Localization of electrons in one-dimensional conductors due to scattering by nondispersing phonons

A. A. Gogolin

L. D. Landau Institute of Theoretical Physics, USSR Academy of Sciences

(Submitted 9 March 1983)
Zh. Eksp. Teor. Fiz. **85**, 1131–1141 (September 1983)

The localization of electrons in one-dimensional conductors, due to scattering by nondispersing phonons at low temperatures, when the phonon occupation numbers are low ($N \ll 1$), is investigated by the Berezinskiĭ diagram technique. It is shown that the localization length $l_{\rm loc}$ in this case is large compared with the mean free path $l_2 \sim l_1/N$ with respect to the parameter $(pl_1)^2 \gg 1$, which is determined by the characteristic electron momentum p. The asymptotic value of the low-frequency conductivity, ${\rm Re}\sigma(\omega) \propto \omega^2|\ln^3\omega|$, deviates noticeably from Mott's law.

PACS numbers: 71.50. + t, 71.38. + i, 72.10.Di

1. INTRODUCTION

The great theoretical and practical interest recently aroused by Mott localization in one-dimensional conductors (see the reviews 1–4) raises the question of the region of existence of this effect and the feasibility of its experimental observation in real quasi-one-dimensional conductors. Since most presently known quasi-one-dimensional organic conductors do not have a strong structural disorder (see Refs. 5 and 6), the question is whether localization effects exist in such systems. This question is closely related to the problem of electron localization via various elastic-scattering mechanisms not due to the presence of impurities and defects that are randomly located in a one-dimensional conductor.

The present paper deals with the elastic-scattering mechanism connected with the nondispersing intramolecular phonons. It is shown that this mechanism leads to electron-state localization but of a type that differs substantially from that in the usual impurity problem.[1,7] The localization length $l_{\rm loc}$, in particular, turns out to be larger than the mean free path l_2 for phonon absorption.

We consider low temperatures $T \ll \omega_0$, where ω_0 is the frequency of the intramolecular phonon. In this case the phonon occupation numbers are extremely small, so that the mean free path l_2 for phonon absorption is long enough: $l_2 \sim l_1/N \gg l_1$, where l_1 is the mean free path for phonon emission. The absorption of the phonons is therefore relatively infrequent and is accompanied by their rapid emission. We get thus an effective electron scattering similar to the usual impurity scattering. This analogy, however, is complete only in the three-dimensional case, first considered by Fröhlich and Mott,[8] when the electron motion is described by the usual kinetic equation.

It is known that a very important problem for one-dimensional systems is that of the phase structure of the scattered wave, and is directly connected with the localization problem.[1–4,7] In this sense, successive two-phonon scattering differs noticeably from impurity scattering, for in the intermediate hot state following the phonon absorption there is a phase change of the order of $pl_1 = 2\pi l_1/\lambda$, a change absent in scattering by impurities. As shown in a preceding paper,[9] at large values $pl_1 \gg 1$ the contribution of the elastic scattering by nondispersing phonons does not lead, in the lowest zeroth order in the parameter $(pl_1)^{-1}$, to localization of the electron states and differs thereby substantially from ordinary impurity scattering. This result, however, was due to neglect of the higher orders of the expansion in $(pl_1)^{-1} \ll 1$, which will be shown in the present paper to lead to localization of the electron states with large value $l_{\rm loc} \sim (pl_1)^2 l_2 \gg l_2$. We note that in the present paper we take into account only single-particle effect, so that we are considering a nondegenerate electron gas of very low density (semiconducting situation), in which the effects of electron-electron interaction do not play a significant role. In real situations such an electron system can be realized in quasi-one-dimensional organic semiconductors, which include at sufficiently low temperature most TCNQ salts.[5,6]

2. ANALYSIS OF THE DIAGRAM SERIES

We consider a one-dimensional system of noninteracting electrons with low density n and with a quadratic dispersion law $\varepsilon(p) = p^2/2m^* = m^*v^2/2$. We assume that the electrons interact with one branch of the nondispersing phonons with frequency ω_0. The Hamiltonian of the interaction is of standard form[1] and is linear in the phonon operators. To investigate the character of the localization, of the electric conductivity, and of the dielectric constant it is necessary to calculate the correlation functions of the current and density operators. A convenient diagram technique for these purposes is described in the preceding papers.[1,7,9,10]

In view of the absence of phonon dispersion, the electron energy returns to its exact initial value after absorption and emission of an equal number of phonons, meaning that the scattering is effectively elastic so that it is necessary to take into account the interference effects connected with scattering by phonons. In diagram language[9] this leads to the need for summing graphs with intersections of the phonon lines, graphs that were found to be insignificant in the case of sufficiently large phonon dispersion.[1,10]

At low temperatures $T \ll \omega_0$ the electron is scattered by phonons via infrequent absorption followed by rapid emission of phonons. The lifetime of the hot electrons with energy $\varepsilon + \omega_0$ is then much shorter (relative to the parameter $N \approx \exp(-\omega_0/T) \ll 1$), than that of the cold states with energy $\varepsilon \sim T$. As a result the damping of a Green's function with

0038-5646/83/090657-08$04.00

energy ε is small compared with the damping of a Green's function with energy $\varepsilon + \omega_0$ (relative to the parameter $N \ll 1$). The electron mean free paths $l^+(\varepsilon)$ and $l^-(\varepsilon)$ for forward and backward scattering, which describe the spatial damping of the Green's functions $G(\varepsilon, x, x')$ (Ref. 1), are given by

$$[l^{\pm}(\varepsilon)]^{-1}=[l_1^{\pm}(\varepsilon)]^{-1}+[l_2^{\pm}(\varepsilon)]^{-1}, \tag{1}$$

$$\frac{1}{l_2^{\pm}(\varepsilon)}=\frac{1}{v(\varepsilon)}\int\frac{d^3\mathbf{q}}{(2\pi)^2}|c_\mathbf{q}|^2\frac{N}{v(\varepsilon+\omega_0)}\delta(q_x+p(\varepsilon)\mp p(\varepsilon+\omega_0)), \tag{2}$$

$$\frac{1}{l_1^{\pm}(\varepsilon)}=\frac{1}{v(\varepsilon)}\int\frac{d^3\mathbf{q}}{(2\pi)^2}|c_\mathbf{q}|^2\frac{N+1}{v(\varepsilon-\omega_0)}\delta(q_x+p(\varepsilon)\mp p(\varepsilon-\omega_0)),\quad \varepsilon>\omega_0, \tag{3}$$

where c_q is the matrix element of the electron-phonon interaction.

At $\varepsilon < \varepsilon_0$ and $\varepsilon > \varepsilon_0$ we have respectively $l^{\pm}(\varepsilon) = l_2^{\pm}(\varepsilon)$ and $l^{\pm}(\varepsilon) \approx l_1^{\pm}(\varepsilon)$, with $l_1^{\pm}(\varepsilon) \ll l_2^{\pm}(\varepsilon)$ to the extent that N is small. We shall assume hereafter for simplicity that $l_i^+(\varepsilon) = l_i^-(\varepsilon) = l_i(\varepsilon)$, $i = 1; 2$. This assumption that the scattering is isotropic is certainly satisfied in the case $c_q = \text{const}$, to which correspond the basic mechanisms of interaction of electrons with intramolecular vibrations of large organic molecules.[11]

Examples of diagrams corresponding to successive absorption and emission of phonons by cold electrons and containing no rapidly oscillating factors are shown in Fig. 1. The rapid damping of the Green's functions with energy $\varepsilon + \omega_0$ causes the integral over the distance between the phonon lines to converge on a length $\sim l_1$ and the integral with respect to the position of pair of phonon lines to converge on a length $\sim l_2$. Therefore, integrating first over the lengths of the hot lines and taking the elasticity of successive two-phonon scattering into account, we obtain for the vertices effective expressions analogous to the usual impurity correlators.[1,7,9,10] It must be emphasized here that rapid damping of the hot lines is ensured by the self-energy insets that contain cold electron lines. These lines can be "drawn out" of the effective two-phonon vertex in the form of long "tongues" connected to other two-phonon vertices. The skeleton diagram of Fig. 2a is therefore transformed into the effective many-point diagram shown in Fig. 2. An effective expression for this vertex can be easily calculated. Indeed, integrating over the positions of the inner phonon lines x_i and y_i and then over the difference $z' - z$ we easily obtain for a diagram with r internal phonon lines in the upper part and s lines in the lower part of the diagram:

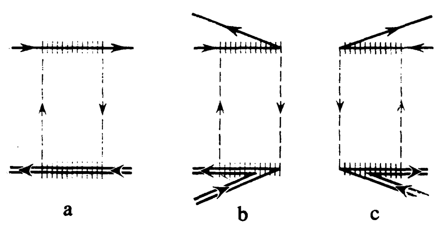

FIG. 1. Skeleton two-phonon vertices containing no rapidly oscilating factors. The hatches mark the hot lines.

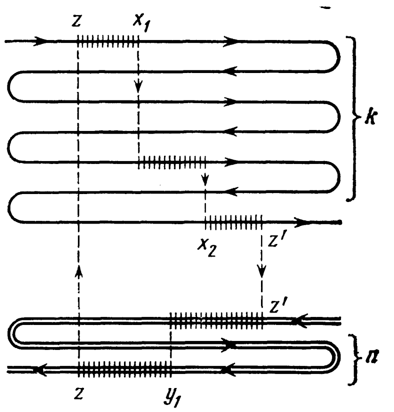

FIG. 2. Elaboration of the skeleton diagram because of drawing out of cold lines.

$$\frac{1}{l_1l_2}\int_0^\infty d(z'-z)\exp\left[-\frac{2}{l_1}(z'-z)\right]$$
$$\times\left(-\frac{2}{l_1}\right)^{r+s}\int_0^{z'-z}dx_1\int_0^{x_1}dx_2\ldots\int_0^{x_{r-1}}dx_r\int_0^{z'-z}dy_1\int_0^{y_1}dy_2\ldots\int_0^{y_{s-1}}dy_s$$
$$=\frac{1}{l_1l_2}\int_0^\infty d(z'-z)\frac{1}{r!s!}\left[-\frac{2}{l_1}(z'-z)\right]^{r+s}\exp\left[-\frac{2}{l_1}(z'-z)\right]$$
$$=\frac{1}{2l_2}(-1)^{r+s}C_{r+s}^r. \tag{4}$$

Summation over all the arrangements of the internal phonon lines leads to the following effective expression for the vertex $\Gamma_{k,n}$ with k and n tongues in the upper and lower parts of the diagram of Fig. 2:

$$\frac{1}{2l_2}\Gamma_{k,n}=\frac{1}{2l_2}\sum_{r,s}(-1)^{r+s}C_{r+s}^rC_{k-1}^{r-1}C_{n-1}^{s-1}. \tag{5}$$

This expression can be easily simplified with the aid of the known integral representation for the binomial coefficients $C_{r+s}{}^r$:

$$C_{r+s}^r=\frac{1}{2\pi i}\oint\frac{dz}{z^{r+1}(1-z)^{s+1}}, \tag{6}$$

where the integration is along a small circle around $z = 0$. Substituting (6) in (5) we obtain after simple transformations

$$\Gamma_{k,n}=(-1)^{k-n}C_2^{k-n+1}=2\delta_{k,n}-\delta_{k,n+1}-\delta_{n,k+1}. \tag{7}$$

As shown in a preceding paper,[9] expressions (5) and (7) correspond to all the skeleton diagrams shown in Fig. 1, with diagrams c and d corresponding also to a phase factor $e^{2i\omega z/v}$, while e and f to a factor $e^{-2i\omega z/v}$, where ω is the external frequency. As a result we have for the right-hand and central parts $R_m(x)$ and $Z_{m'm}(x',x)$ of the polarization loop that describes the correlation functions of the density $\mathscr{H}^a(\omega,k)$ $(a = 0)$ and of the current $(a = 1)$ (Ref. 9)

$$-\frac{d}{dx}R_m=-\frac{4m}{l_2}R_m+\frac{1}{l_2}\Gamma_m(R_{m+1}e^{-2i\omega x/v}+R_{m-1}e^{2i\omega x/v}+2R_m), \tag{8}$$

$$\frac{d}{dx}Z_{m'm}=\frac{i\omega}{v}Z_{m'm}-\frac{2}{l_2}(2m+1)Z_{m'm}$$
$$+\frac{1}{l}\left(\Gamma_m Z_{m'm-1}e^{-2i\omega x/v}+\Gamma_{m+1}Z_{m'm+1}e^{2i\omega x/v}\right)$$
$$+\frac{1}{l_2}(\Gamma_m+\Gamma_{m+1})Z_{m'm}, \qquad (9)$$

where

$$\Gamma_m\equiv\sum_{k,n=0}^{m}(m-k)(m-n)\Gamma_{k,n}=m \qquad (10)$$

is determined by the number of methods of connecting the many-point vertex. The coordinate dependence of the quantities $R_m(x)$ is trivial, $R_m(x)=R_m e^{2im\omega x/v}$, and can be easily separated. The equations for R_m therefore take the form

$$i\tilde{v}mR_m+m(R_{m+1}+R_{m-1}-2R_m)=0,\quad R_0=1,\quad \tilde{v}=2\omega\tau_2=2\omega l_2/v. \qquad (11)$$

The correlation functions $\mathscr{H}^a(\omega,k)$ are expressed in terms of the quantities P_m^a and Q_m^a defined by the formulas

$$P_m{}^0={}^1/_2(R_m+R_{m+1}),\quad P_m{}^1=R_m-R_{m+1}, \qquad (12)$$

$$Q_m{}^a(\omega,k)$$
$$=\frac{1}{l_2}\sum_{m'=0}^{\infty}\int_{x'}^{\infty}dx e^{ik(x'-x)}e^{-2i\omega m'x'/v}Z_{m'm}(x',x)e^{2i\omega mx/v}P_{m'}{}^a \qquad (13)$$

in the following manner[1,7,9,10]:

$$\mathscr{X}^a(\omega,k)=4T\int\frac{d\varepsilon}{2\pi}\left(-\frac{\partial n}{\partial\varepsilon}\right)\frac{1}{v(\varepsilon)}X^a(\varepsilon,\omega,k), \qquad (14)$$

$$X^a(\varepsilon,\omega,k)$$
$$=\frac{2l_2}{v(\varepsilon)}\left[\frac{v(\varepsilon)}{2}\right]^{2a}\sum_{m=0}^{\infty}P_m{}^a(\omega)[Q_m{}^a(\omega,k)+Q_m{}^a(\omega,-k)], \qquad (15)$$

where $n(\varepsilon)$ is the Boltzmann distribution function.

The equations for $Q_m{}^a(\omega,k)$ take then the form

$$i\tilde{v}(m+{}^1/_2)Q_m{}^a+(m+1)(Q_{m+1}^a-Q_m{}^a)-m(Q_m{}^a-Q_{m-1}^a)$$
$$-i\tilde{\varkappa}Q_m{}^a+P_m{}^a=0,\quad \tilde{\varkappa}=kl_2. \qquad (16)$$

Equations (11) and (16) are easily solved by an exponential substitution,[9] and as a result we obtain for the conductivity $\sigma(\omega)$ the usual Drude formula with a finite value $\sigma(0)=\sigma_0=2e^2l_2/\pi S$, where S is the cross section area of one conducting filament. This result can be seen directly from the structure of Eqs. (11) and (16) as $\omega\rightarrow 0$. To this end we compare them with Berezinskiĭ's equations,[7] which take in the same notation the form

$$i\tilde{v}mR_m+m^2(R_{m+1}+R_{m-1}-2R_m)=0, \qquad (17)$$

$$i\tilde{v}(m+{}^1/_2)Q_m{}^a+(m+1)^2(Q_{m+1}^a-Q_m{}^a)-m^2(Q_m{}^a-Q_{m-1}^a)$$
$$-i\tilde{\varkappa}Q_m{}^a+P_m{}^a=0. \qquad (18)$$

It can be easily seen that in (11), (16) and in (17), (18), large $n\gg 1$ are significant at small $\tilde{v}\ll 1$. However, the structure of the difference operators in (11), (16), and (17), (18) is such that in the limit $m\gg 1$ the former contain only terms of the type $m^{n-1}(d/dm)^n$, $n=1;2$, and the latter only terms of the type $m^n(d/dm)^n$, $n=1;2$. Therefore to make (11) and (16) completely nondimensional they must be multiplied by m, as a result of which the continuous parameter becomes $m(\tilde{v})^{1/2}$ [and not $m\tilde{v}$ as in (17) and (18)], and the inhomogeneous term in (16) at $a=1$ (the current correlator) takes the form $mdR_m/dm\sim R_m$, in contrast to $dR_m/dm\sim R_m/m\ll R_m$ in (18). The presence of an extra power of m in the denominator for this term in (18) leads to vanishing of the correlator of the currents and of the conductivity as $\tilde{v}\rightarrow 0$: $\sigma(\tilde{v})\propto(-i\tilde{v})$ (Refs. 1 and 7). In Eq. (16), however, cancellation of the smallness $\sim m^{-1}\ll 1$ leads to the onset of finite conductivity $\sigma(0)=\sigma_0$.[9]

It should be noted that in the presence of both phonons and impurities in the system the resultant equations[9] will include additively the difference operators (11), (15) and (17), (18). Therefore as $\omega\rightarrow 0$, owing to the faster decrease at large m, the phonon terms, starting with a certain sufficiently small $\tilde{v}\ll 1$, become inessential even at low impurity densities, and the static characteristics are again determined by Eqs. (16) and (18) and correpond to complete localization due to scattering by impurities. In this case the phonons can determine only the rate of approach to stationary asymptotic forms and make no contribution to the static characteristics of the localized electron states.

It was concluded on this basis in the preceding paper[9] that scattering by nondispersing phonons makes no contribution to the localization of electron states. In the present paper is shown that this conclusion has restricted applicability and is due to neglect of the higher order terms of the expansion in the small parameter $(pl_1)^{-1}\ll 1$.

In fact, as will be shown in the next section, allowance for these corrections introduces into Eqs. (11) and (16) terms having a structure of the type (17) and (18), and these terms, notwithstanding the smallness of the parameter $(pl_1)^{-1}$, will predominate as $\omega\rightarrow 0$ because of the higher power of m in their expansion at large $m\gg 1$. This relative smallness of these terms $\sim(pl_1)^{-2}$ only increases the localization length $l_{\text{loc}}l_2(pl_1)^2$.

3. DERIVATION OF THE BASIC EQUATIONS OF LOCALIZATION THEORY

All the rapidly oscillating phase factors of the type exp (ipx) are completely cancelled out in the skeleton diagrams of type of Fig. 2 with insets of type 3a, a′, b, and b′. These diagrams determine therefore the term of zeroth order in the expansion in terms of the parameter $(pl_1)^{-1}\ll 1$.

To calculate the first corrections in terms of the parameter $(pl_1)^{-1}$, it is necessary to take into account, besides skeleton diagrams such as in Fig. 1, also skeleton diagrams such as in Fig. 4, in which there is no total cancellation of the rapidly oscillating factors of the type exp(ipx), as well as the corresponding insets such as 3c, c′, d, d′, which have a similar property.

We note that by taking the corrections of order $(pl_1)^{-1}$ into account we neglect the corrections of order $(pl_2)^{-1}\sim N(pl_1)^{-1}\ll(pl_1)^{-1}$, owing to the smallness of the phonon occupation numbers $N\ll 1$. Therefore the skeleton diagrams b, b′, c, c′, d, d′, e, e′, f and f′ of Fig. 4 should contain appropriate numbers of internal insets such as in Figs. 3c, c′, d, and d′, which cancel out the asymmetry in the change of the number of single and double lines in section of the diagram, as asymmetry that can arise only if account is taken of corrections for the parameter $(pl_2)^{-1} \ll 1$ are taken into account.[12] This means that the rapidly oscillating factors such as $\exp(ipx)$ can appear only in the internal integrals of type (4) with characteristic scale $x \sim l_1$, and are absent from the coordinate dependence of the total vertices integrated with respect to the internal variables of Ref. 9. Thus, the numbers of single and double lines in each section of the diagram are equal. In addition we assume that to the extent that $T \ll \omega_0$ is small we have $p(\varepsilon + \omega_0) \gg p(\varepsilon)$ at $\varepsilon \sim T$, and therefore we disregard the corrections for the parameter $[p(\varepsilon + \omega_0) l_1]^{-1} \ll [p(\varepsilon) l_1]^{-1}$. Consequently the phase factors of type $\exp(ip(\varepsilon + \omega_0)x)$, always cancel out in the diagrams of type 1–4 considered by us, and oscillations set in only on account of factors of the type $\exp(ip(\varepsilon)x)$.

By way of example we consider first the elaboration of the skeleton diagrams of Fig. 1 by additional insets such as in Figs. 3c, c′, d, and d′. Two situations are possible here: the numbers of vertices of type 2c, c′ and 3d, d′ inserted in the diagram are either equal or not. In the former case the change of the number of lines in the section of the diagram is due to external lines of the skeleton diagram of Fig. 1 and can therefore not exceed unity. In the latter case, as will be shown below, no asymmetry of the numbers of the single and double lines in the section of the diagram should arise, so that the vertices of the type 3c, 3c′ and 3d, 3d′ should be simultaneously inserted in the upper and lower parts of the effective diagram of the type of Fig. 2. In the lowest nonvanishing order in the parameter $(pl_1)^{-1}$ only one such vertex can be inserted in each (upper and lower) part of the diagram, so that when account is taken of the external lines the number m in the section of the diagram cannot change by more than 2.

We consider initially the first case. In the lowest order in $(pl_1)^{-1}$ one can insert in a diagram such as in Fig. 1 only one vertex of type 3c, c′ and one of type 3d, d′. It is easily seen that the contribution of lowest order in $(pl_1)^{-1}$ can stem from such diagrams as in Fig. 2 in which these vertices are located either on neighboring steps of the hatched ladder, or on every other step. The terms $\sim (ipl_1)^{-1}$ resulting in the first of these methods are pure imaginary and cancel one another in the final equations after summation of the contributions of the single and double lines, in analogy with the cancellation in the preceding work.[1,9,10,12,13] The first nonvanishing terms are therefore of order $(pl_1)^{-2}$.

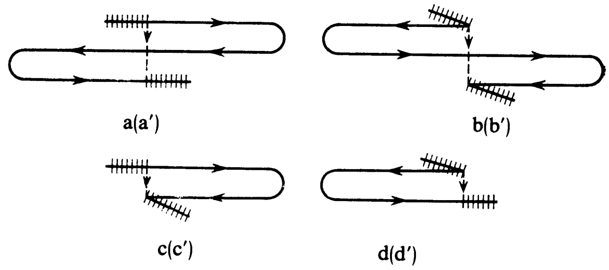
a(a′)
b(b′)
c(c′)
d(d′)

FIG. 3. Method of including cold lines in skeleton diagrams. The hatches correspond to replacement of single lines by double ones.

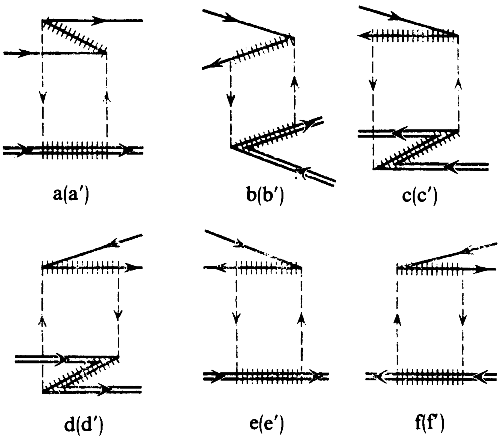
a(a′)
b(b′)
c(c′)
d(d′)
e(e′)
f(f′)

FIG. 4. Additional skeleton vertices containing rapidly oscillating factors. The hatches correspond to replacement of single lines by double ones and vice versa.

Calculating the corresponding integrals with respect to the internal variables of the type (4) with allowance for two rapidly oscillating factors of the type $\exp(2ipx_i)$ and $\exp(-2ipx_{i-n})$, $n = 1; 2$ in the neighboring integrations, and summing over all the possible arrangements of the hatched lines and "cold tongues," we obtain for the total contribution of the skeleton diagrams of the type of Fig. 1 in an equation of the type (11) the following expression:

$$
\begin{aligned}
&(2R_m+R_{m+1}+R_{m-1})\frac{-4}{(pl_1)^2}\\
&\quad\times\sum C_{r+s-1}^{r-1}C_{k-1}^{r-1}C_{n-1}^{s-1}(-1)^{r+s}(m-k)(m-n)\\
&\quad=(2R_m+R_{m+1}+R_{m-1})\frac{-4}{(pl_1)^2}\\
&\quad\times\sum_{k,\,n}(\delta_{n,k}-\delta_{n,k+1})(m-k)(m-n).
\end{aligned}
\tag{19}
$$

In the simplification of (19) we have used the integral representation (6) for C_{r+s-1}^{r-1}.

In perfectly analogous fashion we obtain in the second case the expression

$$
\begin{aligned}
&[2(R_m+R_{m+1}+R_{m-1})+R_{m+2}+R_{m-2}]\frac{2}{(pl_1)^2}\\
&\quad\times\sum_{k,n}(\delta_{n,k}-\delta_{n,k+1})(m-k)(m-n).
\end{aligned}
\tag{20}
$$

Similar expressions correspond also to the contributions of the remaining skeleton diagrams of the type of Fig. 4. Simple calculations, however, show that they cancel one another in the summation. Thus, adding (19) and (20) and summing over k from $k = 1$ to m we easily obtain the following equations for the right-hand sides of R_m, accurate to terms of second order in $(pl_1)^{-1}$:

$$
\begin{aligned}
&i\tilde{\nu}mR_m+m(R_{m+1}+R_{m-1}-2R_m)\\
&\quad+\frac{m(m-1)}{(pl_1)^2}(R_{m+2}+R_{m-2}-2R_m)=0.
\end{aligned}
\tag{21}
$$

In perfectly similar fashion we obtain also equations for Q_m^a:

$$i\tilde{\nu}(m+{}^1/_2)Q_m{}^a+(m+1)(Q_{m+1}^a-Q_m{}^a)-m(Q_m{}^a-Q_{m-1}^a)$$
$$+\frac{1}{(pl_1)^2}[(m+1)(m+2)(Q_{m+2}^a-Q_m{}^a)$$
$$-m(m-1)(Q_m{}^a-Q_{m-2}^a)]-i\tilde{\varkappa}Q_m{}^a+P_m{}^a=0. \tag{22}$$

It can be easily seen that the terms $\sim(pl_1)^{-2}$ in Eqs. (21) and (22) have the same structure as Berezinskiĭ's equations (17) and (18), and therefore predominate at low frequencies $\omega\to0$ in analogy with the corresponding impurity terms.[9] The parameter $(pl_1)^{-2}\ll1$ has here the meaning of a low effective impurity density. It must be emphasized that an analysis of the succeeding terms of the expansion in the parameter $(pl_1)^{-1}$ shows that they have a similar structure of the type $(pl_1)^{-2k}(m)^n(d/dm)^n$ and add only small corrections $\sim(pl_1)^{-2k}$ to all the numerical coefficients. In this sense they are similar to the corresponding terms in the impurity problem.[12,13]

4. DIELECTRIC CONSTANT, CONDUCTIVITY, AND LOCALIZATION LENGTH

It is known[2-4] that localization effects manifest themselves primarily in low-frequency asymptotic correlators of the density and of the current. We therefore investigate first of all the limiting case $\omega\to0$. In this limit, the major role in Eqs. (21) and (22) and in the sums (15) over m is assumed by large $m\gg1$ (Refs. 1, 7, 9). Therefore, expanding (21) and (22) in powers of small $m^{-1}\ll1$, introducing the continuous variable

$$q=(-i\tilde{\nu}m)(pl_1/2)^2 \tag{23}$$

and neglecting the small corrections $\sim(pl_1)^{-1}$ to all the numerical coefficients, we obtain the following differential equations:

$$-qR+q(q-i\nu\alpha)\frac{d^2R}{dq^2}=0, \tag{24}$$

$$-qQ^a+\frac{d}{dq}\left(q(q-i\nu\alpha)\frac{dQ^a}{dq}\right)-i\varkappa Q^a+P^a=0, \tag{25}$$

where

$$\alpha=(pl_1/2)^2,\quad \nu=\tilde{\nu}\alpha,\quad \varkappa=\tilde{\varkappa}\alpha,$$
$$P^a(q)=\alpha\left(i\nu\frac{d}{dq}\right)^aR(q),\quad a=0,1. \tag{26}$$

The expression for the correlators $x^a(\varepsilon,\omega,k)$ takes in this case the form

$$X^a(\varepsilon,\omega,k)$$
$$\approx\frac{2l_2}{v(\varepsilon)}\left[\frac{v(\varepsilon)}{2}\right]^{2a}\frac{1}{-i\nu\alpha}\int_0^\infty dqP^a(q)[Q^a(q,\varkappa)+Q^a(q,-\varkappa)]. \tag{27}$$

It follows from (26) and (27) that the correlators of the densities ($a=0$) and of the currents ($a=1$) take as $\omega\to0$ the asymptotic form

$$X^a(\varepsilon,\omega,k)\infty(-i\omega)^{2a-1}.$$

This means that the density correlator has in the time representation a stationary asymptotic form $p_\infty(x)$ as $t\to\infty$. This asymptotic form can be easily obtained from Eqs. (24) and (25), which go over as $\nu\to0$ into the corresponding equations of the impurity problem[1,7,9,10] with the impurity mean free path l_i replaced by $l=\alpha l_2$. Using the known solution[1,20,24] of these equations we obtain for $P_\infty(x)$ the expression

$$p_\infty(x)=\frac{\pi^2}{16l}\int_0^\infty\eta\,d\eta\,\mathrm{sh}\,\pi\eta\left(\frac{1+\eta^2}{1+\mathrm{ch}\,\pi\eta}\right)^2\exp\left(-\frac{1+\eta^2}{4l}|x|\right).$$
$$l=\alpha l_2. \tag{28}$$

The asymptotic form of $p_\infty(x)$ at $|x|\gg l$, which determines the localization length l_{loc}

$$l_{\mathrm{loc}}=\lim_{|x|\to\infty}|\ln p_\infty(x)/x|, \tag{29}$$

is of the form

$$p_\infty(x)\approx\frac{1}{4l(\pi)^{1/2}}\left(\frac{\pi^2}{8}\right)^2\left(\frac{4l}{|x|}\right)^{3/2}\exp\left(-\frac{|x|}{4l}\right),\quad |x|\gg l. \tag{30}$$

It follows therefore that the localization length l_{loc} is given by

$$l_{\mathrm{loc}}=4l=4\alpha l_2\gg l_2. \tag{31}$$

It is thus found that in contrast to the impurity problem[1,7,9,19,12-14] the localization length l_{loc} is much longer than the mean free path l_2. In this sense the electron localization is weak, i.e., it has a large characteristic dimension. This fact has a very simple qualitative explanation.

Indeed, the main difference between elastic two-phonon successive scattering and impurity scattering lies in the phase shift $\Delta\varphi\sim pl_1$, which takes place in the intermediate state between successive phonon absorption and emission acts. Since, however, the phonon emission probability is uniformly distributed over the entire mean free path l_1, there exists a finite small probability $\sim\lambda/l_1$ that the phonon may be emitted immediately after absorption, i.e., over a distance of the order of the wavelength λ. Therefore the amplitude of successive two-phonon scattering always contains a small admixture (of order λ/l_1) of the amplitude of pure elastic scattering with small phase shift in the intermediate state. This small impurity adds terms $\sim(\lambda/l_1)^2$ to the scattering probability and plays in fact the role of impurities with small relative density $\sim(\lambda/l_1)^2$.

The first term of the low-frequency expansion of the current correlator $X'(\varepsilon,\omega,k)\propto-i\omega$ determines in accord with the Kubo formula the low-frequency asymptotic complex conductivity $\sigma(\omega)\propto-i\omega$, and consequently determines the static dielectric constant

$$\varepsilon'(0)=\lim_{\omega\to0}[4\pi\sigma/(-i\omega)]. \tag{32}$$

The value of $\varepsilon'(0)$ can be easily obtained from Eqs. (24) and (25), which coincide as $\nu\to0$ with the equations of the impurity problem (Refs. 1, 7, 9, and 10). Using the known[1,7,10] solution of these equations we obtain

$$\varepsilon'(\varepsilon,\,0)=\varepsilon_0 2\zeta(3)\,(pl_1/2)^4,\qquad \varepsilon_0=16e^2l_2^2/vS, \tag{33}$$

where $\varepsilon'(\varepsilon, 0)$ is the contribution of electrons of energy ε to the static dielectric constant, while $\zeta(3) = 1.308...$ is the Riemann zeta function. To obtain the total dielectric constant it is necessary to integrate (33) with respect to ε with weight $(-\partial n/\partial\varepsilon)$. The quantity ε_0 in (33) is the absolute value of the usual static dielectric constant determined by the Drude formula.

To calculate the next term of the expansion in ω, which determines the low-frequency asymptotic value of Re $\sigma(\omega)$, we can use the continuous equations (24) and (25). This circumstance distinguishes our problem from the genuine impurity problem[1,7,9,10,12–14] and is due to the presence of terms $\sim\nu\alpha$ with $\alpha\gg1$ in Eqs. (24) and (25). Using the known solution of these equations, obtained[9] by expanding them in the small parameter $|\nu\alpha|\ll1$, we get the contribution made to the conductivity by electrons of energy ε:

$$\sigma(\varepsilon,\omega)=\sigma_0\Big[(-i\nu\alpha)2\zeta(3)+(\nu\alpha)^2\times\Big[-\frac{2}{3}\ln^3(-i\nu\alpha)+(3-4C)\ln^2(-i\nu\alpha)+(12C-8C^2-7+2\zeta(3))\ln(-i\nu\alpha)\Big]+O(\nu^2\alpha^2)\Big]. \tag{34}$$

Here $C=0.577...$ is the Euler constant. We note that the low-frequency expansion is now in powers of $\nu\alpha = 2\omega\tau_2(pl_1/2)^4$, and the characteristic localization time $\tau_{\rm loc}$ is now of the order of $\tau_2(pl_1)^4\sim l_{\rm loc}^2/v^2\tau_2$ and corresponds to the diffusion mechanism of electron motion over distances $\sim l_{\rm loc}$ with the usual diffusion coefficient $D\sim v^2\tau_2$. It must be emphasized, however, that this diffusion is of purely quantum type and does not influence the static characteristics of the localized electron states, but changes only the characteristic time to reach the stationary asymptotic values. It is interesting to note that the low-frequency absorption for the phonon mechanism of localization takes the form Re $\sigma(\omega)\propto\omega^2|\ln^3\omega|$ as against $\omega^2\ln^2\omega$ in the impurity case.[1,7] This indicates that the Mott law for low-frequency absorption is not universal and is subject to noticeable deviations in the logarithmic factor.

We note that in the continuous limit $m\gg1$ the structure of the additional terms $\sim(pl_1)^{-2}$ in Eqs. (21) and (22) coincides with the structure of the impurity terms [see (17) and (18)], which in the presence of impurities in the crystal should be additively included in (21) and (22) with a coefficient l_2/l_i, where l_i is the mean free path for scattering by impurities. Therefore if impurities and phonons are present in the system all the static characteristics are determined as before by Eqs. (28)–(33), but with the effective mean free path $l=al_2$ replaced by

$$l'=(l_i^{-1}+l^{-1})^{-1}. \tag{35}$$

Thus, the presence of nondispersing phonons in the system always leads to the onset of a temperature-dependent increment $(al_2)^{-1}$ to the reciprocal l_i^{-1} of the impurity mean free path. We note that this circumstance expands considerably the region of applicability of the mechanisms of the temperature dependences of $\varepsilon'(T)$ and $\sigma(T)$, proposed earlier[15] to explain the experimental data on the electric properties of conducting TCNQ salts with asymmetric cations. It was shown there that Eq. (35) is valid for non-fully-symmetric intramolecular phonons, scattering from which is fully equivalent to impurity scattering. It follows from our present results that a contribution to the $l'(T)$ temperature dependence is made by intermolecular phonon. In this case the contribution of the fully symmetric oscillations is weakened somewhat because of the presence of the factor $(2/pl_1)^2$. As shown by various estimates,[1,12,15] however, this parameter is of the order of unity in real substances, so that $l'(T)$ has a substantial temperature dependence even in the absence of non-fully symmetric phonons.

Relation (35), however, is valid only at low frequencies $|\nu\alpha|\ll1$ when large $m\gg1$ need only be considered. At high frequencies, $|\nu\alpha|\gg1$, the difference of the terms $\sim(pl_1)^{-2}$ in (21) and (22) from the corresponding impurity terms (17) and (28) becomes essential. In this frequency region Eqs. (21) and (22) can be easily solved directly by perturbation theory in the parameter $(pl_1)^{-2}\ll1$.

Indeed, in the zeroth order in $(pl_1)^{-1}$ Eqs. (21) and (22) can be easily solved with the aid of the exponential susbstitution[9]

$$Q_m{}^a=Q_0{}^ae^{-\gamma m},\qquad R_m=e^{-\gamma m}.$$

Taking into acount the first corrections to $Q_m{}^a$ and R_m for the parameter $\alpha^{-1}\ll1$, we obtain at $a=1$ after simple calculations

$$R_m=e^{-\gamma m}[1+(4\alpha)^{-1}(e^{\gamma}-e^{-\gamma})\,m(m-2)/2], \tag{36}$$

$$Q_m{}^1=e^{-\gamma m}[Q_0{}^1+(4\alpha)^{-1}(Am^2+Bm+C)], \tag{37}$$

where

$$4\,\mathrm{sh}^2(\gamma/2)=-i\tilde\nu,\qquad Q_0{}^1=(1-e^{-\gamma})/\mathrm{sh}\,\gamma,\qquad \tilde\varkappa=0, \tag{38}$$

$$A=(e^{-\gamma}-1)(e^{2\gamma}-1)[{}^1\!/_2e^{-\gamma}+Q_0{}^1(e^{-\gamma}+1)][{}^5\!/_2(e^{-\gamma}+e^{\gamma})+1]^{-1}, \tag{39}$$

$$B=-{}^2\!/_3\{1+{}^3\!/_2e^{-\gamma}+Q_0{}^1(1+3e^{-2\gamma})-(e^{\gamma}-1)(1-e^{\gamma}-3e^{-\gamma})(e^{-\gamma}+2Q_0{}^1(e^{-\gamma}+1))[1+{}^5\!/_2(e^{-\gamma}-e^{\gamma})]^{-1}\}, \tag{40}$$

$$C=-2e^{-\gamma}[1+2e^{\gamma}Q_0{}^1+(A+B)(e^{-\gamma}-e^{\gamma})^{-1}]. \tag{41}$$

From this we get ultimately for the complex conductivity

$$\sigma(\varepsilon,\omega)=\frac{\sigma_0}{1-i\tilde\nu/4}\Big\{1+(4\alpha Q_0{}^1)^{-1}\Big[\frac{1}{2}\frac{1}{e^{\gamma}+1}-1-e^{-\gamma}\Big(1+\frac{3}{2}e^{-\gamma}\Big)+C+B\frac{1}{e^{2\gamma}-1}+A\frac{e^{2\gamma}}{(e^{2\gamma}-1)^2}\Big]\Big\}. \tag{42}$$

It follows from (42) that Reσ and Imσ decrease simultaneously at high frequencies $|\nu\alpha|\gg1$, and the expansion is in powers of $|\nu\alpha|^{-1}\ll1$. The imaginary part of $\sigma(\varepsilon,\omega)$, meaning also the dielectric constant $\varepsilon'(\varepsilon,\omega)$, vanishes and reverses sign while still in the region of applicability of (42). This takes place at $\omega\tau_2=(13/48\alpha)^{2/3}\ll1$. Therefore the dielectric constant acquires the characteristic positive sign while still in the frequency region where the conductivity is well described by the Drude formula. Expressions (34) and (42) are continuously joined at $|\nu\alpha| \sim 1$.

It must be noted that our results were obtained formally for the case of isotropic scattering by the phonons and for a nondegenerate electron gas. The first of these assumptions can be easily dispensed with and all the results are easily generalized to the case of different forward and backward mean free paths, which leads only to some complication of the final results, namely, in Eqs. (21) and (22) l_1 is replaced by $(l_1{}^+ l_1{}^-)^{1/2}$ and l_2 by l (Ref. 9), where the superscripts + and − correspond to forward and backward scattering. Curiously, the localization length $l_{\rm loc}$ (31) in the phonon problem is determined not only by the mean free paths l_1^- and l_2^- for backward scattering, but depends also significantly on the paths l_1^+ and l_2^+, so that this situation differs strongly from the impurity problem.[1–4,7,9,12–15]

As for the second assumption, its physical meaning is that at high electron density the effects of electron-electron interaction via phonons can be excluded only if $(pl_1)^{-1} \ll 1$ (Ref. 10), i.e., they are of the same order of smallness as the corrections for $(pl_1)^{-1}$ in (21) and (22). This, however, does not mean that the approximate results do not hold for one-dimensional metals, since investigations, say, of their thermodynamic properties with allowance for the interaction and localization effects[16] point to a dominant role of the latter. Therefore all the approximate results can be extended in principle to include the case of a degenerate electron gas by simply replacing the Boltzmann function $n(\varepsilon)$ by the Fermi function.

We note in conclusion that we did not take into account here polaron corrections to the electron spectrum, which are small in terms of the interaction constant $g \ll 1$. The reason is that they need not be taken into account in the terms $\sim (pl_1)^{-2}$, while in the terms ~ 1 they introduce in all coefficients corrections that are small relative to g and are inessential for electron localization.

5. CONCLUSION

We investigated here the localization of electrons in one-dimensional conductors on account of elastic scattering by nondispersing intramolecular phonons. Our analysis is formally valid only at low temperatures $T \ll \omega_0$, when the phonon occupation numbers $N \sim \exp(-\omega_0/T) \ll 1$ turn out to be small. Actually, however, all the approximate results are valid at all temperatures, since the only difference between the cases $T \gtrsim \omega_0$ and $T \ll \omega_0$ is the need for taking into account the finite number n of electron states with energies $\varepsilon + n\omega_0$, where $n\omega_0 \sim T$. Allowance for a finite number of electron states connected by arbitrary transitions should lead only to some change of the effective localization length $l'_{\rm loc} \sim n l_{\rm loc}$, as indicated, in particular, by the results for n coupled one-dimensional chains.[17,18]

Thus, one-dimensional localization of the electrons can take place even in ordered systems on account of scattering by nondispersing phonons. The resultant localization length $l_{\rm loc}$ depends quite strongly on temperature, and differs strongly thereby from the usual impurity length. Similar effects can result also from other mechanisms of quasi-elastic scattering, particularly scattering by low-frequency acoustic phonons at high temperatures.[1,15] All these processes, however, always contain a low inelastic-scattering probability, which leads to the onset of weak hopping conduction.[1,10]

In the system considered, the degree of inelasticity of the scattering is determined by the value of the phonon dispersion Δ, which is finite in all real cases, although it can be very small, especially for large organic molecules.[19] An estimate of the contribution Δ to the static conductivity can be obtained from the following simple considerations. The hopping-diffusion coefficient D is of the order of $l^2_{\rm loc}/\tau_{\rm in}$ (Refs. 1 and 10), where $\tau_{\rm in}$ is the characteristic inelastic-scattering time, which can be estimated at small Δ to be the reciprocal probability of accumulating an energy of the order of the reciprocal localization time $\tau_{\rm loc}^{-1}$ via diffusion in energy in elementary steps $\sim \Delta$. This leads at $\Delta \ll \tau_{\rm loc}^{-1}$ to the estimate $\tau_{\rm in}{}^{-1} \sim \tau_2{}^{-1}(\Delta\tau_{\rm loc})^2$ and yields for the conductivity $\sigma(T)$ the estimate

$$\sigma(T) \sim \sigma_0 (\Delta\tau_{loc})^2 (l_{loc}/l_2)^2 \sim \sigma_0 (\Delta\tau_2)^2 \alpha^6.$$

The condition for smallness of σ is therefore the relation $\Delta \ll \tau_2{}^{-1}\alpha^{-3}$. In real quasi-one-dimensional organic conductors[1,12,15] we have $\alpha \sim 1$ and $\tau_2{}^{-1} \sim 100$ K. Therefore the aforementioned criterion is well satisfied for the overwhelming majority of intramolecular oscillations,[19] in which $\Delta \sim 1$ to 10 K.

We wish to note in conclusion that the existence of phonon and other one-dimensional localization mechanisms that are not connected with impurities and can take place in ordered quasi-one-dimensional conductors explains the presence of characteristic maxima in the frequency dependence of Re $\sigma(\omega)$ and the abrupt change of the sign of $\varepsilon'(\omega)$ observed in quasi-one-dimensional TCNQ salts.[1]

The author thanks P. B. Wiegmann, V. I. Mel'nikov, and É. I. Rashba for a helpful discussion of the results.

[1] A. A. Gogolin, Phys. Rep. **86**, 2 (1982).
[2] A. A. Abrikosov and I. A. Ryzhkin, Adv. Phys. **27**, 147 (1978).
[3] P. Erdos and R. C. Herndon, Adv. Phys. **31**, 65 (1982).
[4] I. M. Lifshitz, S. A. Gredeskul, and L. A. Pastur, Vvedenie v statisticheskuyu teoriyu neuporyadochennykh sistem (Introduction to Statistical Theory of Disordered Systems), Nauka (1982).
[5] I. F. Shchegolev, Phys. Stat. Sol. (a) **12**, 9 (1972).
[6] D. Jerome and H. J. Schulz, Adv. Phys. **31**, 299 (1982).
[7] V. L. Berezinskiĭ, Zh. Eksp. Teor. Fiz. **65**, 1251 (1973) [Sov. Phys. JETP **38**, 620 (1974)].
[8] H. Fröhlich and N. F. Mott, Proc. Roy. Soc. **A171**, 496 (1939).
[9] A. A. Gogolin, V. I. Mel'nikov, and É. I. Rashba, Zh. Eksp. Teor. Fiz. **72**, 629 (1977) [Sov. Phys. JETP **45**, 330 (1977)].
[10] A. A. Gogolin, V. I. Mel'nikov, and É. I. Rashba, Zh. Eksp. Teor. Fiz. **69**, 327 (1975) [Sov. Phys. JETP **42**, 168 (1975)].
[11] M. J. Rice and N. O. Lipari, Phys. Rev. Lett. **38**, 437 (1977).
[12] A. A. Gogolin, Zh. Eksp. Teor. Fiz. **83**, 2260 (1982) [Sov. Phys. JETP **56**, 1309 (1982)]; Sol. St. Commun. **45**, 361 (1983).
[13] A. A. Gogolin, Z. Phys. **B50** (1983).
[14] A. A. Gogolin, Zh. Eksp. Teor. Fiz. **71**, 1912 (1976) [Sov. Phys. JETP **44**, 1003 (1976)].
[15] A. A. Gogolin, S. P. Zolotukhin, V. I. Mel'nikov, É. I. Rashba, and I. F. Shchegolev, Pis'ma Zh. Eksp. Teor. Fiz. **22**, 564 (1975) [JETP Lett. **22**,

278 (1975)].
[16] V. L. Berezinskiĭ and L. P. Gor'kov, Zh. Eksp. Teor. Fiz. **78**, 812 (1980) [Sov. Phys. JETP **51**, 409 (1980)].
[17] W. Weller, V. N. Prigodin, and Yu. A. Firsov, Phys. Stat. Sol (b) **110**, 143 (1982).
[18] O. N. Dorokhov, Pis'ma Zh. Eksp. Teor. Fiz. **36**, 391 (1982) [JETP Lett. **36**, 472 (1982)].
[19] M. G. Kaplunov, T. P. Panova, E. B. Yagubskiĭ, and Yu. G. Borod'ko, Zh. strukturnoi khimii **13**, 440 (1972).

Translated by J. G. Adashko