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Discussion of the memory-function method

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Abstract. The recently proposed memory-function method for the calculation of transport coefficients is discussed and criticised in the context of a simple model. In the study of the frequency-dependent conductivity $\sigma(\omega)$ of this model it is shown that this method yields a simple result for $\sigma(0)$ that is, however, different from the standard result. It is then proved that this method commits errors, and when properly corrected it yields the standard result. For $\omega \neq 0$ this method yields an expression for $\sigma(\omega)$ that is valid only for large ω , a result that can be obtained more simply from the standard formula. It is concluded that the method of kinetic equations is the correct and simplest way for the calculation of $\sigma(\omega)$ for all frequencies.

1. Introduction

The problem of electrical conduction in solids has been studied by a large number of theoretical methods [1–17]. Although the techniques differ, they all require [18] the solution of an integral equation. In the lowest approximation for the scattering this is a quantum-mechanical generalisation of the Boltzmann–Bloch transport equation, first proposed by Bloch [19] and Nordheim [20]. The most direct and simple method that derives this transport equation is the method of kinetic equations [3, 12, 14, 17].

Recently a new approach, the memory-function method, has been proposed [21] that yields the conductivity for all frequencies in terms of the memory function, which can be obtained explicitly by a simple perturbation expansion in the small parameter λ such as the strength of the scattering, and thus avoids the difficulty of finding a solution to the integral transport equation. This method has been applied [21–23] to a number of similar problems. This memory-function method is expounded in § 2, where, for the sake of avoiding unnecessary generalisations, we consider the simple but basic model of independent free electrons scattered by randomly distributed centres. An explicit expression for the memory function and the conductivity for all frequencies in terms of the matrix elements of the scattering potential is obtained.

In view of the simplicity of this method, the question naturally arises as to how this explicit formula for the conductivity compares with the corresponding expression of the standard theory [1–17], and whether it is correct. This is discussed in § 3 for the simple system under consideration. It is shown that the memory-function method is not valid for the static case $\omega = 0$; a correct evaluation of the memory function for weak scattering in this case is shown to lead to an integral equation for a distribution function that is

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identical to the standard transport equation for the system. For the case $\omega \neq 0$ the result of the memory-function method is valid only for large frequencies, in which case it presents no particular advantage. This study thus corrects the erroneous claims [21] made for the memory-function method.

In a very recent work [24–26] a more sophisticated version of this approach (Mori's formalism) has been proposed, on the basis of which the conductivity of a quantum particle in a random potential, exhibiting the Anderson transition from the metallic to the insulating phase, was discussed. Clearly, any scheme that describes this transition even qualitatively is quite important. However, our study of the memory function presented here suggests that caution should be exercised in *assuming* (as this work does) that in the metallic regime ($\lambda \rightarrow 0$) the memory function is an analytic function of λ . For example, although this method gives the correct result up to order λ^2 for the specific model considered in this work, this would not be the case for a more general scattering potential and arbitrary temperature, and thus the analytic expressions for the metallic regime ($\lambda \rightarrow 0$) would have to be re-examined.

From this discussion and the work in Appendix 2 it becomes obvious that the method of kinetic equations [3, 12, 14] offers a more direct and simple way for the calculation of the conductivity.

2. The memory-function method

We develop the memory-function formalism for the conductivity of the simple system of independent electrons in the field of randomly distributed static scattering centres, driven by a homogeneous electric field of frequency ω .

Since the centres are stationary, it suffices [3, 12] to consider one electron, without thereby ignoring the exchange effects of the electrons. Its Hamiltonian is $H + F(t)$, where

$$H = H_0 + V = \frac{1}{2m} p^2 + \sum_{\alpha} u(\mathbf{r} - \mathbf{r}_{\alpha}) \quad (2.1)$$

is the kinetic energy and the interaction with the scattering centres $\{\mathbf{r}_{\alpha}\}$, and

$$F(t) = F e^{-i\omega t} + \text{HC} \quad (2.2a)$$

$$F = (ieE/\omega)v \quad (2.2b)$$

is the interaction with the electric field $\mathbf{E}(t) = \mathbf{E}e^{-i\omega t} + \text{cc}$ described in the vector gauge, with $v = p/m$ being the component of the velocity operator in the direction of \mathbf{E} . The linear steady-state density operator satisfies the equation [2, 27] ($\hbar = 1$)

$$(\omega^+ - L)\rho(\omega) = [F, f_0(H)] \quad (2.3a)$$

with the solution

$$\rho(\omega) = G(\omega^+)[F, f_0(H)] = (ieE/\omega)[G(\omega^+)v, f_0(H)]. \quad (2.3b)$$

Here $f_0(H) = \{\exp[\beta(H - \mu)] + 1\}^{-1}$ is the Fermi–Dirac function for temperature $T = 1/k_B\beta$ and chemical potential μ ,

$$G(z) = (z - L)^{-1} \quad (2.4)$$

is the propagator for the Liouville operator L defined by

$$LX = [H, X] \quad (2.5)$$

for any operator X , and $\omega^+ = \omega + i\eta$ with η a positive infinitesimal, where the limit

$\eta \rightarrow 0_+$ is always implied and assumed to be taken after the thermodynamic limit. We obtain then the standard expression [2, 3, 14] for the conductivity for the vector gauge

$$\sigma(\omega) = (e/E) \text{Tr}[v\rho(\omega) - (ieE/m\omega) f_0(H)] \quad (2.6a)$$

$$= -(ie^2/\omega)[\chi(\omega^+) - (n/m)] \quad (2.6b)$$

in terms of the velocity–velocity correlation function

$$\chi(z) = \langle [G(z)v, v] \rangle \quad (2.7)$$

where

$$\langle X \rangle = \text{Tr} f_0(H)X \quad (2.8)$$

and the average over the random distribution of the scatterers will be implicitly understood as part of the trace operation. The density of electrons is denoted by n and it determines the chemical potential μ through $\langle 1 \rangle = n$. (We consider a system of unit volume.) For a normal conductor, i.e. when $\sigma(0) = \text{finite}$, we *must* have

$$\chi(0^+) = n/m \quad (2.9)$$

as can be seen from (2.6). An explicit demonstration of this is given in Appendix 1.

For the implementation of the memory-function method we begin by writing (2.6b) in the form

$$\sigma(\omega) = ie^2(n/m)/(\omega^+ + M(\omega^+)) \quad (2.10)$$

introducing thereby the memory function

$$M(z) = z\chi(z)/[\chi(0^+) - \chi(z)]. \quad (2.11)$$

From this we have equivalently,

$$\chi(z) = \chi(0^+)M(z)/[z + M(z)]. \quad (2.12)$$

Thus $M(0^+) \propto 1/\sigma(0)$, i.e. $M(0^+)$ is proportional to the DC resistivity of the system. It is clear that in the absence of scattering, i.e. for $V = 0$, we have $G(z)v = v/z$, and thus $\chi(z) = M(z) = 0$. We wish to determine $M(z)$ for all z up to $O(\lambda^2)$, where λ denotes the strength of the scattering interaction V , which is the lowest non-vanishing order.

In the memory-function formalism one reasons [21] that, if $M(z)$ has a regular dependence of λ , it follows from (2.12) that

$$\chi(0^+) M(z) + O(\lambda^3) = z\chi(z). \quad (2.13)$$

One then rewrites $\chi(z)$, the velocity–velocity correlation function (2.7), in terms of the acceleration–acceleration correlation function

$$\psi(z) = \langle [G(z)a, a] \rangle \quad (2.14)$$

where

$$a = iLv = (L_0 + L_1)v = iL_1v \quad (2.15)$$

is the acceleration operator. Here we have written $L = L_0 + L_1$, where in accordance with (2.5) and (2.1)

$$L_0 X = [H_0, X] \quad L_1 X = [V, X]. \quad (2.16)$$

The relation between $\chi(z)$ and $\psi(z)$ is established by the use of the equation of motion, which in our notation takes the form

$$zG(z) = 1 + LG(z) = 1 + G(z)L \quad (2.17)$$

as follows from the definition (2.4) of $G(z)$, in the following way. From (2.7), (2.14) and (2.15) we have $z\chi(z) = (-i)\langle [G(z)a, v] \rangle$ and hence

$$\begin{aligned} z^2\chi(z) &= (-i)\langle [a, v] \rangle + (-i)\langle [LG(z)a, v] \rangle \\ &= (-i)\langle [a, v] \rangle + \langle [G(z)a, a] \rangle. \end{aligned} \quad (2.18)$$

But since according to (2.9) $\chi(0^+) = n/m$, we must have from (2.18) for $z = 0^+$ that $i\langle [a, v] \rangle = \langle [G(0^+)a, a] \rangle$ (see Appendix 1 for an explicit demonstration), and thus

$$z^2\chi(z) = \psi(z) - \psi(0^+), \quad (2.19)$$

where $\psi(z)$ is given by (2.14). Combining (2.13) and (2.19) one obtains

$$M(z) = [\psi(z) - \psi(0^+)]/z\chi(0^+) + O(\lambda^3). \quad (2.20)$$

One then reaches the conclusion [21] that an evaluation of the correlation function $\psi(z)$ in the lowest non-vanishing order of λ yields $M(z)$ in the lowest order, according to (2.20). Since, according to (2.15), $a \sim O(\lambda)$, we have from the formal expansion of $\psi(z)$ in powers of λ ,

$$\psi(z) = \sum_{n=0}^{\infty} \lambda^n \psi^{(n)}(z)$$

that the lowest order is

$$\psi^{(2)}(z) = \langle [G_0(z)a, a] \rangle_0 \quad (2.21)$$

where

$$G_0(z) = (z - L_0)^{-1} \quad (2.22)$$

and $\langle \rangle_0$ denotes the average in (2.8) but with $f_0(H)$ replaced by $f_0(H_0)$. Higher-order terms of $\psi(z)$ can be easily found by using the expansion of $G(z)$ in powers of λ , i.e.

$$G(z) = G_0(z) \sum_{n=0}^{\infty} [L_1 G_0(z)]^n \quad (2.23)$$

and the expansion of

$$f_0(H) = f_0(H_0 + V) = \sum_{n=0}^{\infty} \lambda^n f^{(n)}.$$

The memory-function method thus concludes [21] that the conductivity $\sigma(\omega)$ for all ω is given by (2.10), with $M(\omega^+)$ evaluated to the lowest order in λ as

$$\begin{aligned} M^{(2)}(\omega^+) &= [\psi^{(2)}(\omega^+) - \psi^{(2)}(0^+)]/(\omega^+ n/m) \\ &= (m/\omega^+ n) \{ \langle [G_0(\omega^+)a, a] \rangle_0 - \langle [G_0(0^+)a, a] \rangle_0 \}. \end{aligned} \quad (2.24)$$

For the system under consideration we find from (2.21), (2.15), (2.16) and (2.1)

$$\psi^{(2)}(\omega^+) = 2 \sum_k \sum_{k'} \overline{|V_{kk'}|^2} (v_k - v_{k'}) \frac{f_0(\varepsilon_k) - f_0 \varepsilon_{k'}}{\omega^+ - \varepsilon_{k'} + \varepsilon_k}. \quad (2.25)$$

Here $V_{kk'}$ is the matrix element of V between the plane-wave states $|k\rangle$ and $|k'\rangle$, $|k\rangle$ being an eigenstate of H_0 with eigenvalue $\varepsilon_k = k^2/2m$, $v_k = p_k/m = k/m$ is the component of

$v_{kk} = \langle k|v|k \rangle$ in the direction of E , and the bar denotes the average over the random distribution of the scattering centres, so that $\overline{|V_{kk'}|^2} = n_s |u_{kk'}|^2$ with n_s being the density of scatterers and $u_{kk'}$ the matrix element of the single scattering potential $u(r)$. Thus for $\sigma(0)$ to $O(\lambda^{-2})$, the memory-function formulation gives, according to (2.10), (2.24) and (2.25),

$$\sigma(0)_{MF} = e^2(n^2/m^2) \left(\sum_k \sum_{k'} [-f'_0(\epsilon_k)] W_{kk'} (v_k - v_{k'})^2 \right)^{-1} \tag{2.26}$$

where

$$W_{kk'} = 2\pi \overline{|V_{kk'}|^2} \delta(\epsilon_k - \epsilon_{k'}) \tag{2.27}$$

is the Born approximation for the transition probability rate due to the random scatterers and $f'_0(\epsilon) = df_0(\epsilon)/d\epsilon$.

It is important to point out that this formulation yields an *explicit* expression for $\sigma(\omega)$ for all ω , equations (2.10), (2.24) and (2.25), in terms of the matrix elements of the scattering potential $u(r)$. This is in contrast to the standard method [2, 14] which requires the solution of an integral equation. Thus, if it is correct, the memory-function method is of extreme practical importance for the calculation of $\sigma(\omega)$ for various scattering mechanisms, and for similar transport quantities for many systems.

3. Discussion of the memory-function method

In the ensuing discussion of this method we make the following points. First, the result of the memory-function formulation for the DC conductivity is different from that of the standard model. Secondly, we show that the memory-function method is invalid for $\omega = 0$. Thirdly, for $\omega = 0$ it is correct only for $\omega\tau(\omega) \gg 1$, where $\tau(\omega)$ is the appropriate relaxation time, and in this case it does not present any advantage. Fourthly, we show how the memory function can be calculated correctly for all ω including $\omega = 0$, for small λ , and that then this yields a result for the DC conductivity that is identical to that of the standard method.

The standard method for evaluating $\sigma(0)$ is that of kinetic equations [3, 14]. According to this, we evaluate

$$\sigma(0) = (e/E) \text{Tr}[v\bar{\rho}(0)] = -e^2 \text{Tr}\{vG(0^+)[r, f_0(H)]\} \tag{3.1}$$

where $\bar{\rho}(0)$ is the steady-state density operator in the scalar gauge, i.e. for $F = -eEr$, in terms of the distribution function $f_k(0) = \bar{\rho}(0)_{kk}$, namely

$$\sigma(0) = 2(e/E) \sum_k v_k f_k(0). \tag{3.2}$$

Here $f_k(0)$ is determined by a kinetic equation, which takes the form of a Boltzmann-Bloch transport equation, i.e.

$$\sum_{k'} W_{kk'} [f_{k'}(0) - f_k(0)] = eE v_k f'_0(\epsilon_k) \tag{3.3}$$

with $W_{kk'}$ given by (2.27) in the lowest order in λ for the scattering. (For completeness this is derived simply in Appendix 2.) This is an integral equation for $f_k(0)$, which in general has no simple solution, and therefore $\sigma(0)$ from (3.2) cannot be equal to $\sigma(0)_{MF}$ of (2.26), in spite of the fact that both expressions are of $O(\lambda^{-2})$.

In order to make this disagreement more perspicuous, we consider the case of spherically symmetric scatterers. Then (3.3) has the simple solution

$$f_k(0) = -eEv_k \tau(\varepsilon_k) f'_0(\varepsilon_k) \quad (3.4a)$$

in terms of an energy-dependent relaxation time $\tau(\varepsilon_k)$, where

$$\tau(\varepsilon_k)^{-1} = \sum_{k'} W_{kk'} (1 - \cos \theta_{kk'}) \quad (3.4b)$$

and $\theta_{kk'}$ is the angle between the wavevectors \mathbf{k} and \mathbf{k}' . The conductivity is then

$$\sigma(0) = 2e^2 \sum_k [-f'_0(\varepsilon_k)] v_k^2 \tau(\varepsilon_k). \quad (3.5)$$

By contrast, (2.26) in this case becomes

$$\sigma(0)_{\text{MF}} = e^2 (n/m)^2 / 2 \sum_k [-f'_0(\varepsilon_k)] v_k^2 \tau(\varepsilon_k)^{-1} \quad (3.6)$$

which is clearly different from (3.5) even in this especially simple case. Only for completely degenerate statistics, i.e. at $T = 0$ K, is $\sigma(0)_{\text{MF}}$ equal to $\sigma(0)$, since then both are equal to $e^2 n \tau(\varepsilon_F) / m$ where ε_F is the Fermi energy.

We now prove that the explicit expression (2.26) for $\sigma(0)_{\text{MF}}$ up to $O(\lambda^{-2})$ is incorrect in general. We recall that this expression was derived from the exact equation (2.6b) and the relations (2.13) and (2.24). Relation (2.13) was obtained from the definition (2.12) with the recognition that $M(\omega^+) \sim O(\lambda^2)$. But it is wrong for $\omega = 0$, as in this case one would have to have $\lim_{\eta \rightarrow 0_+} M^{(2)}(0^+) / i\eta \ll 1$; equivalently, since according to (2.9) $\chi(0^+) = n/m$, (2.13) gives $M^{(2)}(0^+) = 0$, which is clearly absurd as it would give $\sigma(0) = \infty$ up to $O(\lambda^{-2})$, in contradiction to (2.26). Furthermore, relation (2.24) is correct only if the formal expansion of $\psi(z)$ in powers of λ is valid for $\omega = 0$. We will, however, demonstrate below that in fact this expansion of $\psi(0^+)$ in powers of λ involves terms of order λ^3 and higher, which diverge in the final limit $\eta \rightarrow 0_+$. We thus conclude that the memory-function method of evaluating $\sigma(\omega)$ breaks down for $\omega = 0$.

For $\omega \neq 0$ both of these objections are not applicable, namely (2.13) is correct and, as we shall see below, there are no divergent terms in the formal expansion of $\psi(\omega^+)$ in powers of λ (as $\eta \rightarrow 0_+$), and thus

$$R(\omega) = [\omega^+ + M^{(2)}(\omega^+)] / ie^2 (n/m) \quad (3.7)$$

with $M^{(2)}(\omega^+)$ given by (2.24) and (2.25), is the correct expression for the AC resistivity up to $O(\lambda^2)$. This is, however, nothing more than the reciprocal of $\sigma^{(2)}(\omega)$, i.e. $\sigma(\omega)$ evaluated up to $O(\lambda^2)$. Both expansions are valid for $(\lambda^2/\omega) \ll 1$, or more precisely $\omega\tau(\omega) \gg 1$, where $\tau(\omega) \sim O(\lambda^2)$ is a measure of the appropriate relaxation time. But such a high-frequency expression for $\sigma^{(2)}(\omega)$ can be obtained simply and directly from formula (2.6b). If we use (2.19) to rewrite $\chi(z)$ in terms of $\psi(z)$, we obtain an expression for $\sigma^{(2)}(\omega)$ which is clearly the reciprocal of (3.6) up to $O(\lambda^2)$. In fact, it is worth while to remark that within the memory-function formalism one may use (2.13) and obtain $M^{(2)}(\omega^+)$ in terms of $\chi^{(2)}(\omega^+)$ in the formal expansion of

$$\chi(z) = \sum_{n=0}^{\infty} \lambda^n \chi^{(n)}(z)$$

in powers of λ , namely

$$M^{(2)}(\omega^+) = \omega^+ \chi^{(2)}(\omega^+) / (n/m) = (m/n) \text{Tr} f^{(1)} [G_0(\omega^+) L_1 v, v] \quad (3.8)$$

instead of using (2.20) to obtain $M^{(2)}(\omega^+)$ in terms of $\psi^{(2)}(\omega^+)$, as in (2.24). This is

obviously true due to the fact that the relation (2.19) between $\chi(z)$ and $\psi(z)$ is exact and $\chi = \sum_n \lambda^n \chi^{(n)}$, $\psi = \sum_n \lambda^n \psi^{(n)}$ are formal expansions in powers of λ . The equivalence of (3.8) to (2.24) can of course be proved directly, if use is made of the invariance of the trace under cyclic permutations, the equation of motion (2.17), the relation $L_0 f^{(n)} = -L_1 f^{(n-1)}$ ($n \geq 1$), which follows from $L f_0(H) = 0$, and $[H_0, v] = 0$. We conclude that for the calculation of the AC conductivity in the case of $\omega\tau(\omega) \gg 1$ the memory-function formulation offers no particular advantage.

Let us now show that the formal expansion of $\psi(\omega^+) = \sum_n \lambda^n \psi^{(n)}(\omega^+)$ in powers of λ breaks down for $\omega = 0$, and thus (2.24) is not valid for $\omega = 0$. The reason for this is the same as for the well known [6-9] breakdown of the formal expansion of $\chi(\omega^+) = \sum_n \lambda^n \chi^{(n)}(\omega^+)$ for $\omega = 0$, as evidenced by the fact that $\sigma(0) \sim O(\lambda^{-2})$. Since the formal series is generated by the expansion (2.23) of $G(\omega^+)$, we note that whenever $G_0(\omega^+)$ operates on the part χ_d of any operator X that is diagonal in $|k\rangle$ we have

$$(G_0(\omega^+)X_d)_{kk'} = X_k \delta_{kk'} / (\omega + i\eta) \tag{3.9a}$$

and this diverges for $\omega = 0$ and in the limit $\eta \rightarrow 0_+$. By contrast we note that for the non-diagonal part X_{nd} of X

$$G_0(0^+)X_{nd})_{kk'} = (i\eta - \epsilon_k + \epsilon_{k'})^{-1} X_{kk'} \quad (k \neq k') \tag{3.9b}$$

presents no divergence as $\eta \rightarrow 0_+$, since in the integration over the intermediate states this becomes

$$[-i\pi\delta(\epsilon_k - \epsilon_{k'}) - (\epsilon_k - \epsilon_{k'})_p^{-1}] X_{kk'}$$

after the thermodynamic limit is taken. The subscript p indicates the principal value.

Thus the procedure of keeping only the term of the lowest non-vanishing order in λ in the expansion of $\psi(0^+)$, or $\chi(0^+)$, is invalid. Instead we must sum the infinite subset of terms in the expansion of $\psi(0^+)$, or $\chi(0^+)$, that are of the form $(\lambda^2/i\eta)^n$ ($n \geq 1$). These are the dominant terms for sufficiently small λ . Such a procedure is equivalent to the 'λ²t limit' technique [28] and yields, as we shall see, a DC resistivity of $O(\lambda^2)$. Higher-order terms of the forms $(\lambda^3/i\eta)^n$, $(\lambda^4/i\eta)^n$, etc., can also be summed, and they give rise to the corrections of the DC resistivity of order λ^3 , λ^4 , etc.

Similarly, for the case $\omega \neq 0$ but arbitrary $\omega\tau(\omega)$, we should sum all terms of the form $(\lambda^2/\omega^+)^n$ ($n \geq 1$).

We now demonstrate that when this procedure is followed and $M(\omega^+)$ is correctly evaluated for small λ , an expression for the resistivity $R(\omega)$ up to $O(\lambda^2)$, equation (3.7), obtains which is in full accord with the standard result obtained by the method of kinetic equations for all ω including $\omega = 0$. In order to find the correct expression for $M(z)$ for small λ , we use its definition (2.11) in terms of $\chi(z)$. The correct behaviour of $\chi(z)$ for small λ is obtained by identifying, in its formal expansion in powers of λ , all terms of the form $(\lambda^2/z)^n$ ($n \geq 1$), and summing them.

In order to isolate the desired divergent terms, we introduce the projection operator Δ that projects the part X_d of any operator X that is diagonal in the $|k\rangle$ representation, i.e.

$$(\Delta X)_{kk'} = X_{kk} \delta_{kk'}. \tag{3.10}$$

The operator that projects the non-diagonal part X_{nd} of X is then $\Delta' = 1 - \Delta$. We have

the obvious properties $\Delta^2 = \Delta$, $\Delta'^2 = \Delta'$, $\Delta\Delta' = \Delta'\Delta = 0$. The divergent terms of (see (2.7) and (2.23))

$$\chi(z) = \sum_{n=0}^{\infty} \langle [G_0(z)\{L_1 G_0(z)\}^n v, v] \rangle \quad (3.11)$$

now arise whenever $G_0(z)$ operates on a diagonal operator, since as we saw in (3.9a)

$$G_0(z)\Delta = (1/z)\Delta \quad (3.12)$$

whereas $G_0(z)\Delta'$ yields regular terms. Thus, it is convenient *not* to use the expansion (2.23) of $G(z)$ in powers of λ (i.e. of L_1) as indicated in (3.11), but rather to expand $G(z)$ in powers of ΔL_1 . This is accomplished simply by writing

$$G(z) = (z - L_0 - \Delta' L_1 - \Delta L_1)^{-1} \quad (3.13)$$

since then it follows that

$$G(z) = \sum_{n=0}^{\infty} [G'(z)\Delta L_1]^n G'(z) \quad (3.14)$$

where

$$G'(z) = (z - L_0 - \Delta' L_1)^{-1} = G_0(z) + G_0(z)\Delta' L_1 G_0(z) + \dots \quad (3.15)$$

From the structure (3.15) of $G'(z)$ and the property (3.12) of $G_0(z)$ we note that in $G'(z)\Delta'$ there are no divergent terms, whereas in $G'(z)\Delta$ there are divergent terms with a *single* $(1/z)$ factor. By a simple rearrangement of these divergent terms can be made manifest by noting that

$$G'(z)\Delta = \frac{1}{z}\Delta + \frac{1}{z}G'(z)\Delta' L_1 \Delta \quad (3.16)$$

and therefore

$$\Delta G'(z)\Delta = (1/z)\Delta. \quad (3.17)$$

Since now $\Delta[v, f_0(H)] = 0$, we have from (2.7), (2.8) and (3.14)

$$\begin{aligned} \chi(z) &= -\text{Tr } v G(z)[v, f_0(H)] \\ &= \text{Tr } v \sum_{n=0}^{\infty} [G'(z)\Delta L_1]^n G'(z)\Delta'[v, f_0(H)] \\ &= -\text{Tr } v \Delta G'(z) \sum_{n=0}^{\infty} [\Delta L_1 \Delta' G'(z)\Delta]^n L_1 \Delta' G'(z)\Delta'[v, f_0(H)] \end{aligned} \quad (3.18)$$

where we have used the relations $\Delta G'(z)\Delta' = 0$ and $\Delta L_1 G'(z) = \Delta L_1 \Delta' G'(z)$. Because of (3.16) the last expression (3.18) of $\chi(z)$ can be written in the form

$$\chi(z) = -\text{Tr } v [z - S(z)]^{-1} B(z) \quad (3.19)$$

where

$$S(z) = \Delta L_1 G'(z) L_1 \Delta \quad (3.20)$$

$$B(z) = \Delta L_1 G'(z)[v, f_0(H)] \quad (3.21)$$

The ‘most divergent’ terms of the form $(\lambda^2/z)^n$ are obtained by replacing in (3.20) and (3.21) $G'(z)$ by $G_0(z)$, its first term in (3.15). We thus get for small λ

$$\chi(z) \approx -\text{Tr } v[z - S_2(z)]^{-1} B_2(z) \tag{3.22}$$

where

$$S_2(z) = \Delta L_1 G_0(z) L_1 \Delta \tag{3.23}$$

$$B_2(z) = \Delta L_1 G_0(z) [v, f^{(1)}]. \tag{3.24}$$

We may rewrite this in the form

$$\chi(\omega^+) \approx -\text{Tr } v g(\omega) = -2 \sum_k v_k g_{kk}(\omega) \tag{3.25}$$

where $g(\omega)$ is the solution of

$$[\omega^+ - S_2(\omega^+)]g(\omega) = B_2(\omega^+). \tag{3.26}$$

This is clearly an integral equation for $g_{kk}(\omega)$. However, it is *not* identical to the standard form (3.3) for $\omega = 0$. This is due to the fact that in the description of the effect of the electric field in (2.26) we used the vector gauge, whereas in the standard form one employs the scalar gauge, i.e. one takes $F = -eEr$.

We demonstrate now how the final connection with the standard result for $\sigma(\omega)$ is obtained within this formalism. In (3.21) for $B(z)$ we note that, since

$$[v, f_0(H)] = izD - i(z - L)D \tag{3.27}$$

with

$$D = [r, f_0(H)] \tag{3.28}$$

we have

$$B(z) = izC(z) + iS(z)D \tag{3.29}$$

where

$$C(z) = \Delta L_1 \Delta' G'(z) \Delta' D. \tag{3.30}$$

Using (3.29) in (3.19) we get

$$\chi(z) = -iz \text{Tr } v[z - S(z)]^{-1} [D + C(z)] + i \text{Tr } vD. \tag{3.31}$$

But

$$i \text{Tr } vD = i([p, r])/m = n/m = \chi(0^+). \tag{3.32}$$

Thus, $\chi(\omega^+)$ is found from the expression

$$\chi(\omega^+) - \chi(0^+) = -i\omega^+ \text{Tr } v\bar{\rho}(\omega)/(-eE) \tag{3.33}$$

where $\bar{\rho}(\omega)$ is determined from the equation

$$[\omega^+ - S(\omega^+)]\bar{\rho}(\omega) = (-eE)[\Delta D + C(\omega^+)] \tag{3.34}$$

where S , D and C are given by (3.20), (3.28) and (3.30), respectively. The small- λ behaviour of $\bar{\rho}(\omega)$, and of $\chi(\omega^+)$, is then determined from

$$[\omega^+ - S_2(\omega^+)]\bar{\rho}(\omega) = (-eE)[\Delta(D_0 + D_2) + C_2(\omega^+)] \tag{3.35}$$

where $S_2(\omega^+)$ is given by (3.23) and

$$D_0 + D_2 = [r, f_0(H_0) + f^{(2)}] \tag{3.36}$$

$$C_2(z) = \Delta L_1 G_0(z) \Delta' [r, f^{(1)}]. \tag{3.37}$$

The memory function $M(\omega^+)$ for small λ is thus found from its definition (2.11) and from (3.23) to be

$$M(\omega^+) = -\omega^+ + i(n/m)[\text{Tr } v\bar{\rho}(\omega)/(-eE)]^{-1}. \quad (3.38)$$

In the memory-function method then the conductivity $\sigma(\omega)$ is obtained from (2.10) in terms of $M(\omega^+)$ given by (3.38), and it is

$$\sigma(\omega) = (e/E) \text{Tr } v\bar{\rho}(\omega) = 2(e/E) \sum_k v_k f_k(\omega). \quad (3.39)$$

Here $f_k(\omega) = \bar{\rho}(\omega)_{kk}$ is the steady-state distribution function in the scalar gauge, which for small λ is determined from (3.35). This can be seen to be the integral equation

$$\omega^+ f_k(\omega) - i \sum_{k'} W_{kk'}(\omega) [f_{k'}(\omega) - f_k(\omega)] = (-eE) [D_{0,kk} + D_{2,kk} + C_2(\omega)_{kk}] \quad (3.40)$$

where

$$W_{kk'}(\omega) = i|\overline{V_{kk'}}|^2 [(\omega^+ - \varepsilon_k + \varepsilon_{k'})^{-1} + (\omega^+ - \varepsilon_{k'} + \varepsilon_k)^{-1}] \quad (3.41)$$

$$-eED_{0,kk} = -ieEv_k f'_0(\varepsilon_k) \quad (3.42)$$

and $D_{2,kk}$, $C_2(\omega^+)_{kk}$ are the natural matrix elements of D_2 and $C_2(\omega^+)$, as given by (3.36) and (3.37), the detailed nature of which are not of interest here. In particular, for $\omega = 0$ we find that (3.40), to the lowest order in λ for the inhomogeneous terms, reduces to (3.3) with $W_{kk'}(0) = W_{kk'}$, and thus $\sigma(0)$ up to $O(\lambda^{-2})$ is obtained from (3.2) and (3.3), which is the standard result. More generally, for arbitrary ω equation (3.40) is identical to the standard result, which for completeness is derived [12, 14] simply in Appendix 2 by the method of kinetic equations.

We conclude that correct evaluation of the memory function $M(z)$ for small λ leads to the same result as the standard method, and it certainly does not avoid the mathematical complexities of the standard procedure of kinetic equations. This refutes the claims that have been made [21] for the memory-function formalism.

We should point out that the discussion above is not complete in one important aspect. The important role of the averaging over the random distribution of the scattering centres has not been brought out. We shall forego such a discussion, as it has been given elsewhere [3, 14, 27] in connection with the standard theory of the conductivity.

Finally, we remark that there have been other attempts [29, 30] to simplify the calculation of the conductivity, but they have been shown [24, 27] to be erroneous. In fact, expression (2.26) for $\sigma(0)$ in the memory-function formalism is identical to the expression for $\sigma(0)$ obtained by a different method [27, 29] (see [27], equation (3.12); the extra factor of $\frac{1}{2}$ is due to the fact that spin was ignored there), which was shown [27] to be in error.

Appendix 1

First we prove the relation $\chi(0^+) = n/m$, equation (2.9). Since $G(0^+)^{-1}r = (i\eta - L)r = iv + i\eta r$, we have $G(0^+)v = -ir$ and thus

$$\chi(0^+) = \langle [G(0^+)v, v] \rangle = -i\langle [r, v] \rangle = -i\langle [r, p] \rangle/m = \text{Tr } f_0(H)/m = n/m. \quad (\text{A1.1})$$

Secondly, we prove that $\psi(0^+) = i\langle [a, v] \rangle$, a relation used in the derivation of (2.19).

Since $G(0^+)^{-1}v = (i\eta - L)v$, we get $G(0^+)Lv = -v$. Now, using $a = iLv$, equation (2.15), and this relation, we have

$$\psi(0^+) = \langle [G(0^+)a, a] \rangle = i\langle [G(0^+)Lv, a] \rangle = i\langle [a, v] \rangle. \quad (\text{A1.2})$$

In these formal manipulations we have tacitly assumed the existence of a scattering potential $V(\mathbf{r})$ such that $\sigma(0) \neq \infty$.

Appendix 2

We give here a simple derivation of the transport equation (3.40) within the formalism of kinetic equations.

The steady-state density operator $\bar{\rho}(\omega)$ for the scalar gauge is determined by (2.3a) with $F = -eEr$, i.e.

$$(\omega^+ - L)\bar{\rho}(\omega) = -eED = -eE[r, f_0(H)]. \quad (\text{A2.1})$$

The conductivity is then given by (3.39) as

$$\sigma(\omega) = (e/E) \text{Tr} \, v f(\omega) = 2(e/E) \sum_k v_k f_k(\omega) \quad (\text{A2.2})$$

where now

$$f(\omega) = \Delta \bar{\rho}(\omega) \quad (\text{A2.3})$$

and Δ is the projection operator defined in (3.10). An equation for $f(\omega)$ is obtained from (A2.1) by writing $\bar{\rho}(\omega) = f(\omega) + \Delta' \bar{\rho}(\omega)$, substituting this in (A2.1) and operating on it with Δ and Δ' , separately, to get

$$(\omega^+ - \Delta L)f(\omega) - \Delta L \Delta' \bar{\rho}(\omega) = (-eE)\Delta D \quad (\text{A2.4})$$

$$(\omega^+ - \Delta' L)\Delta' \bar{\rho}(\omega) - \Delta' L f(\omega) = (-eE)\Delta' D \quad (\text{A2.5})$$

Solving (A2.5) for $\Delta' \bar{\rho}(\omega)$ in terms of $f(\omega)$ and substituting it in (A2.4), we get

$$[\omega^+ - S(\omega^+)]f(\omega) = (-eE)[\Delta D + C(\omega)] \quad (\text{A2.6})$$

where

$$S(\omega^+) = \Delta L_1 G'(\omega^+) L_1 \quad (\text{A2.7})$$

$$C(\omega) = \Delta L_1 G'(\omega^+) \Delta' D \quad (\text{A2.8})$$

with $G'(\omega^+)$ given by (3.15). Here we made use of $\Delta L_0 = L_0 \Delta$, $\Delta L_1 \Delta = 0$ and the properties of Δ and Δ' . Equations (A2.6)–(A2.8) are identical to (3.34), (3.20) and (3.30), which were derived by a more involved procedure, and constitute the general kinetic equation for $f(\omega)$ for all ω and λ , and it is clearly an integral equation for the distribution function $f_k(\omega) = \langle \mathbf{k} | f(\omega) | \mathbf{k} \rangle$.

For completeness the operator Δ should include the averaging over the random distribution of the scatterers. For additional discussion of the importance of this point see [3, 14, 27].

For small λ the distribution function $f_k(\omega)$ is determined from (A2.6) with its coefficients S , D , C evaluated up to $O(\lambda^2)$. This is easily seen to be equations (3.40)–(3.42). For $\omega = 0$ the distribution function $f_k(0)$ up to the leading order in λ is then found to be given by the kinetic equation (3.3), with (2.27).

Note that the expansion of $G'(\omega^+)$ in powers of λ , as given in (3.15), which generates the power series expansion of $S(\omega)$ and $C(\omega)$, does *not* introduce the divergent terms (for $\omega = 0$) that we discussed in § 3.

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