

## Discussion of a new theory of electrical resistivity\*

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A discussion is given of the details of our work, the results of which have recently been presented, in connection with the role of projection techniques in the theory of electrical resistivity. It is shown that, contrary to earlier claims, the correct evaluation of the resistivity to the lowest order in the strength of the scattering on the basis of this theory requires, as do other formal expressions, the summation of an infinite number of terms. This leads to the standard expression for the conductivity in terms of the distribution function obtained from the well-known integral transport equation. It is shown in complete generality that the evaluation of this new expression for the electrical resistivity is equivalent to that given by the method of kinetic equations.

### I. INTRODUCTION

Recently, Mori<sup>1</sup> has presented a general theory of irreversible processes, basing his formulation on the use of some general projection operators. In this paper we study the specific problem of electrical conduction in solids by the introduction of a projection operator analogous to those used by Mori.<sup>1</sup>

The problem of electrical conduction in solids has been studied by a large number of theoretical methods.<sup>2-18</sup> Although the techniques differ, they all require<sup>19</sup> the solution of an integral equation, which in the lowest approximation for the scattering and for a weak, homogeneous, and static electric field is identical to the Boltzmann-Bloch transport equation, first proposed by Bloch and Nordheim.<sup>20</sup> The most direct method that leads to this transport equation is the method of kinetic equations.<sup>4,13,15,18</sup>

The introduction of a projection operator of the Mori type yields<sup>21-23</sup> an expression for the conductivity that is different from all the earlier ones, in that all indicated operations in it are performed in the denominator, i. e., it yields a formal expression for the resistivity. The derivation of this expression is given in Sec. II, where it is also shown directly that it is equivalent to the standard formal expression<sup>3</sup> for the conductivity, as it should be. This expression provides the basis for our subsequent study.

The question naturally arises whether this new expression presents any advantages for the practical calculation of the conductivity. This question is examined in Sec. III for a simple system, and for special conditions. It is shown there that for the system under consideration the correct handling of this expression leads to an integral equation for a distribution function that is identical to the standard transport equation for the system. This study thus corrects the erroneous claims made by Kenkre and Dresden<sup>21</sup> and by Kenkre<sup>22</sup> for the prac-

tical usefulness of the new expression for the conductivity.

In Sec. IV we consider the case of electrons in random impurities under general conditions. We show that the new expression for the conductivity in terms of the Mori-type projection operator is entirely equivalent to the one obtained by the method of kinetic equations,<sup>15</sup> which is based on the use of a different projection operator.

From the discussion in Sec. V and the work in Appendices A and B it becomes evident that the method of kinetic equations<sup>13</sup> offers a more direct and simple way for the calculation of the conductivity.

### II. RESISTIVITY IN TERMS OF A PROJECTION OPERATOR

We derive<sup>23</sup> here a formal expression for the resistivity of a system in terms of a projection operator, similar to the one used by Mori<sup>1</sup> in a different context. It will become evident that this method can be used for any transport coefficient.

In order to avoid unnecessary generalities, however, we consider a system of  $N$  electrons in volume  $\Omega$  driven by a uniform electric field  $E(t) = Ee^{-i\omega t} + c. c.$ , of frequency  $\omega$  and in a particular direction, and study the steady-state linear current density in the direction of the field. The Hamiltonian of the unperturbed system is denoted by  $H$ , while its interaction with the electric field is given by  $(-eE)(re^{-i\omega t} + H. c.)$ , where  $r$  is the sum of the components of the position operators for all the electrons in the direction of the field ( $r = \sum_i r_i$ ).

The conductivity can then be written in the form

$$\sigma(\omega) = \left( -\frac{e^2}{\Omega} \right) \text{Tr} v \rho(\omega). \quad (2.1)$$

Here  $v$  is the sum of the components, in the direction of the field, of the velocities of all the electrons, and  $\rho(\omega)$  is the steady-state density operator linear in  $E$  with the factor  $(-eE)$  removed. To de-

termine  $\rho(\omega)$  we consider the system prior to the application of the electric field at  $t=0$  to be in thermal equilibrium, its statistical density operator being denoted by  $f_0(H)$ . For  $t>0$  we then have for the density operator  $\rho(t)$  linear in  $E$  ( $\hbar=1$ )

$$\left(i \frac{d}{dt} - L\right) \rho(t) = D e^{-i\omega t} + \text{H. c.}, \quad (2.2a)$$

$$\rho(t \leq 0) = 0. \quad (2.2b)$$

Here  $L$  is the Liouville operator corresponding to the Hamiltonian  $H$ , i. e., for any operator  $X$

$$LX = [H, X], \quad (2.3)$$

and

$$D = [r, f_0(H)]. \quad (2.4)$$

The solution of (2.2) describes the complete time development of  $\rho(t)$  from  $t=0$  to any later time. After the thermodynamic limit is taken, i. e.,  $\Omega$  and  $N \rightarrow \infty$ , so that  $N/\Omega = n =$  electron density remains finite, the physical steady state is presumably described by

$$\rho(t) \xrightarrow[t \rightarrow \infty]{} \rho(\omega) e^{-i\omega t} + \text{H. c.} \quad (2.5)$$

A convenient method for studying the steady state is provided by the generalized Fourier transform, namely

$$\rho(z) = \int_0^\infty dt e^{izt} \rho(t), \quad (2.6)$$

with  $z$  in the upper half of the complex plane. According to (2.2),  $\rho(z)$  satisfies the equation

$$(z - L)\rho(z) = D \left( \frac{i}{z - \omega} + \frac{i}{z + \omega} \right), \quad (2.7)$$

with the formal solution

$$\rho(z) = G(z)D \left( \frac{i}{z - \omega} + \frac{i}{z + \omega} \right). \quad (2.8)$$

$G(z)$  is the propagator for the Liouville operator  $L$ , defined by

$$G(z) \equiv (z - L)^{-1}. \quad (2.9)$$

Now, since  $\rho(t \leq 0) = 0$ ,  $\rho(z)$  is analytic in the upper-half  $z$  plane above a line parallel to the real axis, while for  $t > 0$  we have

$$\rho(t) = \frac{1}{2\pi} \int_c dz e^{-izt} \rho(z). \quad (2.10)$$

The path of integration  $c$  consists of the line parallel to the real axis in the upper-half plane and an infinite semicircle in the lower-half plane. Evidently  $\rho(z)$  is the analytic continuation in the lower-half plane of the solution (2.8). From (2.8) we note that  $\rho(z)$  will have poles at  $z = \pm\omega$  on the real axis, plus additional singularities (branch cuts, etc.) from  $G(z)$ . The contributions to  $\rho(t)$ , as given by (2.10), of all singularities other than the simple

poles at  $z = \pm\omega$  are presumed to vanish for large times, if we first take the thermodynamic limit, as we should in order to avoid the quantum-mechanical equivalent of the Poincaré cycle for the system. We thus find for large times a steady state described by (2.5), where  $\rho(\omega)$ , according to (2.10) and the residue theorem, is  $(-i)$  times the residue of  $\rho(z)$ , as given by (2.8), at

$$z = \omega + i\epsilon \equiv \omega^*, \quad (2.11)$$

where  $\epsilon$  is a positive infinitesimal. It follows from (2.7) and (2.8) that  $\rho(\omega)$  satisfies the equation

$$(\omega^* - L)\rho(\omega) = D, \quad (2.12)$$

with the formal solution

$$\rho(\omega) = G(\omega^*)D. \quad (2.13)$$

This yields, with the use of (2.1) and (2.13), the formal expression for the conductivity,

$$\sigma(\omega) = \left( -\frac{e^2}{\Omega} \right) \text{Tr} v G(\omega^*)D. \quad (2.14)$$

The limit  $\epsilon \rightarrow 0^+$  is understood to be taken last, in particular after the limit  $\Omega \rightarrow \infty$ ,  $N \rightarrow \infty$ ,  $N/\Omega = n \rightarrow$  finite.

A different expression for  $\sigma(\omega)$  can be obtained<sup>23</sup> by the introduction of a projection operator  $P$ , similar to those used by Mori<sup>1</sup> in a different context. We define this time-independent linear projection operator by the relation

$$PX = D \frac{1}{a} \text{Tr} v X, \quad (2.15a)$$

$$a = \text{Tr} v D, \quad (2.15b)$$

where  $X$  is any operator and  $D$  is given by (2.4). The operator  $P$  exists provided only that  $\text{Tr} v D \neq 0$ . We note that as a direct consequence of this definition we have

$$PD = D, \quad (2.16a)$$

$$P'D \equiv (1 - P)D = 0. \quad (2.16b)$$

Equation (2.16b) defines  $P' \equiv 1 - P$ , with the properties  $P'P = PP' = 0$  and  $P'^2 = P'$ , just like  $P^2 = P$ . We also observe from (2.15a) and (2.1) that

$$P\rho(\omega) = D\sigma(\omega)(-e^2 a/\Omega)^{-1}. \quad (2.17)$$

Thus, in order to get an expression for  $\sigma(\omega)$  we construct an equation for  $P\rho(\omega)$  from (2.12). To accomplish this, we first introduce in (2.12) the splitting  $\rho(\omega) = P\rho(\omega) + P'\rho(\omega)$ , and then operate on it with  $P$  and  $P'$ , separately, to obtain, with the use of (2.16),

$$(\omega^* - PL)P\rho - PLP'\rho = D, \quad (2.18)$$

$$(\omega^* - P'L)P'\rho - P'LP\rho = 0. \quad (2.19)$$

Solving (2.19) for  $P'\rho$  in terms of  $P\rho$ , we get

$$P'\rho(\omega) = G'(\omega^*)P'LP\rho(\omega), \quad (2.20)$$

where we have introduced a new propagator

$$G'(z) \equiv (z - P'L)^{-1}. \quad (2.21)$$

Finally, if we substitute (2.20) into (2.18), we obtain for  $P\rho(\omega)$  the equation

$$\{\omega^* - PL[1 + G'(\omega^*)P'L]\}P\rho(\omega) = D. \quad (2.22)$$

We note that all the terms on the left-hand side of (2.22) are, according to (2.15a), simple scalar multiples of the operator  $D$ , and thus with the help of (2.17) it follows that

$$\sigma(\omega) = \left(-\frac{e^2 a}{\Omega}\right) \left(\omega^* - \frac{1}{a} \text{Tr}vL[1 + G'(\omega^*)P'L]D\right)^{-1}. \quad (2.23)$$

This can also be written in the equivalent form

$$\sigma(\omega) = \left(-\frac{e^2 a}{\Omega}\right) \frac{1}{\omega^*} \left(1 - \frac{1}{a} \text{Tr}vLG'(\omega^*)D\right)^{-1}, \quad (2.24)$$

since from the definition (2.21) of  $G'(\omega^*)$  we have  $1 + G'(\omega^*)P'L = \omega^*G'(\omega^*)$ .

Equations (2.23) and (2.24) are formal expressions for the conductivity  $\sigma(\omega)$ . They have the feature that the trace operations are carried out in the denominator; in other words, they are explicit expressions for the resistivity. In this respect they differ from the expression (2.14) for  $\sigma(\omega)$ , in which the trace operation is performed in the numerator. Thus, the projection operator  $P$  enables us to find formally the reciprocal of (2.14).

From their derivations it is obvious that expressions (2.23) and (2.24), involving the projection operator  $P$ , are equivalent to expression (2.14). This equivalence can be shown directly as follows. We note that the propagator  $G'(\omega^*) = (\omega^* - P'L)^{-1} = (\omega^* - L + PL)^{-1}$  is related to the propagator  $G(\omega^*) = (\omega^* - L)^{-1}$  by the relation

$$G'(\omega^*) = G(\omega^*) - G(\omega^*)PLG'(\omega^*). \quad (2.25)$$

Performing the operation  $\text{Tr}vL \dots D$  on both sides of (2.25) and making use of the definition of  $P$  on the right-hand side, we find an equation for  $\text{Tr}vLG'(\omega^*)D$  with the solution

$$\begin{aligned} \text{Tr}vLG'(\omega^*)D &= \text{Tr}vLG(\omega^*) \\ &\times D \left(1 + \frac{1}{a} \text{Tr}vLG(\omega^*)D\right)^{-1}. \end{aligned} \quad (2.26)$$

From the definition (2.9) of  $G(\omega^*)$  it follows immediately that  $LG(\omega^*) = \omega^*G(\omega^*) - 1$ , which when substituted in (2.26) gives

$$1 - \frac{1}{a} \text{Tr}vLG'(\omega^*)D = \frac{a}{\omega^*} (\text{Tr}vG(\omega^*)D)^{-1}. \quad (2.27)$$

Using this in expression (2.24), we immediately reobtain expression (2.14) for  $\sigma(\omega)$ . This proves directly the equivalence of (2.24) and (2.23) to

$$(2.14).$$

In Appendix A we describe some possible generalizations of the projection technique used in this section, e.g., how we can obtain similar expressions for all elements of the resistivity tensor and the distribution function.

### III. CALCULATION OF THE RESISTIVITY

In this section we examine to what extent expression (2.23), or (2.24), is useful in a practical calculation of the dc and ac resistivity. For concreteness we consider a system of dynamically independent electrons in a periodic potential and a set of fixed impurities, within the one-band approximation. We recall that since the electrons are noninteracting, the problem reduces<sup>4,13</sup> rigorously to a one-electron problem. Thus, the one-electron Hamiltonian of the system is  $H = H_0 + V(\vec{r})$ , where  $V(\vec{r})$  is the momentum-independent "scattering" potential and  $H_0$  commutes with  $\vec{p} = m\vec{v}$ , the momentum operator.  $v$  and  $r$  are now the one-electron velocity and position operators in the direction of the field, while  $f_0(H)$  is the Fermi-Dirac distribution function. This concrete system meets all the specifications of the system considered by Kenkre and Dresden<sup>21</sup> in a similar study.

It is clear that in the absence of scattering, the dc conductivity  $\sigma(0)$  is infinite for this system. If  $\lambda$  denotes the strength of the scattering interaction  $V$ , then  $\sigma(0) \propto \lambda^{-2}$ , to the lowest order in  $\lambda$ . If we use expression (2.14) to calculate  $\sigma(0)$  to order  $\lambda^{-2}$ , we must obviously sum an infinite subset of terms in the expansion of  $\sigma(0) \propto \text{Tr}vG(0^*)D$  in powers of  $\lambda$ . This has been done with the use of the van Hove "λ<sup>2</sup>t limit" technique,<sup>7,8,24</sup> or, equivalently, with the Green's-function technique.<sup>10,16</sup> Both methods<sup>19</sup> lead to the determination of a distribution function through an *integral* equation, which to the order of interest is identical to the Boltzmann-Bloch transport equation, first proposed by Bloch and Nordheim.<sup>20</sup>

It appears that expressions (2.23) and (2.24) give directly an expansion in powers of  $\lambda$ , for  $\sigma^{-1}(0)$ , and thus one might *expect* that  $\sigma^{-1}(0)$  to order  $\lambda^2$  is simply given by the lowest-order term of this expansion and that no summation of an infinite number of terms is necessary. Such an expectation has in fact been asserted<sup>21,22</sup> to be correct. If this assertion were correct, it would be of paramount importance, since one could then bypass the often difficult task of solving the integral transport equation.

We have pointed out,<sup>25</sup> however, that unfortunately this assertion is in error. The correct application of the expression (2.23), or (2.24), for the evaluation of  $\sigma(0)$  to order  $\lambda^{-2}$  requires the summation of an infinite number of divergent terms, and this unavoidably leads back to the integral trans-

port equation for the distribution function. We now show how this conclusion is reached.

For convenience we work with expression (2.24). If we define

$$L_0 X \equiv [H_0, X], \quad L_1 X \equiv [V, X], \quad (3.1)$$

this expression can be written for the system under consideration as

$$\sigma^{-1}(\omega) = \left(-\frac{e^2 n}{m}\right)^{-1} i\omega^* \left(1 - \frac{1}{a} K(\omega)\right), \quad (3.2)$$

where

$$K(\omega) = \text{Tr} v L_1 G'(\omega^*) D. \quad (3.3)$$

In arriving at (3.2) we have made use of the fact that for this system  $a = \text{Tr} v D = \text{Tr} [p, r] f_0(H)/m = -iN/m$  and  $L_0 v = 0$ , from which it follows that  $\text{Tr} v L_0 X = 0$ .

An expansion of  $K(\omega)$  in power series of  $\lambda$  can easily be obtained by expanding the propagator  $G'(\omega^*)$  and  $D$  in powers of  $V$ . We have

$$\begin{aligned} G'(\omega^*) &= (\omega^* - L_0 - P' L_1)^{-1} \\ &= G_0(\omega^*) + G_0(\omega^*) P' L_1 G_0(\omega^*) + \dots \end{aligned} \quad (3.4)$$

and

$$D = [r, f_0(H_0 + V)] = D^0 + D^1 + D^2 + \dots \quad (3.5)$$

The first equality in (3.4) follows from the fact that for the system under study  $P L_0 X \propto \text{Tr} v L_0 X = -\text{Tr} (L_0 v) X = 0$ , since  $L_0 v = 0$ . In (3.4) we have introduced the unperturbed propagator

$$G_0(\omega^*) \equiv (\omega^* - L_0)^{-1}. \quad (3.6)$$

We also note for later reference that for this system  $D^0 = [r, f_0(H_0)] = i v f_0'(H_0)$ , where  $f_0'(x) = df_0(x)/dx$ , and thus  $H_0$ ,  $v$ , and  $D^0$  commute with each other and in particular

$$L_0 D^0 = 0. \quad (3.7)$$

Substituting (3.4) and (3.5) in (3.3) and making use of  $\text{Tr} v L_1 D^0 = \text{Tr} [D^0, v] = 0$  and the definition  $P' = 1 - P$ , we have

$$K(\omega) = \text{Tr} v L_1 G_0(\omega^*) \left( D^1 + \frac{1}{\omega^*} L_1 D^0 \right) + O(\lambda^3). \quad (3.8)$$

The second term in (3.8) follows from the relation

$$G_0(\omega^*) D^0 = \frac{1}{\omega^*} D^0, \quad (3.9)$$

which is a consequence of (3.6) and (3.7). From (3.2) we thus have

$$\begin{aligned} \sigma^{-1}(\omega) &= \left(-\frac{e^2 n}{m}\right)^{-1} i\omega^* \\ &\times \left[ 1 - \frac{1}{a} \text{Tr} v L_1 G_0(\omega^*) \right. \end{aligned}$$

$$\left. \times \left( D^1 + \frac{1}{\omega^*} L_1 D^0 \right) + O(\lambda^3) \right]. \quad (3.10)$$

From the discussion to follow it will become evident that the trace in (3.10) contains no  $(1/\omega^*)$  factors other than the one shown explicitly. One might then expect that the dc resistivity up to order  $\lambda^2$  is obtained from (3.10) by putting  $\omega = 0$  and taking the limit  $\epsilon \rightarrow 0^+$ . According to this expectation then the quantity

$$\tilde{\sigma}^{-1}(0) \equiv (e^2 n)^{-1} (i/a) \text{Tr} p L_1 G_0(0^*) L_1 D^0 \quad (3.11)$$

is the dc resistivity to order  $\lambda^2$ . The trace can be evaluated in the representation  $|k\rangle$  that diagonalizes both  $H_0$  and  $\vec{p}$ , with eigenvalues  $\mathcal{E}_k$  and  $\vec{p}_k$ , respectively. Equation (3.11) thus yields the expression

$$\tilde{\sigma}^{-1}(0) = (e^2 n)^{-1} \frac{1}{2N} \sum_k \sum_{k'} [-f_0'(\mathcal{E}_k)] W_{kk'} (p_k - p_{k'})^2, \quad (3.12)$$

where

$$W_{kk'} = 2\pi |V_{kk'}|^2 \delta(\mathcal{E}_k - \mathcal{E}_{k'}) \quad (3.13)$$

is the Born approximation for the transition probability rate. An identical expression for  $\tilde{\sigma}^{-1}(0)$  is obtained if (2.23) is used to the same order in  $\lambda$ . This is an explicit expression for  $\tilde{\sigma}^{-1}(0)$  in terms of the matrix elements of  $V$  and does *not* involve the solution of an integral equation. Unfortunately, as we shall see,  $\tilde{\sigma}^{-1}(0)$  is *not* the correct expression for the resistivity to order  $\lambda^2$ .

An expression equivalent to (3.12) has been derived,<sup>21,22</sup> and has been claimed to be the correct expression for the dc resistivity to order  $\lambda^2$ . It has been asserted<sup>21,22</sup> that the formal expression (2.23) has a great advantage for the practical evaluation of the dc resistivity over other formal expressions,<sup>3</sup> since, in contrast to these, it does not engender the technique of the " $\lambda^2 t$  limit" of van Hove<sup>8,24</sup> and does not require the solution of an integral equation.<sup>26</sup>

We now prove that this assertion is erroneous and the result (3.11), or (3.12), is incorrect in general. The error lies in the fact that in the expansion of  $K(\omega = 0)$  in powers of  $\lambda$  there are terms of order  $\lambda^3$  and higher that diverge in the final limit  $\epsilon \rightarrow 0^+$ . These divergent terms appear whenever in the expansion (3.4) of  $G'(0^*)$  the unperturbed propagator  $G_0(0^*)$ , given by (3.6), operates on the part  $X_d$  of any operator  $X$  that is diagonal in the  $|k\rangle$  representation. For then

$$[G_0(0^*) X_d]_{kk'} = \frac{1}{i\epsilon} X_{kk'} \delta_{kk'}, \quad (3.14)$$

and thus, as  $\epsilon \rightarrow 0^+$ , such terms diverge. By contrast we note that for the off-diagonal part  $X_{nd}$  of  $X$ ,

$$[G_0(0^*) X_{nd}]_{kk'} = (i\epsilon - \mathcal{E}_k + \mathcal{E}_{k'})^{-1} X_{kk'}, \quad (k' \neq k) \quad (3.15)$$

presents no divergence as  $\epsilon \rightarrow 0^+$ , since in the summation over the intermediate states this becomes  $[-i\pi\delta(\mathcal{E}_k - \mathcal{E}_{k'}) - (\mathcal{E}_k - \mathcal{E}_{k'})_p^{-1}]X_{kk'}$ , after the thermodynamic limit is taken.

Thus the procedure of keeping only the lowest order in  $\lambda$  terms in the expansion of  $K(\omega=0)$  is invalid. Instead, we must sum the infinite subset of terms in the expansion of  $K(0)$  that are of the form  $(\lambda^2/i\epsilon)^n$  ( $n \geq 1$ ). These are the dominant terms for sufficiently small  $\lambda$ . Such procedure is equivalent to the " $\lambda^2 t$  limit" technique<sup>24</sup> and yields, as we shall see, a dc resistivity of order  $\lambda^2$ . Higher-order terms of the form  $(\lambda^3/i\epsilon)^n$ ,  $(\lambda^4/i\epsilon)^n$ , etc., can also be summed, and they give rise to corrections of the dc resistivity of order  $\lambda^3$ ,  $\lambda^4$ , etc.

The isolation of the desired divergent terms is facilitated by the introduction of the operator  $\Delta$  that projects the part of any operator  $X$  that is diagonal in the  $|k\rangle$  representation, i. e.,

$$(\Delta X)_{kk'} \equiv X_{kk} \delta_{kk'} . \quad (3.16)$$

The operator that projects the off-diagonal part of  $X$  is then  $\Delta' \equiv 1 - \Delta$ , with the obvious properties  $\Delta'^2 = \Delta'$ ,  $\Delta' \Delta = \Delta \Delta' = 0$ . The divergent terms now arise whenever  $G_0(0^*)$  operates on a diagonal operator, since, as we saw in (3.14),

$$G_0(0^*)\Delta = \frac{1}{i\epsilon} \Delta , \quad (3.17)$$

whereas  $G_0(0^*)\Delta'$  yields regular terms. Thus, it is convenient *not* to use the expansion (3.4) of  $G'(0^*)$  in powers of  $P'L_1 = L_1 - PL_1$ , but rather to expand  $G'(0^*)$  in powers of  $\Delta L_1$  and  $PL_1$ . This is accomplished simply by writing the first equality of (3.4) as

$$G'(0^*) = (i\epsilon - L_0 - \Delta' L_1 - \Delta L_1 + PL_1)^{-1} , \quad (3.18)$$

since then it follows that

$$G'(0^*) = G''(0^*) + G''(0^*)(\Delta L_1 - PL_1)G''(0^*) + \dots , \quad (3.19)$$

where

$$\begin{aligned} G''(0^*) &\equiv (i\epsilon - L_0 - \Delta' L_1)^{-1} \\ &= G_0(0^*) + G_0(0^*)\Delta' L_1 G_0(0^*) + \dots . \end{aligned} \quad (3.20)$$

From the structure (3.20) of  $G''(0^*)$  and the property (3.17) of  $G_0(0^*)$ , we note that in  $G''(0^*)\Delta'$  there are no divergent terms, whereas in  $G''(0^*)\Delta$  there are divergent terms with a *single*  $(1/i\epsilon)$  factor. By a simple rearrangement, these divergent terms can be made manifest, by noting that

$$G''(0^*)\Delta = \frac{1}{i\epsilon} \Delta + \frac{1}{i\epsilon} G''(0^*)\Delta' L_1 \Delta . \quad (3.21)$$

We note in fact that the quantity of interest  $K(0)$  of (3.3) can be written as

$$K(0) = \text{Trv} \Delta L_1 \Delta' G'(0^*) D , \quad (3.22)$$

since  $\text{Trv} L_1 X = \text{Trv} \Delta L_1 X$  and  $\Delta L_1 \Delta = 0$ . Furthermore, in the expansion (3.19) of  $\Delta' G'(0^*)$ , we can always replace *every*  $G''(0^*)$  by  $\Delta' G''(0^*)$  for the same reasons. It follows then that in the calculation of  $K(0)$  we need only  $\Delta' G''(0^*)$ , the divergent terms of which are

$$\Delta' G''(0^*)\Delta = \frac{1}{i\epsilon} \Delta' G''(0^*)\Delta' L_1 \Delta . \quad (3.23)$$

Specifically, such terms arise in the expansion (3.19) of  $G'(0^*)$  from the terms

$$\Delta' G''(0^*)\Delta L_1 = \frac{1}{i\epsilon} \Delta' G''(0^*)\Delta' L_1 \Delta L_1 , \quad (3.24)$$

$$\Delta' G''(0^*)\Delta D = \frac{1}{i\epsilon} \Delta' G''(0^*)\Delta' L_1 \Delta D , \quad (3.25)$$

where the operator  $D$ , that appears as a result of the  $P$  operation, has been written as  $D = \Delta D + \Delta' D$ . Now we can write the series for  $\Delta L_1 \Delta' G' D$ , which appears in the quantity of interest  $K(0)$  of (3.22), with the use of the expansion (3.19) and the observation that we may replace there every  $G''$  by  $\Delta' G''$ . We observe that, according to the previous discussion,  $\Delta' D = \Delta'(D^1 + D^2 + \dots)$  does not lead to any terms of the form  $(\lambda^2/i\epsilon)^n$ , and that the only terms of this form that arise from  $\Delta D$  and  $\Delta L_1$  are obtained by using  $G_0(0^*)$  for  $G''(0^*)$  and  $D^0$  for  $\Delta D$  in (3.24) and (3.25). Thus we find, keeping the most divergent terms [of the form  $(\lambda^2/i\epsilon)^n$ ] and none others, that

$$\Delta L_1 \Delta' G'(0^*) D \cong \left[ \frac{S}{i\epsilon} + \frac{S}{i\epsilon} \left( 1 - D^0 \frac{1}{a} \text{Trv} \right) \frac{S}{i\epsilon} + \dots \right] D^0 , \quad (3.26)$$

where

$$S \equiv \Delta [L_1 \Delta' G_0(0^*) \Delta' L_1] = \Delta [L_1 G_0(0^*) L_1] . \quad (3.27)$$

The series (3.26) can be rearranged to read

$$\begin{aligned} \Delta L_1 \Delta' G'(0^*) D &\cong \left( \bar{S} - \bar{S} D^0 \frac{1}{a} \text{Trv} \bar{S} \right. \\ &\quad \left. + \bar{S} D^0 \frac{1}{a} \text{Trv} \bar{S} D^0 \frac{1}{a} \text{Trv} \bar{S} - \dots \right) D^0 \\ &= \bar{S} D^0 \left( 1 + \frac{1}{a} \text{Trv} \bar{S} D^0 \right)^{-1} , \end{aligned} \quad (3.28)$$

with

$$1 + \bar{S} = 1 + \frac{S}{i\epsilon} + \left( \frac{S}{i\epsilon} \right)^2 + \dots = \left( 1 - \frac{S}{i\epsilon} \right)^{-1} . \quad (3.29)$$

In order to find  $K(0)$  we perform, according to (3.22), the operation  $\text{Trv} \dots$  on (3.28), and find

$$K(0) \cong \text{Trv} \bar{S} D^0 \left( 1 + \frac{1}{a} \text{Trv} \bar{S} D^0 \right)^{-1} . \quad (3.30)$$

For the dc conductivity  $\sigma(0)$  we need, according to

(3.2), the quantity

$$\left(1 - \frac{1}{a} K(0)\right)^{-1} \cong 1 + \frac{1}{a} \text{Trv} \bar{S} D^0 \\ \cong \frac{1}{a} \text{Trv} (1 + \bar{S}) D^0, \quad (3.31)$$

where we have made use of the relation  $a = \text{Trv} D \cong \text{Trv} D^0$ , to the order of our approximation. Finally, if we use (3.29) for  $(1 + \bar{S})$  in (3.31), and (3.27) for  $S$ , we find from (3.2)

$$\sigma(0) \cong \frac{e^2}{\Omega} \text{Trv} [\Delta L_1 G_0(0^*) L_1]^{-1} D^0. \quad (3.32)$$

Clearly, this gives a dc conductivity of order  $\lambda^{-2}$ . More explicitly, (3.32) can be written in terms of the diagonal operator

$$f \equiv -[\Delta L_1 G_0(0^*) L_1]^{-1} D^0, \quad (3.33)$$

in the form

$$\sigma(0) \cong -\frac{e^2}{m} \frac{1}{\Omega} \sum_k p_k f_k, \quad (3.34)$$

where  $f_k \equiv \langle k | f | k \rangle$ . From (3.33)  $f_k$  is seen to be determined from the integral equation

$$\sum_{k'} W_{kk'} (f_{k'} - f_k) = i D_{kk}^0 = -f'_0(\mathcal{E}_k) p_k / m, \quad (3.35)$$

with  $W_{kk'}$  given by (3.13). This is the standard result<sup>2</sup> of the well-known transport theory<sup>4,5,13,15</sup> of electrical conduction, in the lowest order for the scattering. A simple derivation of it, in the spirit of this paper, is given in Appendix B for comparison.

For completeness, we must point out here that, in order for this procedure to be valid, the "scattering" potential  $V(\vec{r})$  must satisfy certain conditions. We recall that in the expansion of  $K(0)$  in powers of  $\lambda$ , we summed only the terms of the form  $(\lambda^2/i\epsilon)^n$ , as these were taken to be the dominant ones for sufficiently small  $\lambda$  and in the limit  $\epsilon \rightarrow 0^+$ . This is correct, provided all the terms—the ones that were summed and the neglected ones—of every order in  $\lambda$  depend on the volume  $\Omega$  in the same manner in the limit  $\Omega \rightarrow \infty$ . This is clearly essential, since the limit  $\Omega \rightarrow \infty$  must be taken before the  $\epsilon \rightarrow 0^+$  limit. From an examination of the terms appearing in the expansion of  $K(0)$  in powers of  $\lambda$ , we note that this requirement can be expressed in the form

$$\langle k | L_1 (G_0 \Delta' L_1)^n \Delta X | k \rangle \propto \Omega^0, \quad (3.36a)$$

$$\langle k | D^n | k \rangle \propto \Omega^0, \quad (3.36b)$$

$$\langle k | L_1 (G_0 \Delta' L_1)^n \Delta' D^m | k \rangle \propto \Omega^0. \quad (3.36c)$$

Here  $X$  in (3.36a) is any operator with matrix elements  $X_{kk}$  that are smooth functions of  $k$  and independent of  $\Omega$ , and  $D = \sum_n D^n$  denotes the expansion of

$D$  in powers of  $\lambda$ . In other words, the "scattering" potential  $V(\vec{r})$  must have a subtle dependence on the volume  $\Omega$  of the system. A model of such a potential is the one produced by a set of point scatterers distributed randomly. It can be verified<sup>27</sup> that such a potential satisfies (3.36) on the average. From the work of Appendix B it can easily be seen that the method of the kinetic equations also requires the conditions (3.36) on  $V$ . These are analogous to the conditions van Hove<sup>24</sup> proposed for the derivation of the master equation.

In order to make explicit how our result for  $\sigma^{-1}(0)$ , given by (3.34) and (3.35), differs from that proposed by Kenkre and Dresden, Eq. (3.12), we consider the isotropic case of free electrons, i. e.,  $H_0 = \vec{p}^2/2m$ , and spherically symmetric scatterers. The transport equation (3.35) (see also Appendix A) then has a simple solution in terms of an energy-dependent relaxation time

$$\tau^{-1}(\mathcal{E}_k) = \sum_{k'} W_{kk'} (1 - \cos \theta_{kk'}), \quad (3.37)$$

where  $\theta_{kk'}$  is the angle between the wave vector  $\vec{k}$  and  $\vec{k}'$ , namely  $f_k = f'_0(\mathcal{E}_k) p_k \tau(\mathcal{E}_k) / m$ . The dc conductivity is then

$$\sigma(0) = e^2 n \tau / m, \quad (3.38)$$

where according to the standard expression (3.32)

$$\tau = \sum_k \frac{[-f'_0(\mathcal{E}_k)] p_k^2 \tau(\mathcal{E}_k)}{Nm}. \quad (3.39)$$

By contrast, according to expression (3.12),  $\bar{\sigma}(0)$  can be written in the form (3.38) but with

$$\tau \rightarrow \bar{\tau} = Nm / \sum_k [-f'_0(\mathcal{E}_k)] p_k^2 \tau(\mathcal{E}_k)^{-1}. \quad (3.40)$$

The two expressions for  $\tau$  (3.39) and (3.40) are clearly different in general, even in this simple case. Only for completely degenerate statistics are they equal, since then  $\tau = \bar{\tau} = \tau(\mathcal{E}_F)$ , where  $\mathcal{E}_F$  is the Fermi energy.

To sum up the discussion for the dc conductivity, we may say that the expression (2.23), or (2.24), which involves the  $P$  operator, offers no particular advantage in calculating  $\sigma(0)$  over the earlier expressions and methods. Contrary to claims made for it,<sup>21</sup> the correct handling of this expression leads, as does every other method, to the integral transport equation (3.35) for the distribution function.

We now consider the case of the ac conductivity. We note that for  $\omega \neq 0$  there are no divergent terms in the expansion of  $K(\omega)$  in powers of  $\lambda$ , and thus Eq. (3.10) is the correct expression for the ac resistivity up to order  $\lambda^2$ . This, of course, is the reciprocal of  $\sigma(\omega)$  up to second order in  $\lambda$ . Both expansions are valid for  $(\lambda^2/\omega) \ll 1$ , or, more pre-

cisely,  $\omega\tau \gg 1$ . But such an expression for  $\sigma(\omega)$  can be obtained simply from the equation of motion for  $\rho(\omega)$ , Eq. (2.12), by iteration, or equivalently from (2.14) and the expansions of

$$G(\omega^*) = G_0(\omega^*) + G_0(\omega^*)L_1G_0(\omega^*) + \dots \quad (3.41)$$

and  $D = D^0 + D^1 + \dots$  of  $G(\omega^*)$  and  $D$  in powers of  $V$ . We thus find straightforwardly, up to second order in  $\lambda$ ,

$$\sigma(\omega) = \left(\frac{e^2 n}{m}\right) \frac{i}{\omega^*} \left[ 1 + \frac{1}{a} \text{Tr} v L_1 G_0(\omega^*) \times \left( D^1 + \frac{1}{\omega^*} L_1 D^0 \right) + O(\lambda^3) \right], \quad (3.42)$$

which is clearly the reciprocal of (3.10) up to order  $\lambda^2$ . We conclude that for the calculation of the ac conductivity in the case  $\omega\tau \gg 1$ , expressions (2.23) and (2.24) involving the  $P$  operator offer no important advantage. They do, however, yield directly the reciprocal of a series expansion, if one is interested in the resistivity up to a given order in  $\lambda$ .

For the case of arbitrary  $\omega\tau$  it should be emphasized that Eq. (3.10) is *not* valid. One can use Eq. (2.23), or (2.24), to obtain an expression for  $\sigma(\omega)$  for arbitrary  $\omega\tau$ , but again, as in the case of  $\omega = 0$ , one should sum all the terms of the form  $(\lambda^2/\omega^*)^n$  ( $n \geq 1$ ). This yields an expression for  $\sigma(\omega)$  in terms of a distribution function  $f_k(\omega)$  which is determined from an integral transport equation. But again this transport equation can be obtained more simply by other methods (see Appendix B). Rather than demonstrate this now, we shall show it in complete generality in Sec. IV on the basis of a more general and concrete model.

#### IV. ELECTRONS IN RANDOM IMPURITIES

As we mentioned in Sec. III, the scattering potential  $V$  must satisfy certain conditions in order that the usual expansions in powers of  $\lambda$  for the conductivity be valid. A physical model of such a potential is one due to a set of  $N_i$  impurities centered at the points  $\vec{x}_\alpha = 1, \dots, N_i$ , i. e.,  $V(\vec{r}) = \sum_\alpha \varphi(\vec{r} - \vec{x}_\alpha)$ , and distributed randomly. In the thermodynamic limit,  $N_i$  also tends to infinity, so that the density of the impurities  $n_i \equiv N_i/\Omega$  remains fixed. The physical quantities of interest, such as the conductivity, are then their values averaged over all possible distributions of  $\{\vec{x}\}$ , all with the same probability. We denote this averaging by an impurity projection operator  $P_i$ , defined by

$$P_i F(\vec{x}_1, \dots, \vec{x}_{N_i}) \equiv \int \frac{d^3 x_1}{\Omega} \dots \int \frac{d^3 x_{N_i}}{\Omega} \times F(\vec{x}_1, \dots, \vec{x}_{N_i}). \quad (4.1)$$

Thus, the conductivity is now, more precisely,

$$\sigma(\omega) = \left(-\frac{e^2}{\Omega}\right) \text{Tr} v P_i \rho(\omega), \quad (4.2)$$

where  $\rho(\omega)$  is obtained from (2.12).

On the basis of this more precise model for the scattering potential  $V$ , we shall show in this section the complete equivalence of the method developed in Sec. II, which uses the Mori-type projection operator  $P$ , with the method of kinetic equations for all  $\omega$  and  $\lambda$ .

We recall briefly the method of kinetic equations<sup>15</sup> for this system. According to this method, an equation is obtained for  $P_i \rho(\omega)$ , the quantity necessary for the evaluation of  $\sigma(\omega)$  in (4.2), from (2.12) for  $\rho(\omega)$ . This is found simply by eliminating the part  $P_i' \rho \equiv (1 - P_i) \rho$  in terms of  $P_i \rho$ , just as in Eqs. (2.18)–(2.22). The result is quite generally<sup>15</sup> the kinetic equation

$$[\omega^* - S(\omega)] P_i \rho(\omega) = P_i D + C, \quad (4.3)$$

where

$$S(\omega) = P_i L [1 + G_i'(\omega^*) P_i' L] = \omega^* P_i [L G_i'(\omega^*)], \quad (4.4)$$

$$C = P_i L G_i'(\omega^*) P_i' D, \quad (4.5)$$

with the new propagator  $G_i'(\omega^*)$  defined by

$$G_i'(\omega^*) \equiv (\omega^* - P_i' L)^{-1}. \quad (4.6)$$

The second expression for  $S(\omega)$  in (4.4) follows from  $(\omega^* - P_i' L) G_i'(\omega) = 1$ . Expressions (4.4) and (4.5) simplify considerably, if we note that  $P_i L_0 = L_0 P_i$  and  $P_i L_1 P_i = 0$ . In addition, simpler kinetic equations, appropriate to the system under consideration, can be obtained from (4.3) by simply taking appropriate matrix elements of (4.3) (for details see Ref. 15). We are interested, however, only in showing the general equivalence of the expression for  $\sigma(\omega)$  obtained from (4.2) and (4.3), i. e.,

$$\sigma(\omega) = \left(-\frac{e^2}{\Omega}\right) \text{Tr} v [\omega^* - S(\omega)]^{-1} (P_i D + C), \quad (4.7)$$

to that obtained by the method of Sec. II.

Since the quantity of interest is now given by (4.2) which includes the  $P_i$  operator, we redefine the operator  $P$  of the second section as follows:

$$P X \equiv D \frac{1}{a} \text{Tr} v P_i X, \quad (4.8a)$$

$$a \equiv \text{Tr} v P_i D. \quad (4.8b)$$

In terms of this operator the conductivity is given, in direct analogy to (2.24), by

$$\sigma(\omega) = \left(-\frac{e^2 a}{\Omega}\right) \frac{1}{\omega^*} \left(1 - \frac{1}{a} K(\omega)\right)^{-1}, \quad (4.9)$$

where now

$$K(\omega) = \text{Tr} v P_i L G_i'(\omega^*) D. \quad (4.10)$$

We shall show now that (4.9) is equivalent to (4.7). In (4.10) the propagator  $G'(\omega^*)$  is given, as before, by (2.21) and can be written in the form

$$G'(\omega^*) \equiv (\omega^* - P'L)^{-1} = (\omega^* - P'_i L - P_i L + PL)^{-1}. \quad (4.11)$$

Thus, it satisfies the identity

$$G'(\omega^*) = G'_i(\omega^*) + G'_i(\omega^*)(P_i L - PL)G'(\omega^*), \quad (4.12)$$

where  $G'_i(\omega^*)$  is given by (4.6). Performing the operation  $P_i L \dots D$  on (4.12), we obtain

$$P_i LG'D = P_i LG'_i D + P_i LG'_i \left(1 - D \frac{1}{a} \text{Tr}v\right) P_i LG'D, \quad (4.13)$$

if we make use of (4.8a). If we now write  $D = P_i D + P'_i D$ , we can express  $P_i LG'_i D$  in terms of  $S(\omega)$ ,  $P_i D$  and  $C$  from (4.4) and (4.5), namely

$$P_i LG'_i D = \frac{1}{\omega^*} S(\omega) P_i D + C. \quad (4.14)$$

Substituting (4.14) and (4.10) in (4.13) and rearranging terms, we obtain

$$P_i LG'D = [\omega^* - S(\omega)]^{-1} [S(\omega) P_i D + \omega^* C] \times \left(1 - \frac{1}{a} K(\omega)\right). \quad (4.15)$$

Noting that  $(\omega^* - S)^{-1} S P_i D = -P_i D + \omega^*(\omega^* - S)^{-1} P_i D$  and taking  $(1/a)\text{Tr}v$  on both sides of (4.15), we obtain

$$\frac{1}{a} K(\omega) = \left(-1 + \frac{\omega^*}{a} \text{Tr}v[\omega^* - S(\omega)]^{-1} (P_i D + C)\right) \times \left(1 - \frac{1}{a} K(\omega)\right). \quad (4.16)$$

Finally, solving this equation for  $K(\omega)$  and substituting it in expression (4.9) for  $\sigma(\omega)$ , we obtain expression (4.7) for  $\sigma(\omega)$ . This proves the general equivalence of the method of Sec. II to the method of kinetic equations for any  $\omega$  and  $\lambda$ .

One can, of course, recover the results of Sec. III and their generalization for arbitrary  $\omega\tau$  by expanding  $S(\omega)$ ,  $P_i D$ , and  $C$  in powers of  $\lambda$ , keeping them to order  $\lambda^2$  and taking the diagonal in  $|k\rangle$  matrix elements of the kinetic equation (4.3). For details see Ref. 15.

It is also possible<sup>18</sup> to expand  $S(\omega)$ ,  $P_i D$ , and  $C$  in powers of the density  $n_i$  of the scatterers for arbitrarily strong scattering centers. Thus, one can derive a transport equation for  $f_k$ , from which an expression for the dc resistivity to order  $n_i$  can be obtained in terms of the  $t$  matrix for each scattering center. Such an expression can also be obtained from (3.2), but a summation of a more complicated set of infinite terms in the expansion of

$K(0)$  in powers of  $\lambda$  has to be carried out, which leads again to the same integral transport equation.

## V. CONCLUSION

It should be obvious from this discussion that, in spite of their apparent simplicity, formal expressions like (2.14) and (2.24) for  $\sigma(\omega)$  do not afford any particular advantage in the calculation of the conductivity, at least for systems of the type considered. All of them require partial summations of an infinite number of terms that lead to kinetic equations for appropriate distribution functions. The method of kinetic equations leads directly to these, without the necessity of identifying and summing an infinite set of terms; it is thus a simpler technique.

It must be pointed out, however, that there can be special systems for which a particular projection operator of the Mori type can be used, within the method of Sec. II, without having to carry out partial summations. For example, for the isotropic system of free electrons in random impurities, considered toward the end of Sec. III, the dc conductivity can be obtained simply by the method of Sec. II, with the introduction of the projection operator (A9), described in Appendix A. This yields an expression for the distribution function  $f_k$ , rather than the conductivity, namely Eq. (A11). If we evaluate  $f_k(\omega=0)$  to order  $\lambda^{-2}$ , we obtain (A13), namely  $f_k = f'_0(\mathcal{E}_k) p_k \tau(\mathcal{E}_k)/m$ , where  $\tau(\mathcal{E}_k)$  is given by (3.37). As we saw in Sec. III, this gives the correct dc conductivity to order  $\lambda^{-2}$ . In other words, for this system and projection operator, the coefficients of the terms of the form  $(\lambda^2/i\epsilon)^n$  with  $n \geq 2$  in the expansion (A12) vanish.

Our conclusion is then that the technique of Sec. II for the calculation of the resistivity does not live up to the claims made<sup>21,22</sup> for it, in general. It is possible, however, that it may prove useful by a judicious choice of the projection operator for special systems.

These somewhat negative remarks should not be interpreted as applicable to the very general method that Mori<sup>1</sup> has proposed.

## APPENDIX A: RESISTIVITY TENSOR AND DISTRIBUTION FUNCTION

As an example of the possible generalizations of the method used in Sec. II, we derive briefly the expressions corresponding to (2.23) and (2.24) for all the components of the resistivity tensor. The interaction with the electric field is now  $-eE \times (r_\alpha e_\alpha e^{-i\omega t} + \text{H. c.})$  (summation convention), where  $e_\alpha$  ( $\alpha = 1, 2, 3$ ) are the Cartesian components of a unit vector in the direction of the electric field. The resistivity tensor  $[\sigma^{-1}(\omega)]_{\alpha\beta}$  is then defined by the relation



$$[\sigma^{-1}(\omega)]_{\alpha\beta} \left( -\frac{e^2}{\Omega} \right) \text{Tr} v_{\beta} \rho = e_{\alpha}, \quad (\text{A1})$$

where  $\rho$  is given by the equation, analogous to (2.12),

$$(\omega^* - L)\rho = D_{\alpha} e_{\alpha} = [r_{\alpha}, f_0(H)]e_{\alpha}. \quad (\text{A2})$$

An expression for  $(\sigma^{-1})_{\alpha\beta}$  can be obtained by the introduction of a projection operator  $P$  defined by

$$PX = D_{\alpha} (a^{-1})_{\alpha\beta} \text{Tr} v_{\beta} X, \quad (\text{A3})$$

$$a_{\alpha\beta} = \text{Tr} v_{\alpha} D_{\beta}. \quad (\text{A4})$$

We note that  $PD_{\alpha} = D_{\alpha}$ , and thus  $P'D_{\alpha} = 0$ . An equation for  $P\rho = D_{\alpha} (a^{-1})_{\alpha\beta} \text{Tr} v_{\beta} \rho$  can be obtained as in Eqs. (2.18)–(2.22). If the resulting equation for  $\text{Tr} v_{\beta} \rho$  is compared with the definition of  $[\sigma^{-1}(\omega)]_{\alpha\beta}$  in (A1), we get the equivalent expressions for the resistivity tensor

$$\begin{aligned} [\sigma^{-1}(\omega)]_{\alpha\beta} &= \left( -\frac{e^2}{\Omega} \right)^{-1} \{ \omega^* (a^{-1})_{\alpha\beta} \\ &\quad - (a^{-1})_{\alpha\gamma} \text{Tr} v_{\gamma} L [1 + G'(\omega^*) P' L] \\ &\quad \times D_{\delta} (a^{-1})_{\delta\beta} \}, \end{aligned} \quad (\text{A5})$$

$$\begin{aligned} &= \left( -\frac{e^2}{\Omega} \right)^{-1} \omega^* \{ (a^{-1})_{\alpha\beta} \\ &\quad - (a^{-1})_{\alpha\gamma} \text{Tr} v_{\gamma} L G'(\omega^*) D_{\delta} (a^{-1})_{\delta\beta} \}. \end{aligned} \quad (\text{A6})$$

For most systems the matrix  $a_{\alpha\beta} = \text{Tr} v_{\alpha} [v_{\beta}, r_0(H)] = a\delta_{\alpha\beta}$  and (2.31) and (2.32) are somewhat simpler; e.g.,

$$[\sigma^{-1}(\omega)]_{\alpha\beta} = \left( -\frac{e^2 a}{\Omega} \right)^{-1} \omega^* \left( \delta_{\alpha\beta} - \frac{1}{a} \text{Tr} v_{\alpha} L G'(\omega^*) D_{\beta} \right). \quad (\text{A7})$$

Similarly, other modifications of the projection operator  $P$  can be used to get expressions for quantities of interest other than the resistivity. For example, in the case of the system of noninteracting electrons considered in Sec. III, the conductivity can be expressed in terms of a distribution function  $f_k(\omega) \equiv \langle k | \rho(\omega) | k \rangle$  by the relation

$$\sigma(\omega) = -\frac{e^2}{m} \frac{1}{\Omega} \sum_k p_k f_k(\omega), \quad (\text{A8})$$

where  $|k\rangle$  are the eigenstates of  $H_0$  and  $\tilde{p}$ . We can now find a formal expression for  $f_k(\omega)$  by the introduction of the projection operator

$$PX = D \frac{1}{a} \text{Tr} |k\rangle \langle k| X = D \frac{1}{a} X_k, \quad (\text{A9})$$

$$a = \text{Tr} |k\rangle \langle k| D = D_k, \quad (\text{A10})$$

where we have denoted the diagonal in  $|k\rangle$  matrix elements  $\langle k|X|k\rangle$  of any operator  $X$  by  $X_k$ . We note that again  $PD = D$  and  $P'D = 0$ . We can now obtain an equation for  $P\rho(\omega) = Df_k(\omega)/D_k$  as in Eqs. (2.18)–

(2.22). In direct analogy to (2.24) and (3.10), we find then for the distribution function

$$f_k(\omega) = D_k \left( \omega^* - \frac{\omega^*}{D_k} [L G'(\omega^*) D]_k \right)^{-1}, \quad (\text{A11})$$

where  $G'(\omega^*) = (\omega^* - P'L)^{-1}$  as before, but with  $P$  given by (A9) and (A10). If we expand the denominator in powers of  $\lambda$ , we get

$$\begin{aligned} f_k(\omega) &= D_k \left\{ \omega^* - \frac{\omega^*}{D_k} \left[ L_1 G_0(\omega^*) \left( D^1 + \frac{1}{\omega^*} L_1 D^0 \right) \right]_k \right. \\ &\quad \left. + O(\lambda^3) \right\}^{-1}. \end{aligned} \quad (\text{A12})$$

For the case of the isotropic model considered in Sec. III, this gives

$$f_k(\omega = 0) = f'_0(\mathcal{E}_k) p_k \tau(\mathcal{E}_k) / m \quad (\text{A13})$$

where  $\tau(\mathcal{E}_k)$  is given by (3.37). This is correct, as we saw in Sec. III, for this particular model.

#### APPENDIX B: DERIVATION OF THE TRANSPORT EQUATION

We derive here in a simple way the transport equation (3.35) and its generalization for all  $\omega$  and  $\lambda$ . If we evaluate the trace in expression (2.1) for  $\rho(\omega)$ , we get Eq. (3.34), where now

$$f \equiv \Delta \rho(\omega) \quad (\text{B1})$$

with the projection operator  $\Delta$  defined by (3.16). An equation for  $f$  is obtained in the same way as in (2.22) for  $P\rho(\omega)$ . If we write  $\rho(\omega) = f + \Delta' \rho$ , substitute this in (2.12) and operate on it by  $\Delta$  and  $\Delta'$ , separately, we get

$$(\omega^* - \Delta L) f - \Delta L \Delta' \rho = \Delta D, \quad (\text{B2})$$

$$(\omega^* - \Delta' L) \Delta' \rho - \Delta' L f = \Delta' D. \quad (\text{B3})$$

Solving (B3) for  $\Delta' \rho$  in terms of  $f$  and substituting it in (B2), we get

$$[\omega^* - \Delta L - \Delta L G''(\omega^*) \Delta' L] f = \Delta D + \Delta L G''(\omega^*) \Delta' D, \quad (\text{B4})$$

where

$$G''(\omega^*) = (\omega^* - \Delta' L)^{-1}. \quad (\text{B5})$$

For the system of interest  $\Delta L_0 = L_0 \Delta$  and  $\Delta L_1 \Delta = 0$ , and thus (B4) becomes

$$[\omega^* - S(\omega)] f = \Delta D + \Delta L_1 G''(\omega^*) \Delta' D, \quad (\text{B6})$$

where

$$S(\omega) = \Delta [L_1 G''(\omega^*) L_1], \quad (\text{B7})$$

$$\begin{aligned} G''(\omega^*) &= (\omega^* - L_0 - \Delta' L_1)^{-1} \\ &= G_0(\omega^*) + G_0(\omega^*) \Delta' L_1 G_0(\omega^*) + \dots \end{aligned} \quad (\text{B8})$$

In the kinetic equation (B6) for  $f$ , if we take  $\omega = 0$  and keep its coefficients in the lowest nonvanishing

order in  $\lambda$ , we get immediately (3.33) and, thus, the transport equation (3.35).

Equation (B6) is thus a general transport equation for  $f_k$  for all  $\omega$  and  $\lambda$ . We observe that Eq. (A11) of Appendix A is the formal solution of this

equation. From the expansion (B8) of  $G''(\omega^*)$  in powers of  $\lambda$ , we can find the power-series expansion of the coefficients of (B6). The conditions for these series to give meaningful results in the limit  $\Omega \rightarrow \infty$  are easily seen to be Eqs. (3.36).

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<sup>26</sup>In connection with the limit  $\epsilon \rightarrow 0^+$  which occurs in the theory, Kenkre and Dresden (Ref. 21) have asserted emphatically that their evaluation of the dc resistivity to order  $\lambda^2$  is based on the assumption that the limit  $\epsilon \rightarrow 0^+$  is taken before a certain time integration. We should like to point out that this assertion is wrong. The evaluation of their formula (12a) can easily be carried out with the limit  $\epsilon \rightarrow 0^+$  taken last. In fact, one then finds the same result, namely their Eq. (35a). This equivalence is a result of the fact that the use of their Eq. (34) is tantamount to taking the limit  $\epsilon \rightarrow 0^+$  last. Finally, this question of the order of the limits has nothing to do with the main fault of their work, namely, the failure to recognize the divergence of the higher-order terms in the expression for the dc resistivity.

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