Structure of wave functions and ac conductivity in disordered one-dimensional conductors

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(Submitted 21 April 1983)
Zh. Eksp. Teor. Fiz. **85**, 1470–1488 (October 1983)

The correlators of the exact electron wave functions are computed for a one-dimensional system with disorder. It is shown that besides independent localized states, there exist in the system pairs of wave functions whose behavior (in the case of nearly equal energies) is strongly correlated at great distances. Frequency conductivity regimes are considered, and a microscopic expression for the Austin-Mott law is derived for the case when dissipation is due to transitions between independent localized states. Conversely, the zero-phonon contribution to the absorption and the so-called plateau regime are determined by transitions between pairs of strongly correlated states. It is shown that in real quasi-one-dimensional conductors, the expressions for the conductivity in all the frequency regimes are basically insensitive to interaction processes between the electrons, owing to the substantial screening of the Coulomb forces.

PACS numbers: 72.15.Nj, 71.50. + t

1. INTRODUCTION

We consider below a one-dimensional ($1D$) conductor with disorder, examples of which are organic or other linear highly conducting compounds, where the tunneling overlap integrals of the electron wave functions on the different chains are small. It is assumed that the disorder is due to defects that do not distort the conducting chain too greatly. This condition is satisfied either by isostructural chemical defects at low density (henceforth we shall have in mind usually linear defect density), or by structural disorder in a system of one of the components of the donor-acceptor complex if conductivity is due to motion along the $1D$-zone formed in the chains of the second component. There is a rather large number of examples of such systems. However, so as not to complicate the discussion, we will assume that there are no structural Peierls transitions in the considered $1D$-metal. The latter condition restricts by the same token the substances currently known to TCNQ salts, which were first studied in Ref. 1. For what follows, however, we need only know that such complexes exist, since we will be attempting to answer several qualitative questions that arise in the studying of $1D$-localization.

In the $1D$ case, we are basically interested in the fact that all the electron states are localized here, a result first noted by Mott and Twose.[2] In discussing such phenomena as localization and the mobility edge,[3] hopping conduction,[4] etc., models of certain centers on which the electrons are localized are usually employed. The wave function of such electrons drops exponentially far from the center, with a definite atomic scale a. The energy levels of the centers have a random scatter due to local disorder, and wave functions of the centers overlap slightly, since they are distributed randomly in space at low density.[5]

In the $1D$ case localization also occurs in the quasi-classical limit ($k_F\, l \gg 1$, where k_F is the Fermi momentum and l the mean free path relative to back reflection from static defects; at higher dimensionalities such a situation would correspond to metallic conduction). The wave functions in this case are close to the rapidly oscillating wave functions of band electrons, and localization denotes a decrease of the envelope of these oscillations over an approximate length $l \gg k_F^{-1}$. The density of states in the band is high. In this sense, localization is a comparatively weak effect, though it leads to a qualitative restructuring of the electron spectrum.

A rigorous proof of $1D$-localization was first given by Berezinskiĭ,[6] who showed that localization is the result of quantum interference of waves incident on and scattered by the defects, since in all the reflections the electron remains in the same chain. The well-known Mott conductivity law $\sigma(\omega) \propto \omega^2 \ln^2 \omega$ was also deduced in Ref. 6. We recall that in Ref. 2 one more energy scale was needed to derive this law, the quantum level splitting of two close potential wells.

At $T = 0$ we have $\sigma_{dc} = 0$ in the localized states. At low temperatures and low frequencies, therefore, phonons make the basic contribution to the frequency dependence of the conductivity. This contribution is of the nature of "Debye losses," [7] or relaxation of the populations of levels of nearly the same energy (low temperatures) in an alternating electric field, due to transitions caused by equilibrium phonons. The transitions occur between a pair of nearest-neighbor levels. It is physically clear that the pairing mechanism itself must be valid not only in the trapping representation, but also in general, say in amorphous semiconductors,[4,8] since the probability that more than two levels of nearly the same energy may be found close to each other is quite low (i.e., the mean distance between levels lying in the energy range $\sim T$ is large). In the region of practical interest, such absorption may be described by the Austin-Mott formula[8] and yields a nearly linear law for the conductivity as a function of frequency and temperature.

In the one-dimensional problem with weak disorder, the "centers" of the localized functions are determined (as noted above) accurate to l. It is natural to expect that whenever the distances between the centers is great by comparison with l, the pattern just described will be duplicated in the present case. On the other hand, at zero temperature there remains only the zero-phonon contribution to the conductivity which, in phenomenological representations, is due to transitions caused by tunneling splitting of two nearly identical potential wells. Such a formulation is not possible in the one-dimensional localization problem in a conductor with scatterers, where the localized eigenfunctions at a specified realization are the exact solutions of the Schrödinger equation.

The present article has three goals. On the one hand, by making an exact computation of certain mean wave functions and a number of other quantities, we are able to establish the range of applicability of the phenomenological representations. In this light, we then discuss the frequency conductivity modes at low temperatures and, in particular, derive the Austin-Mott formula in a $1D$ conductor with disorder. Finally, under particular very simple assumptions, we study the role of electron–electron interactions and their influence on the conductivity. This influence turns out to be comparatively minor, unlike in semiconductors.[9,10]

2. CORRELATION PROPERTIES AND STRUCTURE OF WAVE FUNCTIONS

As we have remarked, localization qualitatively alters the nature of the wave functions. The Schrödinger equation

$$-\frac{1}{2m}\psi_\mu''(x)+U(x)\psi_\mu(x)=\varepsilon_\mu\psi_\mu(x) \qquad (1)$$

under an appropriate choice of the boundary conditions, for example,

$$\psi_\mu(-L/2)=\psi_\mu(L/2)=0, \qquad (1')$$

has, in the language of mathematics, a point spectrum (see Ref. 11 and the bibliography therein). Here L is the total length of the chain and $U(x)$ is the potential created by the defects in a specified realization of the disorder. The quantities ε_μ and $\psi_\mu(x)$ are the eigenenergies and wavefunctions, respectively, and we put

$$\psi_\mu(x)=R_\mu(x)\sin\varphi_\mu(x). \qquad (2)$$

The amplitude $R_\mu(x)$ describes the behavior of the envelope of the localized wave function, and the phase $\varphi_\mu(x)$ is related directly to the density of states, which in the quasi-classical interval depends weakly on the energy. Assertions that all the functions are localized must be understood, of course in a probabilistic sense. That is, the functions are localized with unity probability as $L\to\infty$.[12] In computing the different physical quantities, it is far more convenient to use their representation in a basis of localized functions.[13]

In this way, the expression for the mean conductivity (when $T=0$) in an alternating field may be represented in the form

$$\sigma(\omega)=2\pi e^2 n_\perp \omega^2 L^{-1}\left\langle\sum_{\mu\nu}\delta(E_F-\varepsilon_\mu)\delta(E_F+\omega-\varepsilon_\nu)x_{\mu\nu}{}^2\right\rangle. \qquad (3)$$

(We write out the specific conductivity at once. Therefore, $n_\perp=d_\perp^{-2}$ in (3) is equal to the number of chains per unit cross-sectional area.) In (3),

$$ex_{\mu\nu}=e\int dx\psi_\mu(x)\psi_\nu(x)x \qquad (3')$$

is the matrix element of the dipole element. Summation in (3) is over all eigenfunctions of the boundary-value problem (1), (1′) for fixed positins of the defects.

The result for the conductivity is, of course, known.[6,14,15] It is, however, of some interest that the conductivity $\sigma(\omega)$ in (3) can be expressed in terms of the correlator

$$F_\omega^{(1)}(z)=\left\langle\sum_{\mu\nu}\delta(E_F-\varepsilon_\mu)\delta(E_F+\omega-\varepsilon_\nu)\psi_\mu(x)\psi_\nu(x)\psi_\mu(x')\psi_\nu(x')\right\rangle, \qquad (4)$$

where $z=|x-x'|$. (In the quasi-classical limit, the result of the averaging depends only on the difference in energies.)

Another important quantity that provides information about the behavior of the localized wave functions is the correlator of the densities of states at different points:

$$F_\omega(z)=\left\langle\sum_{\mu\nu}\delta(E_F-\varepsilon_\mu)\delta(E_F+\omega-\varepsilon_\nu)\psi_\mu^2(x)\psi_\nu^2(x')\right\rangle. \qquad (5)$$

Recall that the density of states per unit length of a chain and per unit energy interval is (disregarding spin):

$$\nu(E_F)=\left\langle\sum_\mu\delta(E_F-\varepsilon_\mu)\psi_\mu^2(x)\right\rangle=(\pi v_F)^{-1}. \qquad (6)$$

The correlations between the true localized wave functions $\psi_\mu(x)$ and $\psi_\nu(x')$ are strongest for nearly equal energies:

$$\varepsilon_\nu-\varepsilon_\mu=\omega\ll1/\tau, \qquad (7)$$

where $\tau=l/v_F$ is mean free time. Therefore, the behavior of the correlators $F_\omega^{(1)}(z)$ and $F_\omega(z)$ is of most interest precisely in the range of energies (7).

A detailed study of the correlator $F_\omega(z)$ has been carried out in a preceding work of ours.[16] A calculation of the function $F_\omega^{(1)}(z)$ using the same method is given in the Appendix to the present article. For the sake of convenience in making comparisons, the results for the functions $F_\omega(z)$ and $F_\omega^{(1)}(z)$ are represented in the Fig. 1 by solid and dashed lines, respectively. Note, first, that a new characteristic scale

$$z_0(\omega)=2l\ln(8/\omega\tau) \qquad (8)$$

appears when condition (7) holds; this scale is much greater than the localization length l. At sufficiently short distances $z\ll z_0(\omega)$, the correlators $F_\omega(z)$ and $F_\omega^{(1)}(z)$ are indistinguishable to within terms $(\omega\tau)^2$. At the point $z\equiv0$, we have

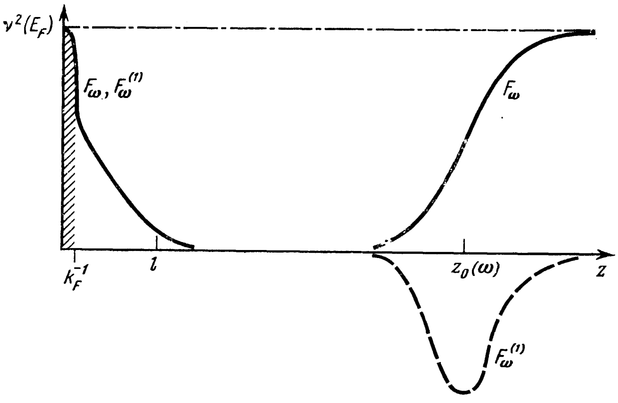

FIG. 1.

$$F_\omega(z=0)=F_\omega^{(1)}(z=0)=\nu^2(E_F), \qquad (9)$$

which corresponds to the complete absence of any correlation. Further, at the atomic scale $z\sim 1/k_F$, there occurs a sharp decrease in the correlators down to a value

$$F_\omega(k_F^{-1}\ll z\ll l)=F_\omega^{(1)}(k_F^{-1}\ll z\ll l)={}^2/_3\nu^2(E_F). \qquad (10)$$

In the region $l \ll z \ll z_0(\omega)$ we can use the asymptotic representation

$$F_\omega(z)=F_\omega^{(1)}(z)=\nu^2(E_F)\frac{\pi^{7/2}}{16}\left(\frac{l}{z}\right)^{3/2}\exp\left(-\frac{z}{4l}\right), \qquad (11)$$

which differs only by a coefficient from a previously derived correlator asymptpte[6,14] that describes the spatial behavior of one eigenfunction

$$\left\langle\sum_\mu \delta(E-\varepsilon_\mu)\psi_\mu^2(x)\psi_\mu^2(x')\right\rangle_{z\gg l}$$
$$=\frac{\nu(E_F)}{l}\frac{\pi^{7/2}}{32}\left(\frac{l}{z}\right)^{3/2}\exp\left(-\frac{z}{4l}\right). \qquad (11')$$

The last relation is usually considered as a proof that all the wave functions for some energy E are localized.

At distances $z\sim z_0(\omega)$, the correlators $F_\omega(z)$ and $F_\omega^{(1)}(z)$ finally begin to diverge markedly, the former becoming positive and assuming the shape of a step function:

$$F_\omega(z)=\frac{1}{2}\nu^2(E_F)\left\{1+\operatorname{erf}\left[\frac{z-z_0(\omega)}{2[lz_0(\omega)]^{1/2}}\right]\right\} \qquad (12)$$

with width

$$z-z_0(\omega)\sim\Delta z_0(\omega)=[lz_0(\omega)]^{1/2} \qquad (13)$$

small in terms of the scale $z_0(\omega)$. The correlator $F_\omega(z)$ in (12) varies from low values $\sim(\omega\tau)^{1/2}\nu^2(E_F)$ when $z<z_0(\omega)-\Delta z_0(\omega)$ to the value $\nu^2(E_F)$ which corresponds to the absence of any correlation when $z>z_0(\omega)+\Delta z_0(\omega)$. When $z>z_0+\Delta z_0$, thus, the states are always statistically independent.

The second correlator $F_\omega^{(1)}(z)$ is negative in this range of values and has the Gaussian form

$$F_\omega^{(1)}(z)=-\nu^2(E_F)\left(\frac{l}{4\pi z_0}\right)^{1/2}\exp\left(-\frac{[z-z_0(\omega)]^2}{4lz_0(\omega)}\right); \qquad (14)$$

its width coincides with the width of the step $\Delta z_0(\omega)$. Note one other property of $F_\omega^{(1)}(z)$:

$$\int_0^\infty dz F_\omega^{(1)}(z)=0, \qquad (15)$$

which follows from the definition (4) and from the fact that the wave functions $\psi_\mu(x)$ and $\psi_\nu(x)$ are orthogonal.

As we noted earlier, expression (3) for the conductivity $\sigma(\omega)$ may be represented in terms of the correlator $F_\omega^{(1)}(z)$ in the form

$$\sigma(\omega)=-2\pi e^2 n_\perp\omega^2\int_0^\infty dz\, z^2F_\omega^{(1)}(z), \qquad (3')$$

where the integral corresponds to the characteristic value of the square of the dipole moment. Substituting the value for the peak (14) in this integral yields a well-known result[6,14,15] for the conductivity in a low-frequency alternating field ($T=0$):

$$\sigma(\omega)=(8/\pi)e^2n_\perp l(\omega\tau)^2\ln^2(\omega\tau). \qquad (16)$$

Thus, according to Fig. 1, the form of the correlators $F_\omega(z)$ and $F_\omega^{(1)}(z)$ indicates that the two localized states cease to be statistically independent if the distances between the "centers" approach $z_0(\omega)$ (to within the interval $\Delta z_0(\omega) \gg l$). At these distances, a level "repulsion" effect sets in.

It has been shown[17] that in a very long chain of length $L\to\infty$ the distribution of the levels is random and obeys a Poisson law. However, as we have already remarked,[16] the distribution is no longer random if the length L is finite and comparable with z_0. We will now supplement certain results of Ref. 16 to explain the assertion just made regarding level repulsion. In fact, the density of states is known and equal to $\nu(E_F)$. Suppose we are interested in the probability $w_N(L,\omega)$ that N levels exist within the energy interval ω for a finite segment of a chain of length $L \ll 1/\omega\nu(E_F)$. If there were no correlations, this probability would be

$$w_N(L,\omega)=(\nu(E_F)\omega L)^N/N!. \qquad (17)$$

We define $\theta_\omega^{\gtrless}(x)=\varphi_{E+\omega}^{\gtrless}(x)-\varphi_E^{\gtrless}(x)$ as the difference between the phases of the two solutions of the Schrödinger equation with energies E and $E+\omega$, a difference that grows from left to right from the value $\theta_\omega=0$ at $x=0$. The probability

$$w_\omega(\theta,x)=\langle\delta(\theta-\theta_\omega^{>}(x))\rangle$$

is an auxiliary quantity in terms of which we can easily express the of which probability of interest to us,

$$w_N(L,\omega)=\int_{N\pi}^{(N+1)\pi}d\theta\, w_\omega(\theta,L)=\Phi((N+1)\pi)-\Phi(N\pi),$$

where according to Eq. (52) of Ref. 16

$$\Phi(N\pi)=\int_{-i\infty}^{+i\infty}(2\pi i\varkappa)^{-1}d\varkappa[1-c_1^{-N}(\varkappa)]\exp i\varkappa L$$

and the coefficient $c_1(\varkappa)$ is given by Eqs. (29) and (30) of Ref. 16 [see also the Appendix, Eqs. (A.20) and (A.21)]. Since we are interested in lengths $L<v_F/\omega$, by expanding $c_1(\varkappa)$ and using the approximation $\varkappa$ is the dimensionless variable of the Laplace representation with respect to coordinate in units of l), we find [see (A.24)]

$$c_1(\varkappa)=(\pi\varkappa/\omega\tau)\exp[(\varkappa-\varkappa^2)2\ln(8/\omega\tau)]. \qquad (18)$$

Substituting (18) in the preceding formulas, we obtain in place of (17)

$$w_N(L,\omega)$$
$$=\left(\frac{\omega\tau}{\pi}\right)^N\int_0^L dx_N\ldots\int_0^{x_2}dx_1\frac{1}{2}\left\{1+\operatorname{erf}\left[\frac{x_1-Nz_0(\omega)}{2[lNz_0(\omega)]^{1/2}}\right]\right\}. \qquad (17')$$

If the width of the transition region is neglected (here it is $(Nlz_0(\omega))^{1/2}$), we arrive at the expression

$$w_N(L,\omega)\approx\begin{cases}[\omega\nu(E_F)(L-Nz_0)]^N/N!, & L>Nz_0\\ 0, & L<Nz_0\end{cases} \qquad (19)$$

The latter contains already the effect the correlation of N levels. It is at once clear that ternary and higher correlations are missing in this approximation. The quantity z_0 serves in

(19) as a rigid dimension related to an individual level, and Nz_0 is the total interval excluded thereby from the accessible part of a segment of length L.

That $F_\omega(z)$ and $F_\omega^{(1)}(z)$ coincide in the region $z\sim l$ at low values of ω from (7) and that Eqs. (11) and (11′) are equivalent (disregarding the numerical coefficient), where the latter equation describes the behavior of one of the localized functions when $z > l$, becomes clear if we study the passage to the limit as $\omega \rightarrow 0$ in Eqs. (9) of Ref. 16 and in (A.6). On the one hand, these equations determine the spatial dependence of the phase difference of two states. On the other, the boundary condition [for example, for the correlator $F_\omega^{(1)}(z)$] contains, for the corresponding function $g_\omega(z)$, a stationary distribution function $w(\theta)$ [$g(\theta\,|z=0) = w(\theta)\cos\theta$], which corresponds to $w(\theta) = \delta(\theta)$ in the limit as $\omega \rightarrow 0$, as in the derivation of (19). The equations themselves turn into an equation for $\zeta = \theta/\omega$, which coincides exactly with Eq. (50) of Ref. 13, which describes the evolution of the mean square modulus of the eigenfunction itself. Therefore, in the region $z\sim l$, the two wave functions behave the same as long as $\omega\tau \ll 1$, e.g., the major contribution to the mean values (4) and (5) is made by those realizations of the potential for which the phase difference of the two states is zero (more precisely, a multiple of π) near $z\sim l$ and amounts to precisely π at distances $z\approx z_0$. The probability of having three or more states in the interval ω is low to long as ω is small [in (19), $\omega\nu(E_F)L$ is small, as was assumed in the derivation]. Therefore, the surges of the correlator (5), which correspond to a phase shift $[\theta] = N\pi$ for $N > 1$, are small. Such surges, which generalize the structure of the correlation $F_\omega^{(1)}(z)$ of the two functions in Fig. 1, would be visible for correlators of functions of three or more states at Nz_0.

The cited phase difference $\theta_\omega(z)$ attains a value of π at great distances $z_0 \gg l$ owing to numerous scattering acts. Therefore the exponential form (14) of the correlator $F_\omega^{(1)}(z)$ [cf. (12)] and the width of the distribution Δz_0 from (13) should be interpreted in terms of the Gaussian fluctuations of the position of the next zero of $\psi_\mu(\varepsilon_\mu > \varepsilon_\nu)$. The pair of strongly correlated states in Fig. 1 is the analog of the two coherent functions that appear in a model of centers[2] in quantum tunnel splitting of levels of two almost identical potential wells.

In fact, suppose that the wave function of the center behaves in the phenomenological picture at great distances as

$$\psi(x) \propto e^{-x/a}. \tag{20}$$

The quantum splitting of the levels of two wells separated by a distance z is, according to Ref. 2,

$$\omega = I_0 e^{-z/a}, \tag{21}$$

where I_0 is the tunneling integral. Hence

$$z_\omega \approx a \ln(I_0/\omega).$$

Identifying z_ω with z_0, we find

$$a = 2l, \quad I_0 = 8/\tau. \tag{22}$$

Equations (22) can answer the question posed in Ref. 10, that of determining the quantitative relation between model representations[2,4,8] and rigorous results in $1D$-systems with disorder.[6]

3. FREQUENCY MODES OF THE CONDUCTIVITY

At zero temperature, the frequency dependence of the conductivity at $\omega\tau \ll 1$ is described by (16). At finite temperatures, a phonon mechanism is turned on. If $T \ll 1/\tau$, the mean distance between the levels participating in the conduction is

$$\bar{R}_T = 1/\nu(E_F)T = (\pi l/T\tau) \gg l, \tag{23}$$

i.e., it is very high. Below we will not be concerned with the dc conductivity, but will limit the discussion to the frequency mode to which the so-called pair approximation is applicable. In this approximation, electron hops are limited to transitions between two nearest centers only. The absorption mechanism is due here to a lag in the changes of the populations of the two levels relative to the alternating external field[7] (Debye losses). Relaxation of the populations is due to thermal phonons. Let us write out an expression for the conductivity $\sigma(\omega)$ in this case[18]:

$$\sigma(\omega) = n_\perp e^2 \iiint \frac{(x_{\mu\mu} - x_{\nu\nu})^2}{4T\,\mathrm{ch}^2(\Delta\varepsilon/2T)} \times \left[\frac{\omega^2/\tau_{\mu\nu}}{\omega^2 + 1/\tau_{\mu\nu}^2}\right] w(\varepsilon_\mu, \varepsilon_\nu, z)\, dz\, d\varepsilon_\nu\, d\varepsilon_\mu, \tag{24}$$

where $ex_{\mu\mu}$ and $ex_{\nu\nu}$ are the matrix elements of the dipole moment in the two states, $\Delta\varepsilon = \varepsilon\mu - \varepsilon_\nu$ is the energy difference between the states, and $1/\tau_{\mu\nu}$ is the corresponding inverse phonon-relaxation time. the triple integral denotes that averaging over the defects for statistically independent states is equivalent to averaging over the energies of both states and their relative distance z. The function w has the form

$$w(\varepsilon_\mu, \varepsilon_\nu, z) = 2\nu^2(E_F)\{n(\varepsilon_\mu)[1 - n(\varepsilon_\nu)] + n(\varepsilon_\nu)[1 - n(\varepsilon_\mu)]\}. \tag{25}$$

We choose electron-phonon Hamiltonian in the form[19]

$$\hat{H}_{e,ph} = d_1 \sum_{\mu\nu} \sum_{k} \left(\left[\frac{\omega(k)}{2V}\right]^{1/2} \cos\theta_k\right) \hat{a}_{\mu\sigma}^{+} \hat{a}_{\nu\sigma} [\hat{b}_k (e^{ikr})_{\mu\nu} + \mathrm{H.c.}]. \tag{26}$$

Here d_1 is the deformation-potential constant. The normalized factor in parentheses, where V is the volume of the crystal, is present because the electron interacts only with a deformation gradient of the form $\partial u_i/\partial x$ in the direction of the chain. The matrix element

$$(e^{ikr})_{\mu\nu} = \int e^{ik_\parallel x} \psi_\mu(x)\, \psi_\nu(x)\, dx \tag{27}$$

enters in the definition of the transition probability from μ to ν and back. The sum of the two inverse relaxation times [cf. Ref. 18]

$$\frac{1}{\tau_{\mu\nu}} = \pi d_1^2 \int \frac{d^3k}{(2\pi)^3}\, \omega(k) \cos^2\theta_k\, \mathrm{cth}\frac{\omega(k)}{2T}\, |e^{ikr}|_{\mu\nu}^2\, \delta(\varepsilon_\mu - \varepsilon_\nu - \omega_k). \tag{28}$$

The time $\tau_{\mu\nu}$ occurs in (24). The main task in the calculation of the losses (24) is to determine the relation between $1/\tau_{\mu\nu}$ and the distance z between the centers. In accordance with

(20), it is usually assumed that[8]

$$1/\tau_{\mu\nu}=\nu_{ph}e^{-2z/a}, \qquad (29)$$

where ν_{ph} is determined by the intensity of electron-phonon interactions. Integration over z in (24) separates the pairs

$$\omega\sim 1/\tau_{\mu\nu}, \qquad (30)$$

which are most effective in this loss mechanism. Thus, the problem involves estimating the matrix element (27) for two independent centers, which may be accomplished in the same way as in Ref. 19. In the domain of localization of the function $\psi_\nu(x)$, a wave function, say $\psi_\mu(x)$, behaves according to (20) and (22) as

$$\psi_\mu(x)\propto\exp\left[-(z+\Delta x)/2l\right]\sin\varphi_\mu(x)$$

when $x = z + \Delta x$. Just like phase $\varphi_\nu(x)$, the phase $\varphi_\mu(x)$ contains rapid variations mainly in the form $k_F\,x$. By averaging the product $\psi_\mu(x)\psi_\nu(x)$ in (27) over the rapid oscillations, we are left with functions which vary about the point of localization of $\psi_\nu(x)$ at distances on the order of l. On the other hand, from (24) and (28) it follows that $k\sim T/s$, where s is the characteristic speed of sounr. If $T\tau\ll 1$, but $T\tau v_F/s\gg 1$, we have in (27) $kl\gg 1$. Therefore, local averaging of the square of the matrix element in (28) yields a result which may be estimated as

$$|e^{ikr}|_{\mu\nu}{}^2\approx(kl)^{-2}e^{-z/l}, \qquad (31)$$

as is confirmed also by computation. We may also introduce for the electrons a dimensionless electron-phonon interaction constant

$$g_{ph}{}^2=2\nu(E_F)\,n_\perp d_1{}^2 \qquad (32)$$

in place of the deformation-potential constant. Using (31) and (32), $1/\tau_{\mu\nu}$ from (28) is conveniently written in the form

$$\frac{1}{\tau_{\mu\nu}}=\alpha g_{ph}{}^2\frac{d_\perp{}^2}{l^2}\frac{v_F}{s}\frac{(T\tau)^3}{\tau}\frac{\Delta\varepsilon}{T}\operatorname{cth}\frac{\Delta\varepsilon}{T}\exp\left[-\frac{z-z_0(T)}{l}\right], \qquad (33)$$

where the competition between the large and small quantities occurring in the pre-exponential factor has been written out in a convenient form. Here α is a numerical coefficient. In deriving (33) from (28), we have assumed that the phonons are three-dimensional. The relaxation (33) is determined by acoustic phonons. The numerical coefficient α depends, of course, on the choice of the acoustic mode with which the electrons interact. In the Hamiltonian (26), this mode has not been specified and, in particular, the polarization vectors of the phonon modes have been omitted from its expression. Unlike (29), expression (33) is already in a form which explicitly takes into account the presence of a correlation radius z_0 for repulsion of the levels. It has the sense of a relaxation time of two independent states only when $z>z_0$.

To prevent any misunderstanding, note that the decrease of the relaxation time with distance between the centers of a pair is characterized by the scale l, whereas the decrease in the correlator of the square of the wave function at two points obeys the law (11′), which contains the characteristic dimension $4l$. This seeming paradox may be explained by the fact that (11′) [just as (4) and (5)] comprises the mean values of products of wave functions which, obviously, are not self-averaged quantities. At the same time, (28) and (33) contain, strictly speaking, the wave functions $\psi_\mu(x)$ and $\psi_\nu(x)$ at a given realization of the random potential. The relevant quantity is the so-called (after Lyapunov) growth factor of the amplitude of thw ave function

$$\frac{1}{z}\lim_{z\to\infty}\ln\frac{R(z)}{R(0)}=\frac{1}{a}, \qquad (34)$$

which in fact determines whether in the wave function is decreasing or increasing. Since the quantity in the logarithm increases linearly with z (at large z), the growth factor is no longer a self-averaged quantity (see also Ref. 11, Sec. 13). The first derivation of $a = 2l$ from (34) was done in Ref. 10. An example of how strongly the mean statistical products of the wave functions differ from the statistical properties of the functions themselves is provided in fact by our computed values of the correlators $F_\omega(z)\,F_\omega^{(1)}(z)$.

Let us now define the quantity

$$\int\limits_{\varepsilon_1,\varepsilon_2\in\varepsilon} d\varepsilon_1\,d\varepsilon_2\left\langle\sum_{\mu\nu}\delta(\varepsilon_1-\varepsilon_\mu)\,\delta(\varepsilon_2-\varepsilon_\nu)\,\frac{1}{\tau_{\mu\nu}}\right\rangle, \qquad (35)$$

which has the sense of the mean total number of all transitions in the system, per unit time, between the states belonging to the energy band ε. The average over the random field of the defects in the integrand is expressed in terms of the correlator $F_\omega^{(1)}(z)$, and is of the order of

$$\sim g_{ph}{}^2\frac{d_\perp{}^2}{l^2}\frac{v_F}{s}\Delta\varepsilon\operatorname{cth}\frac{\Delta\varepsilon}{T}\nu^2(E_F)\,Ll,$$

as can be easily verified either by an estimate similar to that used in determining (31) or by an exact computation by means of (A.6) and (A.8) under the condition $kl\gg 1$. Then (35) yields

$$g_{ph}{}^2\frac{d_\perp{}^2}{l^2}\frac{v_F}{s}\varepsilon^3\operatorname{cth}\frac{\varepsilon}{T}\nu^2(E_F)\,Ll. \qquad (36)$$

Dividing the latter by the total number $\varepsilon\nu(E_F)L$, of states in the energy band of the entire system, we obtain the mean inverse lifetime of a single state at $\varepsilon\sim T$:

$$\frac{1}{\tau_{ph}}(T)\sim g_{ph}{}^2\frac{d_\perp{}^2}{l^2}\frac{v_F}{s}(T\tau)^2\frac{1}{\tau}. \qquad (37)$$

Thus, the mean inverse lifetime of a single state is determined by strongly correlated pairs of states; the interaction between these states does not obey an exponential law. The quantity from (37) always exceeds the rate of relaxation between the states of an independent pair.

Let us now compute the conductivity. Substituting (33) in (24), using (25) for the probability distribution, and integrating, we obtain a one-dimensional variant of the Austin-Mott law[8] which, however, already contains the microscopic parameters, namely,

$$\sigma(\omega)\approx\frac{\pi^3}{4}n_\perp e^2\nu^2(E_F)\,\omega Tl^3\ln^2\frac{64\alpha g_{ph}{}^2d_\perp{}^2v_FT}{l^2s\omega}, \qquad (38)$$

where the logarithmic factor is the result of estimating the dipole moment ez from (30) using the explicity expression (33) for $1/\tau_{\mu\nu}$ and the value of $z_0(T)$ determined from (8).

Moreover, it is necessary that $z - z_0$ exceed the width Δz_0. Therefore (38) is applicable in the frequency range

$$\omega \ll g_{ph}^2 \frac{d_\perp^2}{l^2} \frac{(T\tau)^3}{\tau} \frac{v_F}{s}. \tag{39}$$

On the other hand, the condition that the phonon dissipation mechanism dominate the contribution of the zero-phonon mechanism may be found by comparing (38) and (16):

$$\omega \ll T. \tag{40}$$

Condition (40) introduces real constraints only at very low temperatures.

It is clear even from (40) that at high enough frequencies the conductivity has a plateau mode in which it is independent of frequency.[18] Note the distinctive feature of (24), which in this frequency range naturally is by way of an interpolation only. When the frequency increases and inequality (39) no longer holds, the basic role in the energy dissipation is played by correlated pairs, whose characteristic inverse time is large, according to (37). In other words, when $T_\tau \ll 1$, there exists a range of frequencies higher than the right side of (39) and comparable with (37), where the pair approximation relates to relaxation between the coherent states in Fig. 1. From (24) it is, however, clear that the conductivity can not continue to grow with increasing frequency, since in this region the quantity $(x_{\mu\mu} - x_{\nu\nu})^2$ drops sharply.

The plateau mode for the conductivity has been obtained microscopically[19,21]:

$$\sigma = g_{ph}^2 \frac{\pi^2}{45} \frac{e^2}{\hbar v} \frac{v_F}{s} (2T\tau \ln 2T\tau)^4. \tag{41}$$

It is clear that though

$$\frac{1}{\tau_{ph}} = g_{ph}^2 \frac{d_\perp^2}{l^2} \frac{v_F}{s} T^2\tau \ll \omega \ll T^2 \left(\frac{d_\perp^2}{v_F s} \right)^{1/2} \tag{42}$$

is the condition under which (41) is applicable [the right side of (42) was again obtained by comparing (41) with (16)], the Austin-Mott formula may be matched to (41) even at frequencies on the order of the right side of (39). In light of the above, it is clear that there is a frequency range

$$g_{ph}^2 \frac{d_\perp^2}{l^2} \frac{(T\tau)^3}{\tau} \frac{v_F}{s} \ll \omega \lessgtr g_{ph}^2 \frac{d_\perp^2}{l^2} \frac{v_F}{s} \frac{1}{\tau} (T\tau)^2, \tag{43}$$

which is rather wide when $T\tau \ll 1$ and in which the conductivity varies comparatively slowly, remaining always of the same order of magnitude as in (41). In concluding this section, let us note that the frequency range (42) which describes the plateau region exists if

$$g_{ph}^2 \left(\frac{v_F}{s} \right)^{1/2} \frac{d_\perp}{l} \ll 1.$$

4. ROLE OF ELECTRON-ELECTRON INTERACTIONS

It has been shown[9,10] that the corresponding expressions for zero-phonon conductivity (3), the Austin-Mott formula, and the plateau mode[8,18] substantially change in semiconductors due to effects of long-range Coulomb interaction. Consider, for example, expression (3). That the square of the frequency occurs in it may be attributed to two factors. One of them ($\hbar\omega$) is simply an energy quantum borrowed from the external field in the electron transition from ε_ν into ε_μ. The second factor describes the fraction of electron states below the Fermi level capable of participating in the transition. If there is Coulomb repulsion $e^2/\varepsilon r_\omega$ (where r_ω is the distance to the resonance pair) between the electrons, the fraction of states capable of participating in absorption is increased. In fact, the states ε_μ and ε_ν remain singly occupied if

$$\varepsilon_\mu + \varepsilon_\nu + e^2/\varepsilon r_\omega > 0$$

and the Fermi factors in the expression for the transition probability limit the electron energy from below solely by the condition

$$|\varepsilon_\nu| > \hbar\omega + e^2/\varepsilon r_\omega. \tag{44}$$

The same physical factors expand the energy range of the electrons capable of absorbing a thermal phonon, say, in the Austin-Mott formula. As a result, the expression for the zero-plonon contribution would be obtained by multiplying Mott's result $\sigma(\omega) \propto \omega^2 \ln^2 \omega$ by the fctor $e^2/\varkappa r_\omega \omega$, and, in the case of phonon contributins to the conductivity, by the factor $e^2/\varkappa r_\omega T$. At low temperatures, the absorption would be proportional to the first power of the frequency, whereas in the Austin-Mott formula there would remain only a slow (logarithmic) temperature dependence.

The conductivity properties in a system of one-dimensional electrons are less sensitive to electron-electron (Coulomb) interactions, since these interactions are markedly screened if the system of conducting "chains" constitutes a three-dimensional crystal. At short distances ($z \ll 1$) the screening is metallic in nature. That is, a charge located on one thread is shielded by the displacement of charges on neighboring threads (except, of course, in the transverse direction). The corresponding expressions for the Fourier components of the screened potential[22] (see also Ref. 23) lead to an expression for the inverse Thomas-Fermi screening radius

$$k_{TF}^2 = \frac{4\pi e^2}{\tilde\varepsilon} 2\nu(E_F) n_\perp = \frac{2}{\tilde\varepsilon} \frac{e^2}{\hbar v_F} n_\perp, \tag{45}$$

where $\tilde\varepsilon$ is the dielectric constant of the effective medium produced by the strong polarizability of the large planar molecules. It follows from (45) that metallic screening has a characteristic radius on the order of $k_{TF}^{-1} \sim d_\perp \ll l$. On the other hand, with respect to electrical properties, a system of localized electrons is a dielectric, and therefore at great distances (greater than the *mean free* path) we get a Coulomb interaction but with a very high value of the (longitudinal) dielectric constant[6,15]

$$\varepsilon = \frac{32\zeta(3)}{\pi} \frac{e^2}{\hbar v_F} l^2 n_\perp. \tag{46}$$

Substituting (46) in (44), we obtain for the Coulomb energy

$$\frac{e^2}{\varepsilon z_0(\omega)} \sim \frac{d_\perp^2}{l^2} \frac{\pi}{64\zeta(3)} \frac{\hbar}{\tau} \left[\ln \frac{8}{\omega\tau} \right]^{-1}. \tag{47}$$

To get an idea of the numbers involved here, we use a typical value[19,21] for $1/\tau \sim 100$ K (i.e., $l \sim 10^{-6}$ cm) and $d_\perp \sim 10$ Å. We obtain for (47) an estimate no greater than several tens of degrees. The influence of the long-range Coulomb contribution could therefore affect the zero-phonon contribution to the conductivity (the frequency $f = \omega/2\pi = 10^{10}$ Hz corresponds to about 1 K), but according to (40) the phonon mechanism is dominant at temperatures which are not too low.

Accordingly, we assume that the electron–electron interaction potential $u(x - x')$ is short-range and rather weak. As has been previously shown,[24] under these conditions the basic new factor that alters the systematics of the levels is the interaction of two electrons that occupy the same localized state ε_ν. The energy of this interaction, which we will assume to be repulsion, in is

$$A_\nu = \iint dx\, dx' \psi_\nu^2(x)\, u(x-x')\, \psi_\nu^2(x'). \tag{48}$$

In the model of a short-range δ-function interaction, the latter expression may be rewritten, after averaging (48) over the fast (atomic) oscillations, in the form

$$A_\nu = \frac{\pi v_F}{4} g_{eff} \int R_\nu^4(x)\, dx; \quad g_{eff} = g_2 + \frac{1}{2} g_1, \tag{48$'$}$$

where g_1 and g_2 are the dimensionless electron-electron scattering amplitudes introduced in Refs. 25 and 26, with high $(\sim 2k_F)$ and low momentum transfer, respectively. The assumption that the interaction $u(x - x')$ is weak means that g_1, g_2, and g_{eff} are small. The order of magnitude of these constants is obviously $e^2/\hbar v_F \tilde{\varepsilon}$. Therefore, there is no special reason why this assumption should readily hold in real substances.[1] Model-based arguments that the interaction is weak, however, are useful for understanding the physical picture as a whole.

Owing to the repulsion (48) or (48′) between electrons at the same localized level, the structure of the occupation numbers of the localized states near the Fermi level changes at low temperatures. Near the old Fermi level, only singly occupied electron states remain. These states possess free spin and, consequently, paramagnetic centers can appear in the system.[24] Next, at distances relative to the energies ε_ν on the order of

$$\Delta = \pi g_{eff}/\tau \tag{49}$$

below the Fermi level, there appears a smeared distribution which, turns into ordinary doubly occupied states when $|\varepsilon_\nu| \gg \Delta$. The linear density of the paramagnetic centers, which can be determined from the contribution to the magnetic susceptibility, a contribution that takes at $T \ll \Delta$ the form of the Curie law $\chi \propto T^{-1}$, is equal to[24]

$$n_p = {}^1\!/_3 \nu(E_F)\, \Delta = g_{eff}/3l. \tag{50}$$

The mean distances $\bar{R}$ between the centers are large:

$$\bar{R} = 3l/g_{eff} \gg l \tag{51}$$

in the case of a weak enough interaction.

Let us turn to the frequency dependence of the conductivity of the $1D$-electrons. The zero-phonon contribution (16) as well as the expression (41) for the conductivity in the plateau mode are determined, as we have shown, by transitions between coherent states, whereas the Austin-Mott-type formula (38) is associated with relaxation between pairs of uncorrelated states.

Let us begin with the latter case. If both states ε_ν and ε_μ lie sufficiently close to the Fermi level of non-interacting electrons, they will be not more than singly occupied at $T \ll \Delta$. These transitions would obviously make precisely the same contribution to the frequency-dependent conductivity as (38), the only difference being the factor 1/2, which takes into account the single occupation of these states.

Let us consider again two localized states characterized by energies ε_μ and ε_ν in the absence of interaction. When there is interaction, the new energy levels depend on the occupation. That is, the energy remains the same for single occupation of the levels, whereas for a doubly occupied state (say, the state ε_ν) the total energy is already $\tilde{\varepsilon}_\nu = 2\varepsilon_\nu + A_\nu$. Such a classification is naturally valid only for pairs of independent levels. The interaction energy between the levels ε_ν and ε_μ contains direct and exchange interaction terms

$$A_{\mu\nu}(z) = \iint \psi_\mu^2(x)\, u(x-x')\, \psi_\nu^2(x')\, dx\, dx', \tag{52$'$}$$

$$J_{\mu\nu}(z) = \iint \psi_\mu(x)\, \psi_\nu(x)\, u(x-x)'\, \psi_\mu(x')\, \psi_\nu(x')\, dx\, dx', \tag{52$''$}$$

which are exponentially small in terms of the distance z between the localized states:

$$J_{\mu\nu} \sim A_{\mu\nu} \sim g(1/\tau) \exp(-2z/a). \tag{53}$$

These interactions are too weak and are not capable of creating the situation described by (44), in which a pair of close energy states, ε_μ and ε_ν, are singly occupied in a finite section of phase space. It remains for us to verify the terms of a doubly occupied coherent pair, since in this case the interactions (52) are according to (14) again of order Δ. Splitting of the levels of the coherent pair in the course of interaction will occur for the system of both levels simultaneously. Without presenting the calculations, it is easy to see what the result reduces to if $|\varepsilon_\mu - \varepsilon_\nu| \ll \Delta$. The single occupied pair has, of course, the previous energy ε_μ or ε_ν. In the case of a double occupation, it can be easily verified that interaction leads to two types of states. One of them corresponds so to speak to molecular terms, with each electron is concentrated in the right or left side of Fig. 1, respectively, i.e., in the states $\psi_\pm(x) = 2^{-1/2}[\psi_\mu(x) \pm \psi_\nu(x)]$ localized on the right and left at a distance z_0 from each other. If $|\varepsilon_\mu - \varepsilon_\nu| \ll \Delta$, the levels of this term are $\varepsilon_\mu + \varepsilon_\nu$, while the wave functions ocrrespond to the singlet and triplet spin states of the two electrons. The second type of state constitutes atomic terms in which a pair of electrons is concentrated at the right center and a pair at the left "center." Again, at the close values $\varepsilon_\mu \approx \varepsilon_\nu = \varepsilon$, the levels are equal to $2\varepsilon + A^{(1,2)}$, where $A^{(1,2)}$ is the interaction energy of two electrons concentrated either both on the left or both on the right. The classification of the terms and their energies for the triply or quadraply occupied pairs may be analogously analyzed. To these terms we should add the exchange interactions, which are already exponentially small. Thus, the short-range forces do not hinder double occupation of the molecular terms of the coherent pair.

Let us, however, again consider the initial expression (3) for the zero-phonon contributin to the conductivity. The latter contains the matrix element of a dipole transition, generally speaking, between two arbitrary functions. If the functions correspond to independent states, the square of the matrix element contains the exponential factor $\exp(-2z/a)$, which upon averaging over the distances would indicate that the correlated states with $z \approx z_0$ make the dominant contribution. Interactions alter the structure of the occupation numbers. Therefore, we have the following possibilities for transitions with low energy transfer:

(a) Transition from a singly occupied state ε_ν to an empty state ε_μ near the Fermi level. Such a transition will everywhere yield the earlier results, except for a factor 1/2 that takes into account the spin.

(b) Transition from one singly occupied state to another $(\varepsilon_\mu, \varepsilon_\nu) \to (2\varepsilon_\mu + A_\mu, 0)$. Such a transition requires an energy

$$\varepsilon_\mu + A_\mu - \varepsilon_\nu, \tag{54}$$

which may be low (on the order of ω or T, depending on the problem) if ε_ν and $\varepsilon_\mu + A$ are both small (ε_ν lies near the edge of single occupation, and ε_μ near the edge of double occupation).

(c) The condition for transition from a doubly occupied level $(2\varepsilon_\nu + A_\nu)$ to an empty level ε_ν has a similar form:

$$\varepsilon_\nu + A_\nu - \varepsilon_\mu.$$

(d) A transition from a doubly occupied level $(2\varepsilon_\nu + A_\nu)$ to a singly occupied level ε_μ calls for an energy

$$\varepsilon_\mu + A_\mu - \varepsilon_\nu - A_\nu,$$

which again is possible at the double-occupation boundary.

If in each of these conditions of type (54) the two levels belong to an independent pair, the conditions may hold since each of the quantities A_μ and A_ν is a statistical variable independent of ε_μ and ε_ν (see Ref. 24, where the distribution function $w(A)$ was found). The distribution function $w(A)$ is concentrated at $A \sim \Delta$. The use of condition (54) would formally yield

$$\varepsilon_\mu - \varepsilon_\nu \sim \Delta,$$

i.e., the independent pairs would at first glance seem to resemble each other at a distance of about $z_\Delta = 2l \ln(8/\Delta\tau)$. This apparent paradox, which could have a major impact on the range of applicability of the Austin-Mott formula (see expressions (29) and (33) for $1/\tau_{\mu\nu}$, particularly in the plateau mode, can be resolved if we bear in mind the following simple considerations. If the quantity (54) is small, this will mean that the two-level systems $(2\varepsilon_\mu + A_\mu, 0)$ and $(\varepsilon_\mu, \varepsilon_\nu)$ are degenerate. This energy degeneracy is eliminated by the tunneling splitting caused by nondiagonal matrix elements of the form

$$J_{\mu\mu\mu\nu} = \iint \psi_\mu(x)\psi_\mu(x)\, u(x-x')\, \psi_\mu(x')\psi_\nu(x')\, dx\, dx',$$

the order of magnitude of which is, however, larger than (53), namely,

$$I(z) = J_{\mu\mu\mu\nu}(z) \sim g \frac{1}{\tau} \exp\left(-\frac{z}{a}\right). \tag{54'}$$

The condition under which $I(z)$ attains values on the order of the temperature determines the distances to which the processes (54) are effective for independent pairs ($a = 2l$):

$$z_{min} \sim 2l \ln \frac{\Delta}{T} = 2l \ln g \frac{1}{T\tau} \approx z_0. \tag{55}$$

At lesser distances, the wave function of one of the electrons turns into a quantum superposition of the form $a\psi_\mu(x) + b\psi_\nu(x)$, in which the electron participates in both the state μ and in the state ν, since in the latter state it is repelled by the second electron already there. The dipole-moment matrix element is determined by (55). This is fully identical to the previous representations.[2] Thus, apart from numerical coefficients and the corrections to the leading logarithmic dependences, the zero-phonon contribution to the conductivity and the plateau mode are described by the previously obtained expressions (16) and (41).

In the relaxation mode described by the Austin-Mott formula, greater distances are essential, according to (30). The contributions due to the above processes may be computed (with allowance for interactions at the localized levels) entirely analogously to (24). In the averaging process, however, there is an additional average over the distribution of A_ν and A_μ with independent functions $w(A)$ for each of these quantities. Moreover, Eq. (25) must be replaced by more complicated combinatorial factors that describe the transition probability as a function of the occupation of the states. The occupation state of each level is independently defined, as before, with the sole difference that repulsion of electrons at each level is taken into account. When $T \ll \Delta$, the averaging over A_μ and A_ν actually vanishes. In this case, integration alters the coefficient in (38):

$$\sigma(\omega) = \left(\frac{9}{5} + \frac{16}{5}\frac{\ln^2 2}{\pi^2}\right) \times \frac{\pi^3}{4} n_\perp e^2 \nu^2(E_F)\, \omega T l^3 \ln^2 \left[\frac{64\alpha g_{ph}{}^2 d_\perp{}^2 v_F T}{l^2 s\omega}\right]. \tag{38'}$$

(All possible processes are taken into account in the answer.)

There are several temperature regions in the model with weak interaction. The first such region, to which, in particular, our results relate, correspond to $T \ll \Delta$, in which the paramagnetic centers are still free and in which paramagnetism is manifest. At the temperature T_0, the interaction (52″) essentially couples the paramagnetic centers at the mean distances (51). According to (53),

$$T_0 \approx \Delta \exp(-3/g_{eff}). \tag{56}$$

Since the relation between T_0 and $g_{\rm eff}$ is exponential, even if $g_{\rm eff}$ is not very small expression (56) defines a noticeable temperature interval within which our formulas are applicable. Below the value of T_0 from (56), the spins are "frozen," forming a special type of spin-glass phase. At low temperatures and low frequencies, electronic states in a very narrow energy band of order T or ω, respectively, are essential for the conductivity. As has been previously demonstrated,[27] these states gradually combine into large clusters,[28] so that the effective number of paramagnetic centers falls according to the law[1)]

$$n_p \propto (T/\Delta)^{g_{eff}/3}.$$

Using previous data[1] for $Qn(\text{TCNQ})_2$, we find that $g_{\rm eff} \approx 0.8$. If the localized state is included in a cluster, its participation in absorption will be hindered. It would seem that the same type of effects that lead to exponential temperature dependences of the susceptibility $\chi \alpha T^{-(1-\alpha)}$ could also appear in the frequency dependence of the conductivity at very low temperatures. As yet, no experiments in this temperature range have been carried out, and we are unable to delve into this question to any depth.

APPENDIX

Below we will briefly describe the process of computing the density-density correlation function

$$F_\omega^{(1)}(x-x') = \Big\langle \sum_{\mu\nu} \delta(E-\varepsilon_\mu)\,\delta(E+\omega-\varepsilon_\nu)\,\psi_\mu(x)\,\psi_\nu(x)\,\psi_\mu(x')\,\psi_\nu(x') \Big\rangle . \tag{A.1}$$

The computation is entirely analogous to the computation of the correlator of the density of states in (16) and is carried out by the same method. we introduce the phase φ and amplitude R of the wave function $\psi_\mu(x) = R_\mu(x)\sin\varphi_\mu(x)$ and average in (A.1) over the rapid oscillation sof the wave function, retaining only slow dependences with respect to the phase difference

$$\theta_\omega = \varphi_\mu - \varphi_\nu . \tag{A.2}$$

Then (A.1) is transformed to

$$F_\omega^{(1)}(x-x') = \frac{1}{4}\Big\langle \sum_{\mu\nu} \delta(E-\varepsilon_\mu)\,\delta(E+\omega-\varepsilon_\nu) \times R_\mu(x) R_\nu(x) \cos\theta_\omega(x) R_\mu(x') R_\nu(x') \cos\theta_\omega(x') \Big\rangle . \tag{A.3}$$

The sum over the energy eigenvalues in (A.3) is written as usual[13] in terms of the condition for matching the phases $\varphi^<(x)$ and $\varphi^>(x)$ obtained by solving the Schrödinger equations, from the left and right, respectively, for designated boundary conditions on the ends of the chain. We have

$$F_\omega^{(1)}(x-x') = \frac{1}{v_F^2}\int_0^\pi\int_0^\pi \langle \delta(\varphi_E^>(x')-\varphi_1)\,\delta(\varphi_{E+\omega}^>(x')-\varphi_2)\,\delta(\varphi_1-\varphi_E^<(x')) \times \delta(\varphi_2-\varphi_{E+\omega}^<(x'))\,\alpha_E(x|x')\,\alpha_{E+\omega}(x|x')\cos\theta_\omega(x)\rangle \times \cos(\varphi_1-\varphi_2)\,d\varphi_1\,d\varphi_2,$$

$$\alpha(x|x') = R(x)/R(x').$$

We have taken the matching point at $x' > x$. Because this is a Markov process, we can now average independently to the right and to the left of the point x, respectively. Therefore, we have

$$F_\omega(z) = \frac{\pi}{v_F^2}\int_0^\pi g(z,\theta)\,w(\pi-\theta)\cos\theta\,d\theta, \tag{A.4}$$

where

$$g(z,\theta) = \langle \delta(\theta^>(x)-\theta)\,\alpha_E(x|x')\,\alpha_{E+\omega}(x|x')\cos\theta_\omega(x)\rangle, \tag{A.5}$$

and $w(\theta)$ is the stationary distributin function of the phase difference. A derivation using the matrix of scattering by the defect[13] yields the equation

$$\frac{\partial g}{\partial z} = \frac{\partial}{\partial\theta}\left(\sin^2\theta\,\frac{\partial g}{\partial\theta}\right) - \nu\frac{\partial g}{\partial\theta} - g\sin^2\theta . \tag{A.6}$$

Here and below, $z = (x = x')/l$ and $\nu = \omega\tau$, where l and τ are the range and lifetime relative to back scattering. From (A.5), follows a boundary conditin at $z = 0$:

$$g(0,\theta) = w(\theta)\cos\theta . \tag{A.6'}$$

Taking the Laplace transform with respect to z:

$$g(z,\theta) = \int_{\delta-i\infty}^{\delta+i\infty} \frac{d\varkappa}{2\pi i}\, e^{\varkappa z}\tilde{g}(\varkappa,\theta), \tag{A.7}$$

we find from (A.6) and (A.6') that

$$\frac{\partial}{\partial\theta}\left(\sin^2\theta\,\frac{\partial\tilde{g}}{\partial\theta}\right) - \nu\frac{\partial\tilde{g}}{\partial\theta} - (\varkappa+\sin^2\theta)\,\tilde{g} = -w(\theta)\cos\theta . \tag{A.8}$$

The definition (A.5) leads to the conditions for the aperiodicity of $\tilde{g}(\varkappa,\theta)$ at the end points of the interval $[0,\pi]$:

$$\tilde{g}(\varkappa,\pi) = -\tilde{g}(\varkappa,0) . \tag{A.9}$$

Equation (A.8) cannot be solved in general form. In the case of two nearly equal energies ($\nu \gg 1$), which is of greatest interest to us, we can find a solutin of (A.8) near the boundaries of the interval (i.e., when $\theta \ll 1$, $\pi - \theta \ll 1$), and then match these solutions together through the phase region $\theta \sim 1$. In fact, when $\theta \ll 1$, we have

$$\frac{\partial}{\partial\theta}\left(\theta^2\,\frac{\partial\tilde{g}}{\partial\theta}\right) - \nu\frac{\partial\tilde{g}}{\partial\theta} - \varkappa\tilde{g} = -w(\theta) \tag{A.10}$$

and analogously when $\pi - \theta \ll 1$. The solutions of (A.10) may be expressed in terms of the modified Bessel functions

$$\xi^{1/2}\exp(-\xi)\,\{K_\mu(\xi),\ I_\mu(\xi)\}, \tag{A.10'}$$

where

$$\mu = (\varkappa + 1/4)^{1/2}, \quad \xi = \nu/2\theta .$$

In the region $\theta \sim 1$, we may discard the term $\nu\partial\tilde{g}/\partial\theta$:

$$\frac{\partial}{\partial\theta}\left(\sin^2\theta\,\frac{\partial g}{\partial\theta}\right) - (\varkappa+\sin^2\theta)\,g = -w(\theta)\cos\theta . \tag{A.11}$$

The solutions of (A.11) may be expressed in terms of associated Legendre functions:

$$(\sin\theta)^{-1/2}\{P^{\mu}_{-1/2}(\cos\theta),\ P^{-\mu}_{-1/2}(\cos\theta)\} . \tag{A.11'}$$

The asymptotes (A.11') and (A.10') coincide[29] in the region $\nu \ll \theta \ll 1$

$$\theta^{-1/2+\mu}, \quad \theta^{-1/2-\mu} . \tag{A.12}$$

The condition under which both terms may be distinguished from higher-order corrections to the solutions (A.10) and (A.11) yields

$$\operatorname{Re}\mu < 1 . \tag{A.13}$$

Since the Laplace transformation (A.7) will be required to determine the correlator (A.1), it is best to first represent the solution of (A.8) in a form that possesses the desired analytic properties in the complex plane of the variable $\varkappa$ and only then undertake the indicated matching. For this purpose, we introduce the variable $u = \cot\theta$ and the new function

$$g(\varkappa,\theta) = e^{-\nu u/2}\psi(u) .$$

The function $\psi(u)$ satisfies a sort of Schrödinger equation with right side

$$-\psi''+\left\{\frac{\varkappa}{1+u^2}+\frac{1}{(1+u^2)^2}\right\}\psi+\frac{\nu^2}{4}\psi$$
$$=\frac{uw(u)}{(1+u^2)^{3/2}}e^{\nu u/2}\equiv f(u). \qquad (A.14)$$

The solutions of the homogeneous equation (A.14) are selected in such a way as to ensure that one of them $g_1(\varkappa,\theta)$ will be finite when $\theta=\pi$. The second linearly independent solution is

$$g_2(\varkappa,\ \theta)=e^{-\nu\,\mathrm{ctg}\,\theta}g_1(\varkappa,\ \pi-\theta). \qquad (A.15)$$

Therefore, the choice of the pair of independent solutions in (A.14) $\psi_1(\varkappa,u)$ and $\psi_2(\varkappa,u)$ depends on the condition under which $\psi_1(u)$ decreases exponentially as $u\to-\infty$:

$$\psi_1(\varkappa,\ u)\approx e^{\nu u/2}\quad (u\to-\infty),$$
$$\psi_1(\varkappa,\ u)\approx c_1(\varkappa)e^{\nu u/2}+c_2(\varkappa)e^{-\nu u/2}\quad (u\to+\infty). \qquad (A.16)$$

From (A.14), it follows that $\psi_2(u)=\psi_1(-u)$. The constant in (A.16) is selected so that $g_1(\varkappa,\pi)=1$ and the Wronskian of the selected pair of solutions is

$$\psi_1\psi_2'-\psi_1'\psi_2=-\nu c_1(\varkappa). \qquad (A.17)$$

By means of the pair of independent functions thus determined, the we can write for the inhomogeneous equation (A.14) a solution for which $g(\varkappa,\theta)$ is finite at the end points of the interval and for which (A.9) holds, in the form

$$\psi(u)=\frac{1}{\nu[c_1(\varkappa)+1]}\psi_1(u)\int\limits_{-\infty}^{\infty}f(u')\psi_1(-u')\,du'+\frac{1}{\nu c_1(\varkappa)}$$
$$\times\left\{-\psi_1(u)\int\limits_{-\infty}^{u}f(u')\psi_1(-u')\,du'+\psi_1(-u)\int\limits_{-\infty}^{u}f(u')\psi_1(u')\,du'\right\}. \qquad (A.18)$$

The function $\psi_1(u)$ in different regions of the variable u can be determined by matching the corresponding asymptotes under the condition (A.13). We will require below only the asymptotes near $\theta=0$ $(u=+\infty)$ and $\theta=\pi$ $(u=-\infty)$. In the region with $u\gg1$ $(u'=\nu u/2)$, we have

$$\psi_1(u)=-c_1(\varkappa)\left(\frac{\pi u'}{2}\right)^{1/2}[I_\mu(u')+I_{-\mu}(u')]-\left(\frac{2u'}{\pi}\right)^{1/2}$$
$$\times\frac{\gamma_\mu-\gamma_{-\mu}}{2}\,\mathrm{ctg}\,\mu\pi K_\mu(u'). \qquad (A.19a)$$

In the region with $u<0$ $(|u|\gg1,\ u'=-\nu u/2)$ we have

$$\psi_1(u)=(2u'/\pi)^{1/2}K_\mu(u'), \qquad (A.19b)$$

with

$$c_1(\varkappa)=-[(\gamma_\mu+\gamma_{-\mu})\cos\mu\pi-2]/2\sin^2\mu\pi, \qquad (A.20)$$

where we have introduced

$$\gamma=\frac{\Gamma(1/2-\mu)}{\Gamma(1/2+\mu)}\left[\frac{\Gamma(1+\mu)}{\Gamma(1-\mu)}\right]^2\left(\frac{8}{\nu}\right)^{2\mu}. \qquad (A.21)$$

Substituting (A.18) in (A.4), carrying out simple algebra, and omitting all terms analytic in the left half-plane of the variable $\varkappa$, we obtain

$$F_\omega^{(1)}(\varkappa)=-\frac{\pi}{v_F^2\nu[c_1(\varkappa)+1]}\left(\int\limits_{-\infty}^{+\infty}f(u)\psi_1(-u)\,du\right)^2. \qquad (A.22)$$

The angles θ, which are nearly equal to 0 or π, play the major role in the integral (A.22). In the principal approximation, the integral may be written as a sum of the corresponding contributions $J^{(0)}$ and $J^{(\pi)}$.

In (A.22), we retain initially only the term $(J^{(0)})^2$

$$J\approx(1/4-\mu^2)/\cos\mu\pi\approx1/\pi. \qquad (A.23)$$

The expression for $J^{(0)}$ is the result of integrating $w(\theta)$ from Ref. 13 using (A.19b). In the derivation we have used equation 6.621(3) of Ref. 30. In the denominator of (A.22), the entire expression must be expanded in terms of the small values of $\varkappa$ needed determine the $F^{(1)}(z)$ dependence when $z\gg1$. Here

$$\mu\approx1/2+\varkappa-\varkappa^2,\quad \cos\mu\pi\approx-\pi\varkappa,\quad \gamma_\mu\approx-(1/4\varkappa)(8/\nu)^{2\mu}, \qquad (A.24')$$

and as a result we have

$$c_1(\varkappa)+1\approx(\pi/8)(8/\nu)^{2\mu}. \qquad (A.24'')$$

This contribution to $F_\omega^{(1)}(\varkappa)$ is

$$F_\omega^{(1)}(\varkappa)\approx-\frac{1}{(\pi v_F)^2}\exp\left\{(-\varkappa+\varkappa^2)^2\ln\frac{8}{\nu}\right\},$$

which after substituting in (A.7) yields (14):

$$F_\omega^{(1)}(z)=-\frac{1}{(\pi v_F)^2}\frac{1}{2(\pi z_0)^{1/2}}\exp\left\{-\frac{(z-z_0)^2}{4z_0}\right\},$$

where $z_0=2\ln(8/\nu)$ and the width $Dz\sim[\ln(8/\nu)]^{1/2}$. The asymptotic behavior of $F_\omega^{(1)}(z)$ in the region $1\ll z\ll z_0$ is determined by the term $2J^{(0)}J^{(\pi)}$ in (A.22). The corresponding formulas coincide with the computation of the analygous asymptote in Ref. 16.

[1)] A minor error was made at this point in Ref. 27.

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Translated by Robert H. Silverman