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Abstract

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PHYSICS

N. M. PLAKIDA

ON THE CALCULATION OF THE ELECTRICAL-CONDUCTIVITY TENSOR

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As is known, the kinetic coefficients for weakly nonequilibrium processes are simply expressed in terms of time correlation functions of the equilibrium state. However, the calculation of such quantities in the case of a temperature different from zero presents difficulties. We shall consider two-time temperature Green functions (retarded and advanced) ([1,2]), since the equations for them have a simple form, and the kinetic coefficients are expressed directly in terms of the Fourier component of the retarded Green function. The discussion will be carried out using as an example the calculation of the electrical-conductivity tensor for a system of electrons scattered by lattice phonons or by impurities. This problem has been considered by a number of authors by other methods ([3–5]).

Let us introduce retarded and advanced Green functions of the type ([1,2])

$$\begin{aligned} G^r_{\mu,\nu}(t-t') &\equiv \langle\langle j_\mu(t), j_\nu(t')\rangle\rangle_r = -i\theta(t-t')\langle[j_\mu(t), j_\nu(t')]_+\rangle, \\ G^a_{\mu,\nu}(t-t') &\equiv \langle\langle j_\mu(t), j_\nu(t')\rangle\rangle_a = i\theta(t'-t)\langle[j_\mu(t), j_\nu(t')]_+\rangle, \end{aligned} \tag{1}$$

where $[j_\mu(t), j_\nu(t')]_+$ is the anticommutator of the current operators $j_\mu(t)$ in the Heisenberg representation, and $\langle\cdots\rangle$ denotes averaging over the grand Gibbs ensemble. In what follows we shall omit the indices r, a, since the Fourier components of the Green functions (1)

$$G^{r,a}_{\mu,\nu}(E) = \frac{1}{2\pi}\int_{-\infty}^{\infty} G^{r,a}_{\mu,\nu}(t)e^{iEt}\,dt \tag{2}$$

can be analytically continued into the region of complex E and regarded as a single analytic function with a cut along the real axis ([1,2]).

As is easy to show ([2]), the dissipative part of the electrical-conductivity tensor of the system in the absence of a magnetic field is related to the Fourier component of the Green function (1) in the following way:

$$\operatorname{Re}\sigma_{\mu\nu}(\omega)=\frac{1}{2\omega}\operatorname{th}\frac{\beta\omega}{2}\,2\pi i\lim_{\varepsilon\to+0}\{G_{\mu\nu}(\omega+i\varepsilon)-G_{\mu\nu}(\omega-i\varepsilon)\},\qquad\beta=\frac{1}{kT}.\tag{3}$$

Introducing the mass operator $\mathcal{M}_{\mu\nu}(E)$ for the Green function (1) according to the definition

$$2\pi G_{\mu\nu}(E)=\langle[j_\mu,j_\nu]\rangle/[E-\mathcal{M}_{\mu\nu}(E)],\tag{4}$$

we represent formula (3) in the form

$$\operatorname{Re}\sigma_{\mu\nu}(\omega)=\frac{1}{2\omega}\operatorname{th}\frac{\beta\omega}{2}\langle[j_\mu,j_\nu]_+\rangle\frac{2\gamma_{\mu\nu}(\omega)}{[\omega+M_{\mu\nu}(\omega)]^2+\gamma^2_{\mu\nu}(\omega)},\tag{5}$$

where the real and imaginary parts of the mass operator have been introduced:

$$\lim_{\varepsilon\to+0}\mathcal{M}_{\mu\nu}(\omega\pm i\varepsilon)=M_{\mu\nu}(\omega)\mp i\gamma_{\mu\nu}(\omega).\tag{6}$$

In the case of static conductivity the frequency of the external electric field is $\omega=0$, and the conductivity is

$$\sigma_{\mu\nu}=\frac{\beta}{2}\frac{\langle[j_\mu,j_\nu]_+\rangle}{\gamma_{\mu\nu}(0)}.\tag{7}$$

Thus, the dissipative part of the electrical-conductivity tensor is determined by the imaginary part of the Green' s function of the currents. However, the direct calculation of the Green' s function (1), or of the corresponding time correlation functions, encounters certain difficulties ([5]). Therefore we shall consider the equation for the two-particle Green' s function

$$G_{kk'}(t-t')=\langle\langle a^+_k(t)a_k(t);\,a^+_{k'}(t')a_{k'}(t')\rangle\rangle,\tag{8}$$

from which we shall then determine the Green' s function (1), related to (8) by the relation

$$G_{\mu\nu}(t-t')=e^2\sum_{k,k'}v_\mu(k)v_\nu(k')G_{k,k'}(t-t'),\tag{9}$$

where $a^+_k(t)$ and $a_k(t)$ are the creation and annihilation operators of an electron with momentum k, e is the electron charge, and $v_\mu(k)=\partial\varepsilon_k/\partial k_\mu$ is the μ-th component of the velocity of an electron with energy ε_k.

For definiteness, let us consider a system of metal electrons scattered by lattice phonons, which is described by the Fröhlich Hamiltonian:

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1 = \sum_k \varepsilon_k a_k^+ a_k + \sum_q \omega_q b_q^+ b_q + \sum_{k,q} A_q a_{k+q}^+ a_k (b_q + b_{-q}^+), \quad (10)$$

where ω_q is the energy of a phonon with wave number q, $A_q = \gamma q \omega_q^{-1/2}$, and γ is the interaction constant.

For the Green' s function (8) it is easy to obtain a chain of equations by successively differentiating them with respect to the time t:

$$i\frac{d}{dt} G_{k,k'}(t-t') = \delta(t-t')\langle [a_k^+ a_k, a_{k'}^+ a_{k'}]_+ \rangle + \langle\langle [a_k^+ a_k, \mathcal{H}_1];\, a_{k'}^+(t') a_{k'}(t') \rangle\rangle, \quad (11)$$

$$i\frac{d}{dt} \langle\langle [a_k^+ a_k, \mathcal{H}_1];\, a_{k'}^+(t') a_{k'}(t') \rangle\rangle = \delta(t-t')\langle [[a_k^+ a_k, \mathcal{H}_1], a_{k'}^+ a_{k'}]_+ \rangle + \langle\langle [[a_k^+ a_k, \mathcal{H}_1], \mathcal{H}];\, a_{k'}^+(t') a_{k'}(t') \rangle\rangle. \quad (12)$$

Applying perturbation theory for the mass operator of the two-particle Green' s function ([6]), we represent the higher-order Green' s functions on the right-hand side of equation (12) in terms of the original one. To do this we perform a pairing of operators referring to one instant of time:

$$\langle\langle a_{k+q}^+ a_{p-q}^+ a_p a_k;\, a_{k'}^+ a_{k'} \rangle\rangle = -n_{k+q} G_{k,k'} \delta_{p,k+q} - n_k G_{k+q,k'} \delta_{p-q,k},$$

$$\langle\langle a_{k+q+q'}^+ (b_{q'} + b_{-q'}^+) b_q a_k;\, a_{k'}^+ a_{k'} \rangle\rangle = N_q G_{k,k'} \delta_{-q',q},$$

where n_k and N_q are the mean occupation numbers of electrons and phonons. The inhomogeneous terms in (11) and (12) are calculated in the lowest order, i.e., averaged with the Hamiltonian $\mathcal{H}_0$, for example: $\langle [a_k^+ a_k, a_{k'}^+ a_{k'}]_+ \rangle = 2n_k(1 - n_k)\delta_{k,k'}$. Passing in equations (11), (12) to the Fourier representation and using the approximations made, we obtain a closed equation for the Green' s function $G_{k,k'}(E)$:

$$EG_{k,k'}(E) = \frac{1}{2\pi} 2n_k(1-n_k)\delta_{k,k'} +$$

$$+ \sum_q \left(G_{k,k'}(E) w_{k+q,k}(E) - w_{k,k+q}(E) G_{k+q,k'}(E) \right), \quad (13)$$

where

$$w_{k+q,k}(E) = A_q^2 \left(\frac{-2E(1+N_q-n_{k+q})}{(\varepsilon_{k+q}-\varepsilon_k+\omega_q)^2-E^2} + \frac{-2E(N_q+n_{k+q})}{(\varepsilon_{k+q}-\varepsilon_k-\omega_q)^2-E^2} \right).$$

As is evident, this integral equation is similar to the kinetic equation.

for the nonequilibrium distribution function. In particular, the sum on the right-hand side of (13) is the "collision term" in the approximation linear in the external field; moreover, $w_{k+q,k}(E)$ for $E = i\varepsilon \to 0$ is the probability of transition of an electron from the state with momentum $\mathbf{k}$ to the state with momentum $\mathbf{k}+\mathbf{q}$.

As is known, solving such an equation presents difficulties, but to compute the electrical-conductivity tensor it is necessary to find only the first moment of the function $G_{k,k'}(E)$–the current Green' s function (1). From (13) we find the equation for this function:

$$EG_{\mu\nu}(E) = \frac{1}{\pi}\langle j_\mu j_\nu\rangle_0 + e^2 \sum_{k,k'} v_\mu(k)v_\nu(k')\,\mathcal{M}_k(E)G_{k,k'}(E), \qquad (14)$$

where

$$v_\mu(k)\mathcal{M}_k(E) = \sum_q w_{k+q,k}(v_\mu(k)-v_\mu(k+q)).$$

It is easy to verify that equation (14) is satisfied by the function

$$2\pi G_{k,k'}(E) = [2n_k(1-n_k)\delta_{k,k'} + h_{k,k'}]/[E-\mathcal{M}_k(E)], \qquad (15)$$

where $h_{k,k'}$ is the solution of the homogeneous equation

$$\sum_{k,k'} v_\mu(k)v_\nu(k')h_{k,k'} = 0.$$

Taking into account definition (4) for the mass operator, from (14) we obtain

$$G_{\mu\nu}(E)\mathcal{M}_{\mu\nu}(E) = e^2 \sum_{k,k'} v_\mu(k)v_\nu(k')\mathcal{M}_k(E)G_{k,k'}(E).$$

Substituting here the solution (15) and taking into account that the function $n_k(1-n_k) = -\frac{1}{\beta}\frac{\partial n_k}{\partial \varepsilon_k}$ has a sharp maximum at $|\mathbf{k}| = k_0$, the Fermi momentum, we can obtain the final expression for the mass operator

$$\mathcal{M}_{\mu\nu}(E) = e^2 \sum_k v_\mu(k) v_\nu(k) n_k (1 - n_k) \mathcal{M}_k(E) / \langle j_\mu j_\nu \rangle_0, \tag{16}$$

where we have assumed that the condition

$$\frac{\partial n_k}{\partial \varepsilon_k} \left| \frac{\partial \mathcal{M}_k(E)}{\partial k} \right|_{k=k_0} |k - k_0| \ll \left| \mathcal{M}_k(E) \frac{\partial n_k}{\partial \varepsilon_k} \right|_{k=k_0}$$

is satisfied.

As is evident, the solution $h_{k,k'}$ of the homogeneous equation does not enter into the final expression (16).

In the case of static conductivity, the imaginary part of the mass operator (16), after simple transformations, takes the form

$$\gamma_{\mu\nu}(0) = 2\pi e^2 \sum_{k,q} A_q^2 (v_\mu(k+q) - v_\mu(k))(v_\nu(k+q) - v_\nu(k)) \times$$

$$\times N_q(1 + N_q)(n_k - n_{k+q}) \delta(\varepsilon_{k+q} - \varepsilon_k - \omega_q) / \langle j_\mu j_\nu \rangle_0. \tag{17}$$

This expression leads to the well-known formula for the static conductivity (7):

$$\sigma_{\mu\nu} = \delta_{\mu\nu} 2e^2 k_0^4 v^2(k_0) c^6 \beta^5 / \pi \cdot 3\gamma^2 J_5(\theta/T),$$

where c is the speed of sound and $J_5(\theta/T)$ is a known function of the Debye temperature θ (see, for example, ([3])).

Let us now consider another example: scattering of electrons by impurity centers, which can be described by the Hamiltonian ([7])

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1 = \sum_k \varepsilon_k a_k^+ a_k + \frac{1}{V} \sum_{k,q} I(q) \sum_{j=1}^{N} e^{-iqr_j} a_{k+q}^+ a_k, \tag{18}$$

where N is the number of randomly distributed impurity centers in the volume V, $\mathbf{r}_j$ are their coordinates, and $I(q)$ is the Fourier component of the potential of interaction of an electron with an impurity center; moreover, we shall assume that $I(0) = 0$ ([7]).

The chain of equations for the Green' s function (8) has the same form as (11), (12).

Thus, equation (12) for the Fourier component of the Green' s function takes the form:

$$(E+\varepsilon_k-\varepsilon_{\mathbf{k+q}})G_{k\,\mathbf{k+q},\mathbf{k'}}(E)=\frac{1}{V}\sum_{j=1}^{N}e^{-i\mathbf{q}\mathbf{r}_j}I(\mathbf{q})\{G_{k,\mathbf{k'}}(E)-G_{\mathbf{k+q},\mathbf{k'}}(E)\}+$$

$$+\frac{1}{V}\sum_{q'\neq\mathbf{q}}I(\mathbf{q'})\sum_{j=1}^{N}e^{-i\mathbf{q'}\mathbf{r}_j}\{G_{k\,\mathbf{k+q-q'},\mathbf{k'}}(E)-G_{\mathbf{k+q'},\mathbf{k+q},\mathbf{k'}}(E)\},\qquad(19)$$

where the "off-diagonal" Green' s function has been introduced,

$$G_{k\,\mathbf{k+q},\mathbf{k'}}(t-t')=\langle\langle a_k^+(t)a_{\mathbf{k+q}}(t);a_{k'}^+(t')a_{k'}(t')\rangle\rangle.$$

The usual procedure for decoupling the chain of equations for Green' s functions will consist in neglecting the sum of off-diagonal Green' s functions on the right-hand side of (19), since it gives a contribution of higher order of smallness in the interaction $\mathcal{H}_1$ in comparison with the first term (7). Closing in this way the chain of equations (11), (12) and averaging over the positions of the impurity centers, we obtain equation (13) for the two-particle Green' s function, where now

$$w_{\mathbf{k+q},\mathbf{k}}(E)=\frac{N}{V}|I(\mathbf{q})|^2\left(\frac{1}{\varepsilon_k-\varepsilon_{\mathbf{k+q}}+E}-\frac{1}{\varepsilon_k-\varepsilon_{\mathbf{k+q}}-E}\right).\qquad(20)$$

Repeating the reasoning following formula (13), we arrive at the same expression (16) for the mass operator with the function $w_{\mathbf{k+q},\mathbf{k}}(E)$ (20).

For the static conductivity we obtain the usual formula

$$\sigma_{\mu\nu}=\delta_{\mu\nu}ne^2\tau/m,\qquad(21)$$

where τ is the "transport time" :

$$\frac{1}{\tau}=\frac{N}{V}\frac{1}{2\pi}\frac{k_0^3}{mv^2(k_0)}\int d(\cos\theta)(1-\cos\theta)\,|I(k_0,\cos\theta)|^2.\qquad(22)$$

For impurity conductivity it is easy to obtain higher approximations in the interaction by solving equation (19) iteratively. This leads to the replacement of expression (20) by a more exact one, which can be represented in the form (7)

$$w_{\mathbf{k+q},\mathbf{k}}(E)=\frac{N}{V}|t(\mathbf{q})|^2\left(\frac{1}{\tilde{\varepsilon}_k-\tilde{\varepsilon}_{\mathbf{k+q}}+i\gamma_k+i\gamma_{\mathbf{k+q}}+E}-\frac{1}{\tilde{\varepsilon}_k-\tilde{\varepsilon}_{\mathbf{k+q}}-i\gamma_k-i\gamma_{\mathbf{k+q}}-E}\right),\qquad(23)$$

where $t(\mathbf{q})$ is the exact scattering amplitude, and $\tilde{\varepsilon}_k$ is the renormalized electron energy, with $i\gamma_k$ describing the finiteness of the interaction time of the electron with the impurity center. For $\gamma_k + \gamma_{\mathbf{k+q}} \ll \tilde{\varepsilon}_k + \tilde{\varepsilon}_{\mathbf{k+q}}$ we obtain the previous formula (21), where τ will be determined through the exact scattering amplitude, and not in the first Born approximation, as in (22).

A similar procedure can also be carried out for the scattering of electrons by phonons, which will give qualitatively the same results.

Thus, the method of retarded and advanced Green' s functions makes it possible to calculate kinetic coefficients simply and, moreover, easily to obtain corrections to formulas derived from the solution of ordinary kinetic equations. Let us note that this approach may prove useful in cases where kinetic equations become inapplicable.

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Moscow State University
named after M. V. Lomonosov

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Note: Figure translations are in progress. See original paper for figures.