\mathbf{k}\mathbf{k}'}{}^{-}d_{\mathbf{k}\mathbf{k}''}{}^{-}d_{\mathbf{k}'\mathbf{k}''}{}^{-})-\text{c.c.}], \quad (27)$$

where $C=[\rho,H_F]$, $\langle C_{\mathbf{k}}\rangle=[\langle\rho\rangle,H_F]_{\mathbf{k}}=ie\boldsymbol{\mathcal{E}}\cdot\nabla_{\mathbf{k}}\langle\rho\rangle_{\mathbf{k}}$, and

$$\sum_{\mathbf{k}'}{}'\left[\frac{\langle C_{\mathbf{k}\mathbf{k}'}H'_{\mathbf{k}'\mathbf{k}}\rangle}{d_{\mathbf{k}\mathbf{k}'}{}^{-}}-\text{c.c.}\right]=2ie\boldsymbol{\mathcal{E}}\cdot\sum_{\mathbf{k}'}{}'\,P\frac{\langle|H'_{\mathbf{k}\mathbf{k}'}|^2\rangle}{\omega_{\mathbf{k}\mathbf{k}'}}(\nabla_{\mathbf{k}}+\nabla_{\mathbf{k}'})\frac{f_0(E_{\mathbf{k}})-f_0(E_{\mathbf{k}'})}{\omega_{\mathbf{k}\mathbf{k}'}}; \quad (28)$$

W_2, W_3, and U are the transition rates defined in (14)–(16).

In their treatment, KL reduce (27) to a slightly simpler form, which, however, is still very complicated. Since the conductivity (18) obtained from the Green's-function calculation resembles the result obtainable from an appropriate Boltzmann equation for quasiparticles, one would expect that (27) could be reduced to a Boltzmann form by rewriting it in terms of a quasiparticle description.

A simple method of introducing a quasiparticle distribution function is to recast the expression (5)

$$\mathcal{J}=(e/\Omega)\sum_{\mathbf{k}}\nabla_{\mathbf{k}}E_{\mathbf{k}}\langle f\rangle_{\mathbf{k}} \quad (29)$$

for the current, which involves the free-electron velocity, into a form in which the quasiparticle velocity appears, i.e., we define a distribution function $\mathfrak{F}_{\mathbf{k}}$ such that the current is given by

$$\mathcal{J}=(e/\Omega)\sum_{\mathbf{k}}\nabla_{\mathbf{k}}\epsilon_{\mathbf{k}}\mathfrak{F}_{\mathbf{k}}. \quad (30)$$

But the equation connecting the quasiparticle and free-electron velocities is

$$\nabla_{\mathbf{k}}\epsilon_{\mathbf{k}}=\nabla_{\mathbf{k}}E_{\mathbf{k}}-\tfrac{1}{2}\sum_{\mathbf{k}'}{}'\,\langle|H'_{\mathbf{k}\mathbf{k}'}|^2\rangle$$
$$\times[1/(d_{\mathbf{k}\mathbf{k}'}{}^{-})^2+1/(d_{\mathbf{k}\mathbf{k}'}{}^{+})^2](\nabla_{\mathbf{k}}E_{\mathbf{k}}-\nabla_{\mathbf{k}'}E_{\mathbf{k}'}), \quad (31)$$

which may be derived from the definition $\epsilon_{\mathbf{k}}=E_{\mathbf{k}}+\Delta_{\mathbf{k}}(E_{\mathbf{k}})$ by differentiating (11), making use of the relation $\nabla_{\mathbf{k}}V_{\mathbf{k}\mathbf{k}'}=-\nabla_{\mathbf{k}'}V_{\mathbf{k}\mathbf{k}'}$, and then dropping surface terms of the form[27]

$$\sum_{\mathbf{k}'}\nabla_{\mathbf{k}'}[\langle|H'_{\mathbf{k}\mathbf{k}'}|^2\rangle(1/d_{\mathbf{k}\mathbf{k}'}{}^{+}+1/d_{\mathbf{k}\mathbf{k}'}{}^{-})].$$

From (31) it is apparent that (30) will hold for an $\mathfrak{F}_{\mathbf{k}}$ defined by

$$\langle f\rangle_{\mathbf{k}}=\mathfrak{F}_{\mathbf{k}}-\tfrac{1}{2}\sum_{\mathbf{k}'}{}'\,\langle|H'_{\mathbf{k}\mathbf{k}'}|^2\rangle$$
$$\times[1/(d_{\mathbf{k}\mathbf{k}'}{}^{-})^2+1/(d_{\mathbf{k}\mathbf{k}'}{}^{+})^2](\mathfrak{F}_{\mathbf{k}}-\mathfrak{F}_{\mathbf{k}'}). \quad (32)$$

This equation is the formula for f corresponding to the relation (51) between the equilibrium quantities $\langle\rho\rangle_{\mathbf{k}}$ and $f_0(\epsilon_{\mathbf{k}})$ (note $\rho_T=\rho+f$). $\mathfrak{F}_{\mathbf{k}}$ may therefore be interpreted as the field-dependent part of the quasiparticle distribution function.

The reduction of (27) to a Boltzmann form is comparatively straightforward if the quasiparticle and propagator formalism of III is used as a guide. Since the calculation is somewhat tedious, only a brief outline is given here.[22] From (27) and (28) we have for the explicitly field-dependent part of the KL transport equation

$$X_{\mathbf{k}}=ie\boldsymbol{\mathcal{E}}\cdot\nabla_{\mathbf{k}}\langle\rho\rangle_{\mathbf{k}}+\tfrac{1}{2}ie\boldsymbol{\mathcal{E}}\cdot\sum_{\mathbf{k}'}{}'\,\langle|H'_{\mathbf{k}\mathbf{k}'}|^2\rangle\left(\frac{1}{d_{\mathbf{k}\mathbf{k}'}{}^{-}}+\frac{1}{d_{\mathbf{k}\mathbf{k}'}{}^{+}}\right)(\nabla_{\mathbf{k}}+\nabla_{\mathbf{k}'})\left\{[f_0(E_{\mathbf{k}})-f_0(E_{\mathbf{k}'})]\left(\frac{1}{d_{\mathbf{k}\mathbf{k}'}{}^{-}}+\frac{1}{d_{\mathbf{k}\mathbf{k}'}{}^{+}}\right)\right\}. \quad (33)$$

After making use of (51), differentiating, dropping surface terms, and rearranging, we find

$$X_{\mathbf{k}}=ie\boldsymbol{\mathcal{E}}\cdot\nabla_{\mathbf{k}}\epsilon_{\mathbf{k}}f_0'(\epsilon_{\mathbf{k}})+\tfrac{1}{2}ie\boldsymbol{\mathcal{E}}\cdot\sum_{\mathbf{k}'}{}'\,\langle|H'_{\mathbf{k}\mathbf{k}'}|^2\rangle\left[\frac{1}{(d_{\mathbf{k}\mathbf{k}'}{}^{-})^2}+\frac{1}{(d_{\mathbf{k}\mathbf{k}'}{}^{+})^2}\right][\nabla_{\mathbf{k}}f_0(E_{\mathbf{k}})-\nabla_{\mathbf{k}'}f_0(E_{\mathbf{k}'})]$$
$$+\sum_{\mathbf{k}'}{}'\,\langle|H'_{\mathbf{k}\mathbf{k}'}|^2\rangle\frac{s^2}{(\omega_{\mathbf{k}\mathbf{k}'}{}^2+s^2)^2}\left[\nabla_{\mathbf{k}}f_0(E_{\mathbf{k}})-\nabla_{\mathbf{k}'}f_0(E_{\mathbf{k}'})-\frac{f_0(E_{\mathbf{k}})-f_0(E_{\mathbf{k}'})}{\omega_{\mathbf{k}\mathbf{k}'}}(\nabla_{\mathbf{k}}E_{\mathbf{k}}-\nabla_{\mathbf{k}'}E_{\mathbf{k}'})\right]. \quad (34)$$

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[27] The neglect of these surface terms is certainly justified for the special case of the screened Coulomb potential, since $|H_{\mathbf{k}\mathbf{k}'}|^2(1/d_{\mathbf{k}\mathbf{k}'}{}^{-}+1/d_{\mathbf{k}\mathbf{k}'}{}^{+})$ vanishes at least as fast as $|\mathbf{k}'|^{-6}$ for $|\mathbf{k}'|$ large.

The third term on the right of (34) vanishes in the limit of small s, since the integrand has a zero at $\omega_{\mathbf{kk}'}=0$. The first term is the field-dependent term which one would expect in a Boltzmann equation for the quasiparticles. The second term should not appear in the final result; we shall show that it can be absorbed into the collision term of the Boltzmann equation.

If (32) and (34) are substituted into (27), the transport equation becomes

$$0=ie\boldsymbol{\mathcal{E}}\cdot\nabla_{\mathbf{k}}\epsilon_{\mathbf{k}}f_0'(\epsilon_{\mathbf{k}})+i\sum_{\mathbf{k}'}{}'\,[W_2(\mathbf{k},\mathbf{k}')+W_3(\mathbf{k},\mathbf{k}')+U(\mathbf{k},\mathbf{k}')](\mathcal{F}_{\mathbf{k}}-\mathcal{F}_{\mathbf{k}'})+R_{\mathbf{k}}\,, \tag{35}$$

where

$$\begin{aligned}R_{\mathbf{k}}=\sum_{\mathbf{k}'}{}'\,(\mathcal{F}_{\mathbf{k}}-\mathcal{F}_{\mathbf{k}'})&\left\{\frac{\langle|H'_{\mathbf{kk}'}|^2\rangle}{d_{\mathbf{kk}'}^-}\left[1+\frac{1}{d_{\mathbf{kk}'}^-}\left(\sum_{\mathbf{k}''}{}'\,\frac{\langle|H'_{\mathbf{k}'\mathbf{k}''}|^2\rangle}{d_{\mathbf{kk}''}^-}-\sum_{\mathbf{k}''}{}'\,\frac{\langle|H'_{\mathbf{kk}''}|^2\rangle}{d_{\mathbf{kk}''}^+}\right)\right]-\text{c.c.}\right\}\\
&-\sum_{\mathbf{k}'\mathbf{k}''}{}'\,(\mathcal{F}_{\mathbf{k}'}-\mathcal{F}_{\mathbf{k}''})\langle|H'_{\mathbf{kk}'}|^2\rangle\langle|H'_{\mathbf{k}'\mathbf{k}''}|^2\rangle[1/(d_{\mathbf{kk}'}^-d_{\mathbf{kk}''}^-d_{\mathbf{k}'\mathbf{k}''}^-)-\text{c.c.}]\\
&+\tfrac{1}{2}ie\boldsymbol{\mathcal{E}}\cdot\sum_{\mathbf{k}'}{}'\,\langle|H'_{\mathbf{kk}'}|^2\rangle[1/(d_{\mathbf{kk}'}^-)^2+1/(d_{\mathbf{kk}'}^+)^2][\nabla_{\mathbf{k}}f_0(E_{\mathbf{k}})-\nabla_{\mathbf{k}'}f_0(E_{\mathbf{k}'})]\\
&-i\sum_{\mathbf{k}'\mathbf{k}''}{}'\,(\mathcal{F}_{\mathbf{k}}-\mathcal{F}_{\mathbf{k}''})\langle|H'_{\mathbf{kk}'}|^2\rangle\langle|H'_{\mathbf{kk}''}|^2\rangle[1/(d_{\mathbf{kk}''}^-)^2+1/(d_{\mathbf{kk}''}^+)^2]\pi\delta(\omega_{\mathbf{kk}'})\\
&\qquad+i\sum_{\mathbf{k}'\mathbf{k}''}{}'\,(\mathcal{F}_{\mathbf{k}'}-\mathcal{F}_{\mathbf{k}''})\langle|H'_{\mathbf{kk}'}|^2\rangle\langle|H'_{\mathbf{k}'\mathbf{k}''}|^2\rangle[1/(d_{\mathbf{k}'\mathbf{k}''}^-)^2+1/(d_{\mathbf{k}'\mathbf{k}''}^+)^2]\pi\delta(\omega_{\mathbf{kk}'})+O(\lambda^3)\,.\end{aligned} \tag{36}$$

The KL transport equation will reduce to the appropriate Boltzmann equation if

$$R_{\mathbf{k}}=i\sum_{\mathbf{k}'}{}'\,W_1(\mathbf{k},\mathbf{k}')(\mathcal{F}_{\mathbf{k}}-\mathcal{F}_{\mathbf{k}'})+O(\lambda^3)\,, \tag{37}$$

where W_1, defined by (13), is the first-Born-approximation transition probability per unit time for incoherent scattering of the quasiparticles by the impurities. To prove (37) we first note, from (7), (10), and (13), that W_1 is related to the quasiparticle spectral distribution $\langle A(\mathbf{k}',\mathbf{k}';\epsilon_{\mathbf{k}})\rangle$ and hence to the propagators $\langle G(\mathbf{k}';\epsilon_{\mathbf{k}}\pm is)\rangle$. To order λ^2, $\langle G\rangle$ may be expanded as

$$\langle G(\mathbf{k}';\epsilon_{\mathbf{k}}\pm is)\rangle=(1/d_{\mathbf{kk}'}^{\pm})\{1+(1/d_{\mathbf{kk}'}^{\pm})[\Delta_{\mathbf{k}'}(E_{\mathbf{k}})-\Delta_{\mathbf{k}}(E_{\mathbf{k}})\mp i\Gamma_{\mathbf{k}'}(E_{\mathbf{k}})]+O(\lambda^3)\}\,, \tag{38}$$

where both the dressing function

$$\Delta_{\mathbf{k}}(\omega)=\sum_{\mathbf{k}'}P\langle|H'_{\mathbf{kk}'}|^2\rangle/\omega_{\mathbf{kk}'}$$

and the width function

$$\Gamma_{\mathbf{k}}(\omega)=\pi\sum_{\mathbf{k}'}\langle|H'_{\mathbf{kk}'}|^2\rangle\delta(\omega-E_{\mathbf{k}'})$$

are of order λ^2.

In order to recast (36) into a form in which the expansion of $\langle G\rangle$ can be identified, it is necessary to eliminate the electric-field-dependent terms and to find an interpretation for the term containing $1/d_{\mathbf{kk}'}^-d_{\mathbf{kk}''}^-d_{\mathbf{k}'\mathbf{k}''}^-$. The field-dependent terms can be eliminated by using the zeroth-order Boltzmann equatian (26) and then noting that, to the order in λ of interest, the zeroth-order distribution function may be replaced by $\mathcal{F}_{\mathbf{k}}$. If we now use the identity

$$\frac{1}{d_{\mathbf{kk}'}^-d_{\mathbf{kk}''}^-d_{\mathbf{k}'\mathbf{k}''}^-}-\text{c.c.}=\pi i[\delta(\omega_{\mathbf{k}'\mathbf{k}''})-\delta(\omega_{\mathbf{kk}''})]\left[\frac{1}{(d_{\mathbf{kk}'}^-)^2}+\frac{1}{(d_{\mathbf{kk}'}^+)^2}\right]+\pi i\delta(\omega_{\mathbf{kk}'})\left[\frac{1}{(d_{\mathbf{k}'\mathbf{k}''}^-)^2}+\frac{1}{(d_{\mathbf{k}'\mathbf{k}''}^+)^2}\right], \tag{39}$$

which is valid in the limit of small s, and introduce the dressing function Δ, the differentiated dressing function $\Delta_{\mathbf{k}}'(E_{\mathbf{k}})$, and the width function Γ, $R_{\mathbf{k}}$ can be rewritten as

$$\begin{aligned}R_{\mathbf{k}}=\sum_{\mathbf{k}'}\mathcal{F}_{\mathbf{k}}&\left\{\frac{\langle|H'_{\mathbf{kk}'}|^2\rangle}{d_{\mathbf{kk}'}^-}\left[1+\frac{1}{d_{\mathbf{kk}'}^-}[\Delta_{\mathbf{k}'}(E_{\mathbf{k}})-\Delta_{\mathbf{k}}(E_{\mathbf{k}})+i\Gamma_{\mathbf{k}'}(E_{\mathbf{k}})]\right]-\text{c.c.}\right\}\\
&-\sum_{\mathbf{k}'}\mathcal{F}_{\mathbf{k}'}\left\{\frac{\langle|H'_{\mathbf{kk}'}|^2\rangle}{d_{\mathbf{kk}'}^-}\left[1+\frac{1}{d_{\mathbf{kk}'}^-}\left[\Delta_{\mathbf{k}'}(E_{\mathbf{k}})-\Delta_{\mathbf{k}}(E_{\mathbf{k}})+i\pi\sum_{\mathbf{k}''}\frac{\mathcal{F}_{\mathbf{k}''}}{\mathcal{F}_{\mathbf{k}'}}\langle|H'_{\mathbf{k}'\mathbf{k}''}|^2\rangle\delta(\omega_{\mathbf{kk}''})\right]\right]-\text{c.c.}\right\}\\
&\qquad+i\Delta_{\mathbf{k}}'(E_{\mathbf{k}})\sum_{\mathbf{k}'}2\pi\langle|H'_{\mathbf{kk}'}|^2\rangle\delta(\omega_{\mathbf{kk}'})(\mathcal{F}_{\mathbf{k}}-\mathcal{F}_{\mathbf{k}'})+O(\lambda^3)\,.\end{aligned} \tag{40}$$

To the relevant order in λ, the free-electron first-Born-approximation transition probability $2\pi\langle|H'_{\mathbf{kk}'}|^2\rangle\delta(\omega_{\mathbf{kk}'})$ may be replaced by the quasiparticle first Born term W_1. By analogy with the expansion of $\langle G\rangle$, we can rewrite (40) in the form

$$R_{\mathbf{k}}=\sum_{\mathbf{k}'}\mathfrak{F}_{\mathbf{k}}\langle|H'_{\mathbf{kk}'}|^2\rangle\{1/[\epsilon_{\mathbf{k}}-E_{\mathbf{k}'}-\Delta_{\mathbf{k}'}(E_{\mathbf{k}})-i\Gamma_{\mathbf{k}'}(E_{\mathbf{k}})]-\text{c.c.}\}$$
$$-\sum_{\mathbf{k}'}\mathfrak{F}_{\mathbf{k}'}\langle|H'_{\mathbf{kk}'}|^2\rangle\{1/[\epsilon_{\mathbf{k}}-E_{\mathbf{k}'}-\Delta_{\mathbf{k}'}(E_{\mathbf{k}})-i\pi\sum_{\mathbf{k}''}(\mathfrak{F}_{\mathbf{k}''}/\mathfrak{F}_{\mathbf{k}'})\langle|H'_{\mathbf{k}'\mathbf{k}''}|^2\rangle\delta(\omega_{\mathbf{kk}''})]-\text{c.c.}\}$$
$$+i\Delta_{\mathbf{k}}'(E_{\mathbf{k}})\sum_{\mathbf{k}'}W_1(\mathbf{k},\mathbf{k}')(\mathfrak{F}_{\mathbf{k}}-\mathfrak{F}_{\mathbf{k}'})+O(\lambda^3).\quad(41)$$

If we assume, as in Sec. III, that the imaginary parts of the denominators in (41) are small, the functions $\langle G\rangle-\text{c.c.}$ and

$$[\epsilon_{\mathbf{k}}-E_{\mathbf{k}'}-\Delta_{\mathbf{k}'}(E_{\mathbf{k}})-i\pi\sum_{\mathbf{k}''}(\mathfrak{F}_{\mathbf{k}''}/\mathfrak{F}_{\mathbf{k}'})\langle|H'_{\mathbf{k}'\mathbf{k}''}|^2\rangle\delta(\omega_{\mathbf{kk}''})]^{-1}-\text{c.c.}$$

may be replaced by the equivalent energy-conserving δ function $2\pi i\delta(\epsilon_{\mathbf{k}}-\epsilon_{\mathbf{k}'})/[1-\Delta_{\mathbf{k}'}'(E_{\mathbf{k}'})]$, and hence (41) reduces to the required form (37). It is of interest to note that the natural width of the δ function corresponding to scattering out of the initial-state $\mathbf{k}$ is determined by the "forward-scattering" width function

$$\Gamma_{\mathbf{k}'}=\tfrac{1}{2}\sum_{\mathbf{k}''}2\pi\langle|H'_{\mathbf{k}'\mathbf{k}''}|^2\rangle\delta(\omega_{\mathbf{kk}''}),$$

while that for the scattering into the state $\mathbf{k}$ is determined by the "back-scattering" width function

$$\Gamma_{\mathbf{k}'}{}^{b}=\tfrac{1}{2}\sum_{\mathbf{k}''}2\pi\langle|H'_{\mathbf{k}'\mathbf{k}''}|^2\rangle\delta(\omega_{\mathbf{kk}''})\cos\theta_{\mathbf{k}'\mathbf{k}''}.$$

An analogous result has been found[22] in the Green's-function calculation.

On substituting (37) into (35), we find that the second-order KL transport equation reduces to the quasiparticle Boltzmann equation

$$0=e\mathcal{E}\cdot\nabla_{\mathbf{k}}\epsilon_{\mathbf{k}}f_0'(\epsilon_{\mathbf{k}})+\sum_{\mathbf{k}'}[W_1(\mathbf{k},\mathbf{k}')+W_2(\mathbf{k},\mathbf{k}')+W_3(\mathbf{k},\mathbf{k}')+U(\mathbf{k},\mathbf{k}')](\mathfrak{F}_{\mathbf{k}}-\mathfrak{F}_{\mathbf{k}'}).\quad(42)$$

For the special case of an isotropic system this equation may be solved for $\mathfrak{F}_{\mathbf{k}}$, the result being

$$\mathfrak{F}_{\mathbf{k}}=-e\mathcal{E}\cdot\nabla_{\mathbf{k}}\epsilon_{\mathbf{k}}f_0'(\epsilon_{\mathbf{k}})\tau(\mathbf{k}),\quad(43)$$

where $\tau(\mathbf{k})$ is the relaxation time defined by (19). After substituting (43) into (30) and introducing the extra spin factor of 2, we obtain the identical conductivity formula (18) resulting from the Green's-function calculation. Thus, the decoupling assumption and the KL assumption of $f_{\mathbf{k}}\sim\lambda^{-2}$ for $s\rightarrow 0$ lead to the correct result for the conductivity of the isotropic system.

V. DISCUSSION

As mentioned above, two assumptions are made in the transport equation approach which prevent it from being a completely self-contained theory. We have seen that these assumptions lead to the correct conductivity for an isotropic system, but it is not completely clear why they do or whether they also lead to correct results for an anisotropic system. These points may be clarified by developing an expansion of the Van Hove $\lambda^2t(\equiv\lambda^2/s)$ type for $f_{\mathbf{k}}$ and $f_{\mathbf{kk}'}$. The Van Hove expansions are obtained by examining (21) and (22) for finite s and arbitrary λ^2/s. In lowest order, $f_{\mathbf{k}}$ and $f_{\mathbf{kk}'}$ then go, respectively, as λ^0 and λ. On iterating, we find that $f_{\mathbf{kk}'}$ can be written as a sum of off-diagonal products of the H' impurity matrix elements of the form $H'(\mathbf{kk}'\mathbf{k}''\cdots\mathbf{k}^{(n)})$. The average of each of these off-diagonal products vanishes, and hence we can prove rigorously that $\langle f\rangle_{\mathbf{kk}'}=0$. We also find that $f_{\mathbf{k}}$ can be written as a sum of diagonal products of the H' elements i.e., of products $H'(\mathbf{kk}'\mathbf{k}''\cdots\mathbf{k}^{(m)}\mathbf{k})$. The validity of the decoupling assumption (25) can then be seen to depend on the result, which may easily be proved,[28] that

$$\langle H'(\mathbf{kk}'\cdots\mathbf{k}^{(i)}\cdots\mathbf{k}^{(n)}\mathbf{k})H'(\mathbf{k}^{(i)}\mathbf{k}_1\cdots\mathbf{k}\cdots\mathbf{k}_r)\rangle$$
$$=\langle H'(\mathbf{kk}'\cdots\mathbf{k}^{(i)}\cdots\mathbf{k}^{(n)}\mathbf{k})\rangle\langle H'(\mathbf{k}^{(i)}\mathbf{k}_1\cdots\mathbf{k}\cdots\mathbf{k}_r)\rangle$$
$$\times[1+0(\Omega^{-1})].\quad(44)$$

This result is closely related to the diagonal singularity condition of Van Hove,[12] which requires that diagonal products be an order of N higher than off-diagonal products. These results hold for both the anisotropic and the isotropic cases.

In general, the Van Hove expansions may be regrouped and the Boltzmann equation (42) recovered. Thus the KL approach must also be valid for an anisotropic system.

The existence of the Boltzmann equation (42) means that a variational principle of the Kohler type must exist.[15,22] This principle should be of importance in estimating the quantum conductivity of anisotropic materials.

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[28] Appendix A of Ref. 22.

APPENDIX: MOMENTUM MATRIX ELEMENTS

For the various parts of the Hamiltonian H_T we have

$$H_{0\mathbf{kk}'}=E_{\mathbf{k}}\delta_{\mathbf{kk}'}=\delta_{\mathbf{kk}'}(k_x^2/2m_x+k_y^2/2m_y+k_z^2/2m_z)\,, \tag{45}$$

$$H_{F\mathbf{kk}'}=-e\mathbf{\mathcal{E}}\cdot\mathbf{r}_{\mathbf{kk}'}e^{st}=-ie\mathbf{\mathcal{E}}\cdot\nabla_{\mathbf{k}}\delta_{\mathbf{kk}'}e^{st}=ie\mathbf{\mathcal{E}}\cdot\nabla_{\mathbf{k}'}\delta_{\mathbf{kk}'}e^{st}\,, \tag{46}$$

and

$$H'_{\mathbf{kk}'}=\frac{\lambda}{\Omega}\sum_{j=1}^{N}e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_j}V_{\mathbf{kk}'}\,, \tag{47}$$

with

$$V_{\mathbf{kk}'}=\int_{\Omega}V(\mathbf{r})e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}}d\mathbf{r}\,. \tag{48}$$

The diagonal elements $H'_{\mathbf{kk}}$ are independent of $\mathbf{k}$ and, by a redefinition of the energy zero, can be set equal to zero. The matrix elements of the current-density operator are

$$\mathbf{J}_{\mathbf{kk}'}(\mathbf{r})=(e/2m\Omega)(\mathbf{k}+\mathbf{k}')\exp[-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}]\,. \tag{49}$$

With the exception of $H'_{\mathbf{kk}'}$, all of the above matrix elements are independent of the impurity positions and of λ.

To order λ^2 the equilibrium density matrix is given by

$$\begin{aligned}\rho_{\mathbf{kk}'}=\delta_{\mathbf{kk}'}&\left\{f_0(E_{\mathbf{k}})\left(\sum_{\mathbf{k}''}P\frac{|H'_{\mathbf{kk}''}|^2}{\omega_{\mathbf{kk}''}}\right)-\sum_{\mathbf{k}''}P\frac{|H'_{\mathbf{kk}''}|^2}{\omega_{\mathbf{kk}''}}\frac{f_0(E_{\mathbf{k}})-f_0(E_{\mathbf{k}''})}{\omega_{\mathbf{kk}''}}\right\}\\&+[1-\delta_{\mathbf{kk}'}]\left\{H'_{\mathbf{kk}'}\frac{f_0(E_{\mathbf{k}})-f_0(E_{\mathbf{k}'})}{\omega_{\mathbf{kk}'}}-\sum_{\mathbf{k}''}\frac{H'(\mathbf{kk}''\mathbf{k}')}{\omega_{\mathbf{k}''\mathbf{k}}}\left[\frac{f_0(E_{\mathbf{k}})-f_0(E_{\mathbf{k}'})}{\omega_{\mathbf{kk}'}}-\frac{f_0(E_{\mathbf{k}})-f_0(E_{\mathbf{k}''})}{\omega_{\mathbf{kk}''}}\right]\right\}\,,\end{aligned} \tag{50}$$

where P indicates principal value, $f_0(E_{\mathbf{k}})=\exp[\beta(E_{\mathbf{k}}-\mu_0)+1]^{-1}$ is the Fermi distribution for the free electrons, $\omega_{\mathbf{kk}'}=E_{\mathbf{k}}-E_{\mathbf{k}'}$ is an energy difference, and $H'(\mathbf{kk}_1\mathbf{k}_2)=H'_{\mathbf{kk}_1}H'_{\mathbf{k}_1\mathbf{k}_2}$. When the average of (50) over an ensemble of solids with random impurity distributions is taken, the off-diagonal terms vanish and the diagonal terms can be written in the concise form

$$\langle\rho\rangle_{\mathbf{k}}=f_0(\epsilon_{\mathbf{k}})-A_{\mathbf{k}}\,, \tag{51}$$

where

$$f_0(\epsilon_{\mathbf{k}})=[\exp\beta(\epsilon_{\mathbf{k}}-\mu)+1]^{-1}=f_0(E_{\mathbf{k}})\left\{1-\beta N\frac{\lambda^2}{\Omega^2}\sum_{\mathbf{k}'}P\frac{|V_{\mathbf{kk}'}|^2}{\omega_{\mathbf{kk}'}}+\beta\sum_{\mathbf{k}_1}f_0(E_{\mathbf{k}_1})N\frac{\lambda^2}{\Omega^2}\sum_{\mathbf{k}_2}P\frac{|V_{\mathbf{k}_1\mathbf{k}_2}|^2}{\omega_{\mathbf{k}_1\mathbf{k}_2}}\right\}+O(\lambda^3) \tag{52}$$

is the Fermi distribution for the quasiparticles of energy $\epsilon_{\mathbf{k}}$. The second term in (51) is given by

$$A_{\mathbf{k}}=N\frac{\lambda^2}{\Omega^2}\sum_{\mathbf{k}'}P\frac{|V_{\mathbf{kk}'}|^2}{\omega_{\mathbf{kk}'}}\frac{f_0(E_{\mathbf{k}})-f_0(E_{\mathbf{k}'})}{\omega_{\mathbf{kk}'}}\,. \tag{53}$$

At first sight one might expect the Fermi distribution for the quasiparticles to be equal to the averaged equilibrium distribution $\langle\rho\rangle_{\mathbf{k}}$. However, this cannot be the case, since $\langle\rho\rangle_{\mathbf{k}}$ is taken with respect to the plane-wave (free-electron) states rather than the quasiparticle states.