N. M. PLAKIDA

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Abstract

Full Text

N. M. PLAKIDA

ON THE CALCULATION OF THE DIELECTRIC PERMITTIVITY AND CONDUCTIVITY OF AN ELECTRON-PHONON SYSTEM

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Recently many works have appeared devoted to the study of kinetic processes in an electron-phonon system (see, for example, ([1–8])). A certain difficulty here is presented by the consistent inclusion of screening effects that arise in this system and lead to screening of the external perturbing field. As was noted in ([1]), an important role in this case is played by the direct Coulomb interaction between electrons, and therefore calculations ([2–5]) based on the Fröhlich Hamiltonian, in which this interaction is not taken into account, are not as consistent in this respect as the calculations ([6–8]) using the Bardeen-Pines Hamiltonian ([9]), in which the Coulomb interaction between electron-electrons and ions is explicitly taken into account. At the same time, the method of two-time Green's functions ([10,11]), apparently, is the most convenient in this case, and therefore it is of interest to carry out a consistent inclusion of screening effects in an electron-phonon system on the basis of this method, which is the aim of the present work. We shall calculate the dielectric permittivity and conductivity of the system on the basis of a Hamiltonian of the Bardeen-Pines type.

First of all let us obtain a general expression for the dielectric permittivity of the system. Suppose that an external perturbation acts on the equilibrium system, determined by the Hamiltonian

$$\mathcal{H}'(t) = -e^{\varepsilon t}\int dr\, eN(r,t)\varphi(r,t), \qquad \varepsilon \to +0,$$

where

$$\varphi(r,t) = \frac{1}{V}\sum_k \int d\omega\, \varphi(k,\omega)e^{ikr-i\omega t} \tag{1}$$

is the scalar potential of the external field, determining in the medium the induction vector

$$D(r,t) = -\nabla\varphi(r,t);$$

$$-eN(r,t) = e[\rho(r,t) - ZN - ZR(r,t)] \tag{2}$$

is the charge-density operator of the system; $\rho(r,t)$ is the electron-density operator (e is the electron charge); N is the mean equilibrium density of ions with charge Z, forming the crystal lattice; $R(r,t)$ is the deviation of the ion density from the equilibrium one (cf. [1]). The mean density of polarization charges $\mathcal{N}(r,t)$, arising in the system under the action of the external perturbation, according to the general theory of weakly nonequilibrium processes in the approximation linear in the external field, can be represented in the form [11]

$$\mathcal{N}(k,\omega) = \frac{2\pi e^2}{V}\langle\langle N_k \mid N_{-k}\rangle\rangle_\omega, \tag{3}$$

where we have passed to Fourier components according to (1) and introduced the retarded two-time Green' s function [10,11] for the operators (2):

$$\langle\langle N(r,t); N(r',t')\rangle\rangle = -i\theta(t-t')\langle[N(r,t), N(r',t')]_-\rangle. \tag{4}$$

We define the dielectric permittivity of the system by the equality

$$\mathbf{D}(\mathbf{k},\omega) = \varepsilon(k,\omega)\mathbf{E}(\mathbf{k},\omega), \tag{5}$$

where $\mathbf{E}(\mathbf{r},t)$ is the vector of the electric field in the medium, determined by the equation

$$\operatorname{div}\mathbf{E}(\mathbf{r},t) = \operatorname{div}\mathbf{D}(\mathbf{r},t) + 4\pi\mathcal{N}(\mathbf{r},t). \tag{6}$$

Passing to Fourier components in (5), (6), and defining $\mathbf{D}(\mathbf{k},\omega) = -i\mathbf{k}\varphi(\mathbf{k},\omega)$, with the use of (3) we obtain (cf. [1,9]):

$$\varepsilon^{-1}(k,\omega) = 1 + \frac{4\pi e^2}{k^2}\frac{2\pi}{V}\left[\langle\langle\rho_k \mid N_{-k}\rangle\rangle_\omega + \langle\langle -ZR_k \mid N^z_{-k}\rangle\rangle_\omega\right], \tag{7}$$

where we have represented the Green function (4) in the form of two functions: $G_k(\omega) = \langle\langle\rho_k \mid N_{-k}\rangle\rangle_\omega$, determining the linear response of the electrons, and $D_k(\omega) = \langle\langle -ZR_k \mid N_{-k}\rangle\rangle_\omega$, the response of the ions to the action of the external perturbing field. We now proceed to the determination of these functions.

We shall describe the equilibrium state of the system by a Hamiltonian of the Bardeen-Pines type [9]:

$$\mathcal{H} = \sum_p \varepsilon_p a_p^+ a_p + \frac{1}{2V}\sum_q v(q)\rho_q\rho_{-q} + \sum_q \Omega_q b_q^+ b_q + \sum_q \chi_q\rho_{-q}(b_q + b_{-q}^+), \tag{8}$$

where ε_p is the energy of Bloch electrons in the state with quasimomentum p;

$$\rho_q = \sum_p \rho_{pq} = \sum_p a_p^+ a_{p+q}$$

is the Fourier component of the electron density. The interaction of electrons only with longitudinal phonons is considered; their frequency Ω_q is determined by the normal vibrations of the ions against the background of the uniform negative charge (cf. ([6])). $\chi_q = (2V\Omega_q)^{-1/2} v q^i$, where $vq^i = (v^i_{-q})^*$ is the matrix element of the electron-phonon interaction, which, for convenience, we represent through the matrix element of the Coulomb interaction $v(q)$ in the form $|vq^i|^2 = \Omega_q^2 v(q)$ ([9]). The electron-phonon interaction, according to ([9]), may also be written in the form

$$\sum_q \chi_q \rho_{-q}(b_q + b^+_{-q}) \equiv -\frac{1}{V}\sum_q v(q) Z R_q \rho_{-q}, \tag{9}$$

whence the Fourier components of the ion-density oscillations R_q are directly determined. Although the explicit form of the functions $v(q)$, χ_q, Ω_q is not important to us in solving the equations, for estimates we may use their values obtained when neglecting periodicity effects ([9]): $v(q) = 4\pi e^2/q^2$, $\Omega_q^2 \simeq \Omega_p^2 = 4\pi N Z^2 e^2/M$.

Using the equations of motion for the creation and annihilation operators of electrons and phonons, constructed on the basis of the Hamiltonian (8), it is easy to find the equations for the Green functions. Thus, using relation (9), for the phonon Green function $D_k(\omega)$ we readily obtain

$$\frac{V\chi_k}{v(k)} \langle\langle (b_k + b^+_{-k}) \mid N_{-k} \rangle\rangle_\omega = \frac{V}{2\pi v(k)} \frac{\Omega_k^2}{\omega^2 - \Omega_k^2} \left(1 + \frac{2\pi v(k)}{V} G_k(\omega)\right). \tag{10}$$

In what follows it is convenient to introduce polarization operators for the electrons and ions according to the relations

$$\frac{2\pi}{V} G_k(\omega) = -\frac{\pi_e(k,\omega)}{\varepsilon(k,\omega)}, \qquad \frac{2\pi}{V} D_k(\omega) = -\frac{\pi_i(k,\omega)}{\varepsilon(k,\omega)}, \tag{11}$$

where the dielectric permittivity $\varepsilon(k,\omega)$ (7) takes the form

$$\varepsilon(k,\omega) = 1 + v(k)\pi_e(k,\omega) + v(k)\pi_i(k,\omega). \tag{7a}$$

From equation (10) it is now easy to determine the ionic polarizability

$$v(k)\pi_i(k,\omega) = -\frac{\Omega_a^2}{\omega^2 - \Omega_k^2 + \Omega_a^2}. \tag{12}$$

Let us note that this expression was obtained by neglecting the effects of anharmonicity of the lattice vibrations (phonon collisions), whose inclusion is necessary in some cases, for example, when considering processes of phonon drag by electrons in an external field [4], since they substantially reduce this effect, especially at high temperatures.

The equation for the electron Green' s function $G_k(\omega)$ is more complicated. It can be obtained from the equation

$$(\omega + \varepsilon_p - \varepsilon_{p+k})\langle\langle \rho_{pk} \mid N_{-k}\rangle\rangle_\omega = \frac{1}{2\pi}(n_p - n_{p+k}) +$$

$$+\frac{1}{V}\sum_q \{\langle\langle \rho_{p\,k-q}\rho_q \mid N_{-k}\rangle\rangle_\omega - \langle\langle \rho_{p+q\,k-q}\rho_q \mid N_{-k}\rangle\rangle_\omega\} +$$

$$+\sum_q \chi_q[\langle\langle \rho_{p\,k-q}(b_q + b^+_{-q}) \mid N_{-k}\rangle\rangle_\omega - \langle\langle \rho_{p+q\,k-q}(b_q + b^+_{-q}) \mid N_{-k}\rangle\rangle_\omega]. \qquad (13)$$

Let us consider the simplest approximation, in which in the sums on the right-hand side of (13) only the terms with $q = k$ are retained and the electron number operator is replaced by its mean value $n_p = \langle a^+_p a_p\rangle$, which leads, for example, to terms usually not taken into account in such decouplings [2,5]:

$$\langle\langle \rho_{p\,k-q}(b_q + b^+_{-q}); N_{-k}\rangle\rangle \simeq \delta_{q,k} n_p \langle\langle (b_k + b^+_{-k}); N_{-k}\rangle\rangle.$$

Obviously, this approximation corresponds to the approximation of random phases [9], in which neither the processes of exchange electron–electron scattering nor the processes of electron-phonon relaxation are taken into account. To include them, one should consider equations for more complicated Green' s functions on the right-hand side of (13). In the adopted approximation we immediately obtain

$$(\omega + \varepsilon_p - \varepsilon_{p+k})\langle\langle \rho_{pk} \mid N_{-k}\rangle\rangle^{(0)}_\omega = \frac{1}{2\pi}(n_p - n_{p+k})\varepsilon^{-1}(k,\omega). \qquad (14)$$

As is seen from equations (7a), (12), (14), we have arrived at well-known results [8,9], and therefore we shall not dwell on their discussion. We note only that, since the explicit form of the interaction χ_q was not used by us, we can directly obtain the results of the work [12] concerning the spectrum of real phonons, in which an interaction χ_q, somewhat different from [9], is considered.

When calculating the mean current in the system $\mathbf{J}(k,\omega) = \sigma(k,\omega)\mathbf{E}(k,\omega)$, one should take into account the screening of the external field, as a result of which

for the conductivity $\sigma(k,\omega)$, analogously to the consideration carried out in (1) –(7), we obtain the expression (for more details see [13])

$$\sigma(k,\omega)=\varepsilon(k,\omega)\frac{2\pi i}{V}\frac{e^2}{mk^2}\sum_p\left(\mathbf{p}+\frac{\mathbf{k}}{2}\right)\cdot\mathbf{k}\,\langle\langle\rho_{pk}\mid N_{-k}\rangle\rangle_\omega, \tag{15}$$

which has the additional factor $\varepsilon(k,\omega)$ in comparison with the expression in [7], where screening of the external field was not taken into account. The solution (14), obtained in fact in the same approximation as in [7], leads to the conductivity of a free electron gas, as was to be expected, since electron-phonon relaxation processes are not taken into account in it. Taking into account equations for Green' s functions of higher order in (13), similarly to [2,3,6], should lead to the usual expression for the conductivity of a metal.

Thus, by the method of two-time Green's functions it is possible, very simply, to obtain the known results concerning the dielectric permittivity of the electron-phonon system (9), and also to take proper account of the screening of the external field in calculating the conductivity.

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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.