Thermal effects in spatial dispersion of the conductivity of one-dimensional systems

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The low-temperature conductivity $\sigma(\omega,q)$ of one-dimensional disordered metals in an external field with an arbitrary frequency ω and a wave vector q is calculated allowing for the scattering of electrons by thermal phonons. It is shown that the dependence of the electrical conductivity on q is oscillatory with a period $\pi[l_i|\ln(\tau_i/2\tau_{ph})|]^{-1}$, which is governed by the characteristic separation between two quasistationary localized states which appear as a result of quasielastic scattering of electrons by vibrating impurities. An analysis is made of the characteristic features of the temperature dependence of the frequency of the electron-phonon interaction and of the value of $\sigma(\omega,q)$ associated with the one-dimensional nature of carrier motion.

1. INTRODUCTION

A rigorous theory of the electrical conductivity $\sigma(\omega,q)$ of one-dimensional disordered metals subjected to an alternating inhomogeneous external field with a frequency ω and a wave vector q was developed by Berezinskiĭ.[1] The complex mathematical structure of the main equations of this theory has been the reason why for several years the main topics in studies of the kinetics of such systems has been the frequency dependence of the conductivity in homogeneous fields ($q=0$). Detailed studies have been made of $\sigma(\omega)$ both at $T=0$ (Refs. 1 and 2) and at finite temperatures (see the review in Ref. 3 and the literature cited there).

The problem of the conductivity of $1d$ metals in an inhomogeneous electric field was solved relatively recently.[4] This was done by solving the Berezinskiĭ equations for an arbitrary value of the spatial dispersion parameter ql_i, where l_i is the mean free path of an electron governed by the scattering on impurities. It was found that the dependence of the conductivity of a $1d$ metal on the wave vector is quite different from that in the three-dimensional case. One of the results of Ref. 4 was a prediction of a geometric resonance effect manifested by an oscillatory dependence of the conductivity on the wave number q. One should also mention that all these results were obtained only for the temperature $T=0$.

A solution of the problem of the temporal and spatial dispersion of the conductivity $\sigma(\omega,q)$ of a disordered $1d$ metal at finite temperatures is related closely to the problem of the interaction of electrons with phonons in systems of this kind. It is known[3,5] that phonons in one-dimensional metals have a dual influence. First of all, the induced transitions of electrons between localized states can give rise to delocalizing effect tending to increase the conductivity. On the other hand, the scattering by short-wavelength phonons with a momentum $q\sim 2p_0$ (p_0 is the Fermi momentum) is an additional factor which results in electron localization.

The delocalizing role of the electron-phonon interaction is manifested most clearly in the case when the displacement field varies rapidly during the mean free time of an electron between collisions, i.e., when

$$\omega_{ph}\gg\max\{\tau_i^{-1},\tau_{ph}^{-1}\}. \tag{1}$$

Here, ω_{ph} is the characteristic phonon frequency; τ_i and τ_{ph} are the mean free times of electrons scattered by impurities and by phonons, respectively. It was shown in Ref. 6 that in this limiting case the scattering of electrons by phonons can be simply allowed for in the ladder approximation, whereas the scattering by impurities has to be included exactly. In other words, the conductivity $\sigma(\omega,q)$ of a one-dimensional metal at a finite temperature can be calculated, according to Ref. 6, using the Berezinskiĭ equations in which the real frequency ω is replaced with the sum $\omega+i/\tau_{ph}$.

A calculation of the conductivity of a $1d$ metal at low temperatures when $T\tau_i\ll 1$ is a difficult task. The first reason for this situation is that at temperatures of this kind the localization due to phonons is also important and this requires an accurate description of the repeated scattering of electrons by both impurities and phonons allowing for the mutual interference between these processes. Moreover, at low temperatures the very mechanism of the interaction between electrons and phonons changes. This is due to the fact that at temperatures below the Debye value the main role is played by long-wavelength phonons and the interaction of these with electrons is greatly weakened by the electron screening effect.[7] Consequently, the familiar deformation mechanism does not operate in the case of $1d$ metals and the electron-phonon interaction in the metals is governed largely by the weaker cross-deformation and inertial mechanisms.

We shall consider the spatial dispersion of the electrical conductivity in the range of temperatures defined by the inequality of Eq. (1), which makes it possible to ignore the effect of localization of electrons in the course of their scattering by phonons. For this purpose we have to regard the temperatrue as low compared with the Debye frequency ω_D. Then, the characteristic phonon frequency ω_{ph} is determined by temperature and Eq. (1) yields the condition

$$1/\tau_i\ll T\ll\omega_D. \tag{2}$$

Naturally, the inequalities of Eq. (2) can be satisfied only if $\omega_D\tau_i\gg 1$, i.e., when the scattering of electrons by impurities is sufficiently weak.

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2. INITIAL RELATIONSHIPS

In the range of temperatures defined by the inequalities of Eq. (2) the spatial and temporal dispersion of the electrical conductivity $\sigma(\omega,q)$ of a one-dimensional metal is described[6] by the Berezinskiĭ equations in which the substitution $\omega \to \omega + i/\tau_{ph}$ is made. This replacement is correct subject to the condition (2) and subject to the inequality

$$|\omega+i/\tau_{ph}|\tau_i \ll 1. \tag{3}$$

It means[6] that the scattering by phonons is practically isotropic, i.e., that the probability of such scattering is independent of the sign of the electron velocity. We shall show below that if $T \ll \omega_D$, then the ratio τ_i/τ_{ph} is always small compared with unity and, consequently, the inequality of Eq. (3) reduces to $\omega\tau_i \ll 1$.

Using the results of Ref. 4, where the Berezinskiĭ equations were solved for arbitrary wavelengths and complex frequencies, we shall write down the conductivity equation in the form

$$\sigma(\omega, q)=\sigma_0 \sum_{\pm} \pi \int_0^{\infty} d\mu \frac{\mu \operatorname{sh}(\pi\mu/2)}{\operatorname{ch}^2(\pi\mu/2)} \frac{D_\mu(z)}{(\mu^2+\Delta_\pm^2)}. \tag{4}$$

The following notation is used above:

$$z=-2i(\omega+i/\tau_{ph})\tau_i, \quad \Delta_\pm^2=1+2z\pm 4iql_i, \tag{5}$$

$l_i = v\tau_i$ is the mean free path of electrons in the case of backscattering by impurities, v is the Fermi velocity, and $\sigma_0 = ne^2\tau_i/m$ is the dimensional factor which is identical in form with the static conductivity of a three-dimensional metal. The delocalization factor $D_\mu(z)$ describes the influence of localization of electron states on the electrical conductivity. Its asymptotic forms for low and high values of z can be found in Ref. 4.

It is clear from Eqs. (4) and (5) that the delocalization factor is governed by the complex parameter z and depends strongly on the ratio of the times τ_i and τ_{ph}. We shall first consider possible values of the ratio τ_i/τ_{ph}. We shall estimate the mean free time τ_{ph}. In the range of temperatures of interest to us the usual deformation interaction is absent and the scattering of electrons by phonons is due to the cross-deformation and inertial mechanisms. For the first of these mechanisms the frequency $1/\tau_{ph}$ of the scattering of electrons by phonons is proportional to the square of the modulus of the product of the effective constant Λ of the cross-deformation interaction and the strain tensor $u \sim (q/Ms)^{1/2}$ (s is the velocity of sound and M is the mass of an ion) multiplied by the relative number of phonons participating in the scattering process (which in the one-dimensional case is of the order of $q/p_0 \sim T/\omega_D$) and by the delta function which describes the law of conservation of energy (on the $1/\varepsilon_F$ scale because of the absence of intergration over angles in one measurement). We consequently obtain the estimate

$$\frac{1}{\tau_{ph}} \sim |\Lambda|^2 \frac{q}{Ms} \frac{q}{p_0} \frac{1}{\varepsilon_F} \sim |\Lambda|^2 \frac{T^2}{\varepsilon_F^2 \omega_D}. \tag{6}$$

In the case of the cross-deformation interaction the role of the constant Λ is played by the x-dependent quantity[7]

$$\Lambda(x)=(\Delta/\tau_i)\zeta(x),$$

where x is the electron coordinate, Λ is the cross-deformation potential tensor (of the scale of unity), and $\zeta(x)$ is a complex random Gaussian field with a correlation function

$$\langle \zeta(x)\zeta^+(x')\rangle = l_i\delta(x-x'). \tag{7}$$

The delta function appears in the above expression because the correlation function (7) is calculated for the limit $\xi \to 0$ (Ref. 8), where ξ is the correlation radius of a random field $\zeta(x)$. We therefore have to assume that in the case of identical arguments the delta function is of the order of $1/\xi$. Bearing in mind that the correlation radius ξ is of the atomic size, we obtain from Eq. (7) the following estimate

$$\zeta(x) \sim (p_0 l_i)^{1/2}. \tag{8}$$

Consequently, the effective cross-deformation interaction constant can be estimated from

$$\Lambda \sim (|\Delta|/\tau_i)(p_0 l_i)^{1/2} \sim (\varepsilon_F/\tau_i)^{1/2}. \tag{9}$$

Substituting this result into Eq. (6), we obtain

$$1/\tau_{ph} \sim T^2/\tau_i \varepsilon_F \omega_D, \quad T \ll \omega_D. \tag{10}$$

A calculation carried out using the transport equation makes it possible to obtain the exact result:

$$1/\tau_{ph}=\tau_i^{-1}(4\pi|\Delta|^2 a/3Ms^3)T^2, \tag{11}$$

where a is the lattice constant in the direction of the chains.

We therefore reached the conclusion that in the case under discussion the frequency of the scattering of electrons by thermal phonons is much less than the frequency of the scattering of electrons by impurities:

$$\tau_i/\tau_{ph} \sim T^2/\varepsilon_F \omega_D \ll 1. \tag{12}$$

Consequently, at low temperatures the electrons are scattered mainly by impurities. Collisions with phonons are relatively rare and in the intervals between them the electron states become localized.

The inertial electron-phonon interaction mechanism at low temperatures $T \ll \omega_D$ does not contribute to the transport time τ_{ph}, because the number of photons with the momentum $2p_0$ is exponentially small.

3. ANALYSIS OF SPATIAL DISPERSION OF THE CONDUCTIVITY

The simplest results are obtained in the limiting case of high frequencies $\omega\tau_i \gg 1$. In this frequency range the scattering of electrons by phonons can be ignored. Therefore, the conductivity is independent of temperature and is described by the appropriate formula from Ref. 4. In particular, the imaginary part of the conductivity is given by the Drude formula and the dissipative part differs numerically from the Drude formula because of the localization of electron states.

The most interesting is the frequency range $\omega\tau_i \ll 1$. We then have $|z| \ll 1$ and the function $D_\mu(z)$ is a sum of two different terms[4]:

$$D_\mu(z)=\pi z/\operatorname{ch}(\pi\mu/2) - {}^1/_4 \pi z \operatorname{sh}^{-2}(\pi\mu/2)\left[\Gamma^{-2}(1+i\mu/2)(z/4)^{i\mu} + \Gamma^{-2}(1-i\mu/2)(z/4)^{-i\mu}\right], \tag{13}$$

where $\Gamma(x)$ is the gamma function. The corrections to each of the terms in Eq. (13) are characterized by a relative smallness of the order of z. It should be pointed out that representation of the delocalization factor $D_\mu(z)$ in the form of Eq. (13) does not literally represent an expansion in terms of z. In the absence of phonons the first term in Eq. (13) allows for the localization of the electron states and gives the dominant contribution to the polarizability. The low-frequency dissipative conductivity due to the hopping mechanism appears because of the second term in Eq. (13). When an allowance is made for the scattering by phonons, the parameter z of Eq. (5) becomes complex (and not just purely imaginary) and an additional contribution to the dissipative conductivity is made by the first term in Eq. (13).

In accordance with Eq. (13), we shall represent the complex conductivity as a sum of two terms, $\sigma = \sigma^{(1)} + \sigma^{(2)}$, and we shall analyze the dependence $\mathrm{Re}\sigma^{(2)}$ on the wave number q. We shall first discuss the case when $\omega = 0$. Then, $\sigma^{(1)}(0,q)$ is given by the expression

$$\sigma^{(1)}(0,q)=2\sigma_0\frac{\tau_i}{\tau_{ph}}\int_0^\infty d\mu\, w(\mu)\frac{\nu(\mu)}{\nu^2(\mu)+(ql_i)^2}[1+O(\tau_i/\tau_{ph})], \tag{14}$$

where

$$w(\mu)=\frac{\pi^2}{2}\frac{\mu\,\mathrm{sh}(\pi\mu/2)}{\mathrm{ch}^3(\pi\mu/2)}, \qquad \nu(\mu)=\frac{1+\mu^2}{4}.$$

The formula (14) describes the contribution made to the static conductivity by those electrons which are in localized states, that now become quasistationary states because of the electron-phonon scattering.

The spatial dispersion of $\sigma^{(1)}(0,q)$ is governed essentially only by the mean free path in the case of the scattering by impurities l_i, because $l_i \ll l_{ph} = v\tau_{ph}$. In the limiting case of low values of q when $(ql_i)^2 \ll 1$ Eq. (14) yields the following result first obtained in Ref. 6:

$$\sigma^{(1)}(0,\ q)=4\zeta(3)\sigma_0\tau_i/\tau_{ph}. \tag{15}$$

At high values of ql_i this conductivity decreases strongly because of the spatial dispersion,

$$\sigma^{(1)}(0,\ q)=\sigma_0(\tau_i/\tau_{ph})\,(ql_i)^{-2}, \tag{16}$$

and is independent of the time τ_i in the case of the scattering of electrons by impurities.

The form q of the part of the conductivity $\sigma^{(2)}(0,q)$ which is due to the second term on the right-hand side of Eq. (13) is more complex. The reason is that the second term in the expression for $D_\mu(z)$ contains not only l_i but also an additional large parameter with the dimension of length, which represents the length of a jump of an electron between localized states, proportional to $\ln|z|$. Consequently, the range of low values of q when $ql_i \ll 1$ splits into two intervals with different dependences of the conductivity on the wave number q. In the range of low values of q, when

$$2ql_i|\ln(\tau_i/2\tau_{ph})| \ll 1, \tag{17}$$

we find that

$$\sigma^2(0,\ q)=-4\sigma_0(\tau_i/\tau_{ph})^2\ln^2(\tau_i/2\tau_{ph}). \tag{18}$$

This quantity is small compared with $\sigma^{(1)}(0,q)$ of Eq. (15) because of the smallness of the parameter $\alpha\ln^2\alpha$, where $\alpha = \tau_i/\tau_{ph}$. On the other hand, in view of the large value of the logarithm $[\ln^2(\tau_i/2\tau_{ph}) \gg 1]$ the quantity given by Eq. (13) exceeds the corrections to the main term $\sigma^{(1)}$ representing the higher powers of α.

It should be noted that in the limit of very low values of q the static conductivity $\sigma^{(2)}(0,q)$ exhibits spatial dispersion in the range $q \sim l_{ph}^{-1}$: if $ql_{ph} \ll 1$, then $\sigma^2(0,q)$ contains the factor $1+4(ql_{ph})^2$ whereas for $ql_{ph} \gg 1$ the factor is $1+3(ql_{ph})^{-2}$, i.e., if $ql_{ph} \sim 1$ there is a minimum of $\sigma^{(2)}(0,q)$.

It follows from Eq. (18) that the corresponding contribution to the conductivity is due to transitions of electrons between localized states separated on the average by the distance

$$L=2l_i|\ln(\tau_i/2\tau_{ph})|. \tag{19}$$

The order of magnitude of this distance is readily obtained on the basis of the familiar arguments of Mott[9] if we bear in mind that localized electron states become quasistationary because of the scattering by phonons. A characteristic broadening of the energy levels of the localized states is then $1/\tau_{ph}$.

When q is increased, so that the inequality in Eq. (17) is reversed, an oscillatory dependence of $\sigma^{(2)}(0,q)$ on q is obtained:

$$\sigma^{(2)}(0,q)=\frac{2\sigma_0}{1+(qv\tau_{ph})^2}\left\{\frac{1-(qv\tau_{ph})^2}{1+(qv\tau_{ph})^2}+2\frac{\tau_i}{\tau_{ph}}\ln\frac{\tau_i}{2\tau_{ph}}\right.$$
$$\left.-\exp\left[-2\left((ql_i)^2+\frac{\tau_i}{\tau_{ph}}\right)\left|\ln\frac{\tau_i}{2\tau_{ph}}\right|\right]\right.$$
$$\left.\times\cos\left[2ql_i\ln\frac{\tau_i}{2\tau_{ph}}-2\tan^{-1}(qv\tau_{ph})\right]\right\}. \tag{20}$$

Equation (20) is obtained as a result of an explicit calculation of the integral (4) involving the substitution in place of $D_\mu(z)$ of the second term from Eq. (13). Therefore, the effects of spatial dispersion are allowed for asymptotically accurately in respect of the parameter α. A theoretical analysis of the dependence $\sigma^{(2)}(q)$ in the range where $2qL \gtrsim 1$ is cumbersome and does not give clear results. Therefore, we calculated numerically the values of $\sigma^{(2)}(0,q)$ and the results are plotted in Fig. 1. The abscissa represents the parameter ql_i and the ordinate the function $\mathrm{Re}\sigma^{(2)}\tau_{ph}/\sigma_0\tau_i$. We can clearly

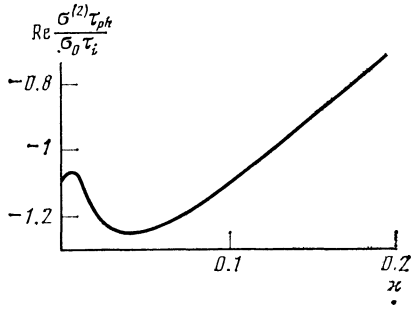

FIG. 1. Dependence of the oscillatory part of the conductivity $\sigma^{(2)}(0,q)$ on the spatial dispersion parameter $\varkappa = ql_i$, calculated for $\tau_i/\tau_{ph} = 10^{-2}$.

see one oscillation of the conductivity in the range of q where $ql_i < 0.1$. The significant difference of the corresponding part of the curve from the sinusoid is due to the presence of a term $\tan^{-1}(qv\tau_{ph})$ in the argument of the cosine of Eq. (20). The structure of the curve in the region of $q \sim l_{ph}^{-1}$ cannot be seen in Fig. 1 because of the inequality $l_{ph} \gg l_i$.

These oscillations are of the same origin as the corresponding oscillations in the geometric resonance effect predicted in Ref. 10. They are due to the oscillatory dependence of the matrix element of a transition on the phase advance qL experienced by an external wave in a distance L representing an electron jump. The second and subsequent periods cannot be seen in Fig. 1 because they fall in the range of values of q where their amplitude becomes exponentially small. Such an exponential damping of the conductivity oscillations is explained by the fact that in reality the length L is not rigorously fixed but exhibits a normal distribution near its average value given by Eq. (19).

Finally, in the range $ql_i > 0.1$, the quantity $\sigma^{(2)}(0,q)$ decreases proportionaly to $1/q^2$:

$$\sigma^{(2)}(0, q) = -2\sigma_0/(qv\tau_{ph})^2. \quad (21)$$

In this region the value of $\sigma^{(2)}(0,q)$ is small compared with the main term in the expression where the parameter is τ_i/τ_{ph}

The temporal dispersion of the low-temperature conductivity is governed by the parameter $\omega\tau_{ph}$ and becomes significant already at low frequencies where $\omega\tau_i \ll 1$. We can allow for the dependence of $\mathrm{Re}\sigma^{(2)}$ on the frequency ω simply by replacing the arguments of the logarithms in Eq. (20) with the quantity

$$|z|/4 = (\tau_i/2\tau_{ph})[1 + (\omega\tau_{ph})^2]^{1/2} \quad (22)$$

and multiplying the whole of Eq. (20) by $1 - (\omega\tau_{ph})^2$. In the case of the principal term of $\sigma^{(1)}(0,q)$ in Eq. (15), the frequency-dependent corrections are proportional to the small parameter $(\omega\tau_i)^2 \ll 1$.

We shall conclude by considering briefly the temperature dependence of the electrical conductivity. The value of the conductivity is governed primarily by the term $\sigma^{(1)}$ of Eq. (15). Since, as already pointed out, in a one-dimensional metal the collision frequency $1/\tau_{ph}$ is proportional to T_2, the dependence $\mathrm{Re}\sigma(T)$ at temperatures defined by the inequalities of Eq. (2) is basically quadratic.

In the inhomogeneous case it is worth noting the dependence on T of the positions of extrema of the oscillatory part of the conductivity $\mathrm{Re}\sigma^{(2)}$. We can see from Eq. (20) that this dependence is fairly complex. However, the general tendency is that as predicted and this is confirmed by numerical calculations, so that cooling shifts the conductivity oscillations toward lower values of the parameter ql_i.

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