region of the resultant degeneracy of the conical point contacts, magnetic breakdown can account for both the behavior of the magnetoresistance and of the thermoelectric power. If this explanation is valid, then the results above are the first observation of magnetic breakdown of this type.

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1) The value $\langle l_p \rangle \approx 3.1\times10^{-12}$ was taken from[11].

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Translated by J. G. Adashko

Conductivity of disordered one-dimensional metal with half-filled band

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The density correlator, the conductivity, and the dielectric constants are calculated for an impurity-containing one-dimensional metal with half-filled band. If the Fermi level coincides exactly with the center of the band, and the amplitude for forward scattering by an individual impurity is equal to zero, then at zero temperature the localization length is infinite. In the frequency region $T\ll\omega\ll1/\tau$ (T is the temperature and τ is the free-path time) the conductivity is constant and the dielectric constant increases with decreasing frequency like $(|\omega|\ln^2|\omega|)^{-1}$. When the Fermi level does not coincide with the center of the band, the static conductivity is equal to zero and the dielectric constant increases in the region $\epsilon\ll1/\tau$ in proportion to $|\epsilon|^{-1}$, where ϵ is the distance from the Fermi level to the center of the band.

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1. INTRODUCTION

Theoretical investigations of disordered one-dimensional systems have by now reached a level such that many properties of real crystals with one dimensional spectra can be explained.[1] We point out, in particular, the electronic-state localization that leads to the vanishing of static conductivity,[2,3] and to the change in the character of this localization when account is taken of the interaction with the phonons.[4,5] These studies make use of continual models that do not take into account the periodicity of real crystals. Dyson[6] has shown that such a characteristic as the density of states in a one-dimensional disordered harmonic chain has singularities in special points of the Brillouin zone. Analogous singularities should take place also in the electron spectrum. The appearance of a singularity in the state density near the center of the zone was observed by Weissman and Cohan,[7] who considered a model with nondiagonal disorder. As shown by Bush[8] the localization length of such a model becomes infinite when the center of the band is approached.

Gor'kov and Dorokhov[9] considered a model in which impurities with fixed potential were randomly distributed over the sites of a one-dimensional lattice with a period a. In the Born approximation, the potential of an individual impurity is characterized by two amplitudes corresponding to forward and backward scattering. It was shown that the electronic-state density becomes infinite at the center of the band only if the forward scattering amplitude is equal to zero. Gor'kov and Dorokhov had demonstrated the possibility of satisfying this condition using as examples TCNQ salts with asymmetric cations.[1]

The appearance of singularities in the state density and in the localization length should lead to a nontrivial behavior of the kinetic characteristics near the center

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of the band. In this paper, assuming vanishing of the forward scattering amplitude, we calculate the conductivity σ and the real part of the permittivity ε' for electrons with one-dimensional disordered lattice as functions of the external frequency ω and the distance ε from the Fermi level to the center of the band. It is shown that in the limit $(\varepsilon, T, \omega) \ll 1/\tau$ (T is the temperature and τ is the free-path time) the conductivity and the dielectric constant behave differently, depending on the order in which ε, T, and ω tend to zero.

We shall assume that the band is exactly half-filled if the limit is taken under conditions $\varepsilon \ll \omega$ and $T \ll \omega$. In this case the conductivity has a finite value $\sigma(0)$ in the limit as $\omega \to 0$, while the permittivity increases with decreasing frequency. Namely

$$\sigma(0) = \frac{2\pi e^2 l_-}{\hbar S}, \quad l_- = v\tau, \tag{1}$$

$$\varepsilon'(\omega) \approx \frac{8\pi^3 e^2 l_-^2 B}{\hbar v S |\omega\tau| \ln^2 |2\omega\tau|}, \tag{2}$$

where v is the Fermi velocity, l_- is the mean free path with respect to backward scattering, and S is the cross section of the crystal area per filament. Formula (2) contains a constant $B \sim 1$, which we were unable to determine.

If the band is not half-filled, i.e., in the limit $\varepsilon \gg \omega$, there is no static conductivity: $\sigma(0) = 0$ and the static permittivity takes the form

$$\varepsilon'(0) \approx \frac{16\pi e^2 l_-^2}{3\hbar v S |\varepsilon\tau|}, \quad |\varepsilon\tau| \ll 1. \tag{3}$$

If the forward scattering amplitude differs from zero, then the conductivity always vanishes in the static limit, the localization becomes finite, and the singularities of the state density and of the permittivity become smoothed out.

To calculate the kinetic coefficients we used the method proposed by Berezinskiĭ[4] for the summation of interference diagrams.1) A generalization of this method to the case of a metal with half-filled band will be carried out using as an example the calculation of the state density for which an analytic expression can be obtained.

2. DENSITY OF STATES

We consider a system of electrons having a dispersion $\varepsilon(p)$ and interacting with randomly distributed impurities

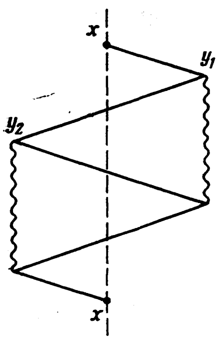

FIG. 1.

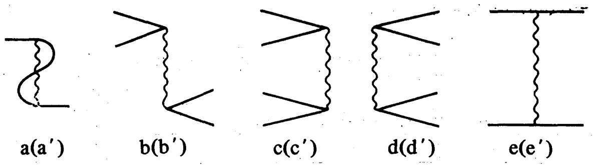

FIG. 2. Types of impurity vertices that enter in the essential diagrams. The prime denotes replacement of single lines by double lines. The vertices correspond to the factors: a) $(-\frac{1}{2})(1/l_- + 1/l_+)$, b) $(-1/l_-)$, c) $(-1/l_-)e^{4i(p-p_0)y}$, d) $(-1/l_-)e^{4i(p-p_0)y}$, e) $(-1/l_+)$, where l_+ is the mean free path for forward scattering.

In contrast to the earlier studies[3,4] we take into account here the periodicity of the real crystal, assuming that the impurities can be located only at the lattice sites with a period a. As will be shown below, this limitation leads to the appearance of a new class of diagrams, the contribution of which increases as the electron energy approaches the center of the band.

To calculate the state density we use the known formula

$$\rho(\varepsilon) = -\frac{1}{\pi} \operatorname{Im} \langle G^+(00|\varepsilon)\rangle, \tag{4}$$

where $G^+(n_1 n_2|\varepsilon)$ is the retarded Green's function of the electron, n_1 and n_2 are the numbers of the sites, while the angle brackets denote averaging over the locations of the impurities. The diagram expansion for expression (4) is constructed in analogy with[3,4]. The only difference is that the integration with respect to the coordinates is replaced by summation over the sites. The first significant diagram is shown in Fig. 1. This diagram corresponds to the expression

$$\delta G^+(00|\varepsilon) = G_0^+(00|\varepsilon) \left(\frac{a}{l_-}\right)^2 \left(\sum_{n_1=0}^{\infty} e^{4ipan_1}\right)^2$$
$$= G_0^+(00|\varepsilon) \left(\frac{a}{l_-}\right)^2 \left(\frac{1}{1-e^{4ipa}}\right)^2 \tag{5}$$

where $G_0^+(00|\varepsilon) = -i/v(\varepsilon)$ and $p = p(\varepsilon)$. It is seen that in the general case the relative increment to G^+ is small like $(a/l_-)^2 \ll 1$. For this reason we can neglect in the continual model the change introduced in the Green's function by the interaction with the impurities.[3] However, as $p \to p_0 = \pi/2a$ the increment (5) increases like $((p-p_0)l_-)^{-2}$. In other words, the vertex shown in Fig. 2c oscillates more and more weakly as $p \to p_0$ and therefore must be taken into account when the significant diagrams are selected. At $l_- \gg a$ the sums over n cover the region $n \sim l_-/a \gg 1$, so that we can change over from summation to integration, and simultaneously replace p by $p - p_0$.

All the essential types of impurity lines are shown in Fig. 2. The lines a(a′), b(b′), and e(e′) were introduced earlier,[3] while the lines c(c′) and d(d′) are significant if the Fermi level is close to the center of the band. It is seen only when the lines c(c′) and d(d′) are taken into account can we construct diagrams of the type of Fig. 1 which contribute to the Green's function.

For the subsequent calculations it will be convenient to cut the diagrams of Fig. 1 at the point x and consider separately the right- and left-hand sides of the diagram $R_m(x)$ and $\tilde{R}_m(x)$. The subscript m means that $4m$ lines pass through the point x. By shifting the point x, we obtain for the right-hand sides of $R_m(x)$ the equation

$$\frac{dR_m}{dx}=\left(\frac{2}{l_+}+\frac{1}{l_-}\right)4m^2R_m+\frac{1}{l_-}m(2m-1)R_{m-1}e^{4i(p-p_0)x}+\frac{1}{l_-}m(2m+1)R_{m+1}e^{-4i(p-p_0)x}. \tag{6}$$

Making the substitution $R_m(x)=R_m(-1)^m\exp[4im(p-p_0)x]$, we obtain for R_m after cancelling m the following equation:

$$isR_m=(2\gamma+1)4mR_m-(2m-1)R_{m-1}-(2m+1)R_{m+1},$$
$$\gamma=l_-/l_+,\quad s=4(p-p_0)l_-,\quad m>0. \tag{7}$$

The difference equation (7) must be solved with the boundary condition $R_0=1$. It is easily seen that the left-hand side is $\tilde{R}_m(x)=R_m(-1)^m\exp[-4i(p-p_0)xm]$. We obtain therefore the state density $\rho(\varepsilon)$ the expression

$$\rho(\varepsilon)=\rho_0(\varepsilon)\left(1+2\operatorname{Re}\sum_{m=1}^{\infty}R_m^2\right). \tag{8}$$

Here $\rho_0(\varepsilon)=1/\pi v(\varepsilon)$ is the state density in the pure crystal. The coefficient 2 in relation (8) arises when account is taken of diagrams that are the mirror images of the diagrams of Fig. 1 relative to the dashed line.

Equation (7) interrelates the quantities R_m with $m>0$. We introduce quantities R_m with $m<0$ by means of the relation $R_m=R^*_{-m}$. Then the recurrence relation (7) is satisfied for all signs of m, and relation (8) can be rewritten in the form

$$\rho(\varepsilon)=\rho_0(\varepsilon)\sum_{-\infty}^{\infty}R_m^2. \tag{9}$$

Multiplication of Eq. (7) by $me^{im\varphi}$ followed by summation with respect to m from $-\infty$ to $+\infty$ makes it possible, in analogy with[9], to transform (7) into a second-order differential equation for the function

$$R(\varphi)=\sum_{-\infty}^{\infty}R_m e^{im\varphi}.$$

Its first integral is[2)]

$$(8\gamma+4-4\cos\varphi)\frac{dR}{d\varphi}+(2\sin\varphi+s)R=D_1. \tag{10}$$

The integration constant D_1 must be chosen to satisfy the normalization condition

$$\int_0^{2\pi}\frac{d\varphi}{2\pi}R(\varphi)=R_0=1. \tag{11}$$

We introduce a new variable χ by the substitution

$$\operatorname{tg}\frac{\varphi}{2}=\left(\frac{\gamma}{\gamma+1}\right)^{1/2}\operatorname{tg}\frac{\chi}{2}.$$

Then Eq. (10) takes the form

$$2\frac{dR}{d\chi}+\left(\frac{\sin\chi}{2\gamma+1+\cos\chi}+\frac{s}{4[\gamma(\gamma+1)]^{1/2}}\right)R=\frac{D_1}{4[\gamma(\gamma+1)]^{1/2}}. \tag{12}$$

This equation has a solution that satisfies the condition of periodicity $R(0)=R(2\pi)$ and the normalization condition (11) is

$$R(\chi)=\frac{D}{h(\chi)}\left[h(2\pi)\int_0^{\chi}h(\psi)d\psi+h(0)\int_{\chi}^{2\pi}h(\psi)d\psi\right], \tag{13}$$
$$h(\chi)=(2\gamma+1+\cos\chi)^{-1/2}\exp\left(\frac{s\chi}{8[\gamma(\gamma+1)]^{1/2}}\right),$$
$$[\gamma(\gamma+1)]^{1/2}\int_0^{2\pi}\frac{d\chi}{\pi}\frac{R(\chi)}{2\gamma+1+\cos\chi}=1.$$

Ultimately we obtain for the density of states

$$\rho(\varepsilon)=\rho_0\frac{[\gamma(\gamma+1)]^{1/2}}{\pi}\int_0^{2\pi}\frac{d\chi R(\chi)R(2\pi-\chi)}{2\gamma+1+\cos\chi}. \tag{14}$$

The function $\rho(s,\gamma)$ is illustrated in Fig. 3. The increment to the state density is positive near the center of the band, reverses sign in the region $s\sim 1$ and then decreases in absolute magnitude like $|s|^{-2}$ at $|s|\gg 1$. The total number of states remains unchanged:

$$\Delta N=\int_{-\infty}^{\infty}\Delta\rho(\varepsilon)d\varepsilon=0.$$

The maximum of $\rho(s)$ is reached at $s=0$. The height of the peak does not depend on the potential of the impurity and is determined by the parameter γ, i.e., by the ratio l_-/l_+. From (13) and (14) with $s=0$ we obtain

$$\rho(0)=\rho_0\left(\frac{\gamma+1}{\gamma}\right)^{1/2}\left[\pi/2K\left(\sqrt{\frac{1}{\gamma+1}}\right)\right]^2, \tag{15}$$

where K is a complete elliptic integral of the first kind. With decreasing γ, the value of $\rho(0)$ increases like

$$\rho(0)\approx\rho_0\pi^2/\sqrt{\gamma}\ln^2\gamma. \tag{16}$$

For impurities with an δ-function potential ($\gamma=1$) the change of the state density at the center of the band is 1.5%.

It is seen from (16) that at $\gamma=0$ the state density as a function of s has a singularity at the center of the band. At $\gamma=0$ Eq. (7) can be conveniently solved by making the substitution

$$R_m=\int d\zeta\,\zeta^m w(\zeta).$$

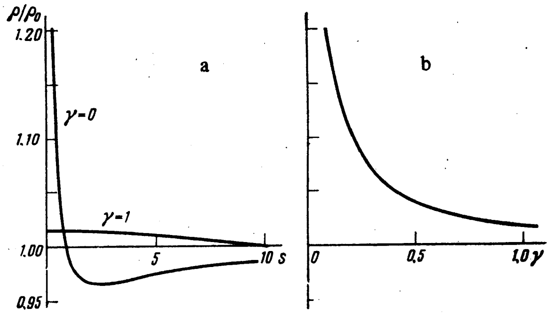

FIG. 3. Plot of $\rho(s)$ at $\gamma=0$ and $\gamma=1$ (a) and of $\rho(\gamma)$ at $s=0$ (b).

We then obtain for $w(\zeta)$ the equation

$$-isw+\left(\frac{1}{\zeta}-\zeta\right)w+2\frac{d}{d\zeta}((\zeta-1)^2w)=0. \tag{17}$$

Allowance for the condition $R_0=1$ yields next

$$R_m=\frac{e^{is/4}}{K_0(-{}^1/_4is)}\int_0^\infty\frac{dt}{[t(t+1)]^{1/2}}\left(\frac{t}{t+1}\right)^m e^{ist/2}. \tag{18}$$

where K_0 is a Bessel function. Substituting (18) in (8) we obtain at $|s|\ll 1$

$$\rho(s)\approx\rho_0\frac{4\pi}{|s|}\frac{-C-\ln|s/8|}{[(\ln|s/8|+C)^2+\pi^2/4]^2}. \tag{19}$$

We note that the form of the singularity in the density of the electronic states (19) coincides with the form of phonon state density singularity obtained by Dyson.[6]

The singularity in the density of the electron states should lead to a singularity in the temperature dependence of the magnetic susceptibility:

$$\chi(T)=2\mu_B{}^2\int_{-\infty}^{\infty}\frac{d\varepsilon}{4T}\operatorname{ch}^{-2}\left(\frac{\varepsilon}{2T}\right)\rho(\varepsilon)\approx\frac{\pi\rho_0\mu_B{}^2}{2T\tau_i\ln^2(T\tau_i)}, \tag{19a}$$

where μ_B is the Bohr magneton.

Using expression (19a), we can explain the temperature dependence of the magnetic susceptibility of NMP-TCNQ in the interval 0.1–7 K.[11] The best agreement between the theoretical curve and the experimental data is reached at $1/\tau_i=140$ K and $\rho_0=2$ states/eV-molecule. It should be noted that this estimate for the free-path time in TCNQ salts with asymmetric cations agrees well with an analogous estimate based on the permittivity.[5] The need to take the disorder into account in order to explain the $\chi(T)$ dependence in these substances was already noted by Bulaevskiĭ, Lyubovskiĭ, and Shchegolev.[12]

Our calculations were made in the Born approximation in the interaction of the electrons with the impurities. As a result, the formal criteria for the applicability of Eq. (7) and of formulas (16) and (19) should be $|s|\gg\sqrt{\alpha}$ and $\gamma\gg\alpha$, where α is the Born parameter. We point out, however, that for two particular forms of the potentials it is possible to take into account also the next term of the expansion in the Born parameter in Eq. (7) and to verify that the singularity of $\rho(s,\gamma)$ remains of the same form. The relative corrections to $\rho(s,\gamma)$ are in this case of the order of $\alpha^2\ll 1$.

3. CORRELATION FUNCTION OF ELECTRON DENSITY

To clarify the character of the localization of the electrons having an energy close to the center of the band, we calculated the electron-density correlator. As seen from the preceding section, greatest interest attaches to the case $\gamma=0$, when a singularity of the electron spectrum appears at the center of the band.

The general procedure for calculating the density correlator was described in detail earlier.[3,4] In our case, besides the impurity vertices that were taken into account in[3,4], there are also the essential vertices c(c′) and d(d′) of Fig. 2 as well as c and d of Fig. 4. The change in the number of single lines in the vertices a(a′), b(b′), and e(e′) of Fig. 2 and of a and b of Fig. 4, considered in[3,4], is accompanied by exactly the same change in the number of the double lines. The new impurity vertices c(c′) and d(d′) of Fig. 2 and c and d of Fig. 4 can have separately different numbers of the single and double lines. The bisection of the diagram must therefore now be characterized not by a single integer but by two integers m_1 and m_2, which denote respectively the numbers of the pairs of single and double lines.

Just as before, we break up the diagram for the density correlator into right-hand $R_{m_1m_2}(x)$ on the central $Z^{m_1'm_2'}_{m_1,m_2}(x',x)$, and left-hand $\tilde{R}_{m_1'm_2'}(x')$ parts. In analogy with[3,4], we separate explicitly the coordinate dependence of the right-hand side:

$$R_{m_1m_2}(x)=R_{m_1m_2}(-1)^{(m_1-m_2)/2}\exp[{}^1/_2ix(m_1(\nu+s)+m_2(\nu-s))]. \tag{20}$$

Here and below we use the dimensionless variables $\nu=2\omega\tau$ and $s=4\varepsilon\tau$, and x is measured in units of l_-. We assume $\gamma=0$, i.e., $l_+=\infty$, and therefore omit the vertices $e(e')$ of Fig. 2. Taking into account the remaining vertices, the equations for $R_{m_1m_2}$ take the form

$$\begin{aligned}&-{}^1/_2i(m_1(\nu+s)+m_2(\nu-s))R_{m_1m_2}\\&=-(m_1{}^2+m_2{}^2)R_{m_1m_2}+m_1m_2R_{m_1-1,\,m_2-1}+m_1m_2R_{m_1+1,\,m_2+1}\\&\quad+{}^1/_2m_1(m_1-1)R_{m_1-2,\,m_2}+{}^1/_2m_2(m_2-1)R_{m_1,\,m_2-2}\\&\quad+{}^1/_2m_1(m_1+1)R_{m_1+2,\,m_2}+{}^1/_2m_2(m_2+1)R_{m_1,\,m_2+2}\\&\quad-m_1m_2R_{m_1-1,\,m_2+1}-m_1m_2R_{m_1+1,\,m_2-1}.\end{aligned} \tag{21}$$

We now introduce the quantities

$$\begin{aligned}Q^a_{m_1m_2}(\nu,\varkappa)&=(-1)^{(m_1-m_2)/2}\sum_{m_1',m_2'=0}^{\infty}\int_x^{\infty}dx\,e^{i\varkappa(x'-x)}\\&\times Z^{m_1'm_2'}_{m_1,m_2}(x',x)P^a_{m_1'm_2'}(-1)^{(m_1'-m_2')/2}\\&\times\exp[{}^1/_2i((\nu+s)(m_1x-m_1'x')+(\nu-s)(m_2x-m_2'x'))].\end{aligned} \tag{22}$$

The index a takes on the values 0 and 1. The correlators of the density ($a=0$) and of the currents ($a=1$) are expressed in terms of the quantities

$$Q^0_{m_1m_2},\quad P^0_{m_1m_2}={}^1/_2(R_{m_1m_2}+R_{m_1+1,m_2+1}),$$

and

$$Q^1_{m_1m_2},\quad P^1_{m_1m_2}=R_{m_1m_2}-R_{m_1+1,m_2+1}$$

by a single formula

FIG. 4. Types of impurity vertices that enter in the essential diagrams. The vertices correspond to the following factors: a) $l_-^{-1}e^{2i\omega y/v}$, b) $l_-^{-1}e^{-2i\omega y/v}$, c) $l_-^{-1}e^{4i(\varphi-\varphi_0)y}$, d) $l_-^{-1}e^{-4i(\varphi-\varphi_0)y}$.

$$\mathfrak{X}^a(s,\nu,\varkappa)=\frac{2l_-}{v}\left[\frac{v}{2}\right]^{2a}\sum_{m_1,m_2=0}^{\infty}P^a_{m_1m_2}(\nu)\,[Q^a_{m_1m_2}(\nu,\varkappa)+Q^a_{m_1m_2}(\nu,-\varkappa)]. \tag{23}$$

The equations for $Q^a_{m_1m_2}$ take the form

$$\begin{gathered}-{}^1/{}_2 i(m_1(\nu+s)+m_2(\nu-s)+\nu)\,Q_{m_1m_2}=P^a_{m_1m_2}-i\varkappa Q^a_{m_1m_2}\\ -(m_1+m_2+1)\,Q^a_{m_1m_2}-(m_1{}^2+m_2{}^2)\,Q^a_{m_1m_2}+m_1m_2Q^a_{m_1-1,m_2-1}\\ +(m_1+1)\,(m_2+1)\,Q^a_{m_1+1,m_2+1}+{}^1/{}_2(m_1+1)\,(m_1+2)\,Q_{m_1+2,m_2}\\ +{}^1/{}_2(m_2+1)\,(m_2+2)\,Q^a_{m_1,m_2+2}+{}^1/{}_2m_1(m_1-1)\,Q^a_{m_1-2,m_2}\\ +{}^1/{}_2m_2(m_2-1)\,Q^a_{m_1,m_2-2}-(m_1+1)\,m_2Q^a_{m_1+1,m_2-1}-m_1(m_2+1)\,Q^a_{m_1-1,m_2+1}.\end{gathered} \tag{24}$$

Expression (23) takes into account the contribution of diagrams of the type 5a. Near the middle of the band, a comparable contribution is made by the diagrams of the type 5b, the calculation of which will be discussed later on.

At $m_2=0$ or $m_1=0$, Eq. (21) admits of the exact solution

$$R_{m_10}=R_{m_1}(\nu+s),\quad R_{0m_2}=R_{m_2}(\nu-s), \tag{25}$$

where $R_m(s)$ are defined in (18).

We now investigate the solutions of (21) and (24) in the limit when $\nu\ll 1$ and $s\ll 1$. In this limit, the essential values are $m_1\gg 1$ and $m_2\gg 1$, so that in (21) and (24) we can change over from difference equations to differential equations. We introduce new variables:

$$p={}^1/{}_2\nu(m_1+m_2)\ \text{и}\ t={}^1/{}_2s(m_1-m_2).$$

Equations (21) and (24) then take the form

$$-i(p+t)R=2\left(p^2\frac{\partial^2R}{\partial p^2}+2pt\frac{\partial^2R}{\partial p\,\partial t}+t^2\frac{\partial^2R}{\partial t^2}\right)+2\left(p\frac{\partial R}{\partial p}+t\frac{\partial R}{\partial t}\right), \tag{26}$$

$$\begin{gathered}-i(p+t)\,Q^a=P^a-i\varkappa Q^a+2Q^a\\ +2\left(p^2\frac{\partial^2Q^a}{\partial p^2}+2pt\frac{\partial^2Q^a}{\partial p\,\partial t}+t^2\frac{\partial^2Q^a}{\partial t^2}\right)+6\left(p\frac{\partial Q^a}{\partial p}+t\frac{\partial Q^a}{\partial t}\right).\end{gathered} \tag{27}$$

Equation (26) has a general solution that decreases at infinity in the form

$$R(p,t)=K_0(\sqrt{-2i(p+t)})\,\varphi\left(\frac{p-t}{p+t}\right), \tag{28}$$

where φ is an unknown function. The appearance of this function is due to the degeneracy of the differential operator (26). This operator vanishes on any function of p/t. The degeneracy takes place in the transition from the difference equation to the differential equation, and therefore the actual form of the function φ should be determined from the solution of Eq. (21) at m_1, $m_2\sim 1$. We were unable to obtain such a solution. However, as shown below, to calculate a number of physical characteristics it suffices to use those properties of the function φ which follow from identical relations. Comparison of (28) with the asymptotic forms of the exact solutions (25) yields the boundary conditions

$$\begin{aligned}\varphi\left(\frac{\nu-s}{\nu+s}\right)&=2e^{i(\nu+s)/4}/K_0\left(-\frac{i}{4}(\nu+s)\right),\\ \varphi\left(\frac{\nu+s}{\nu-s}\right)&=2e^{i(\nu-s)/4}/K_0\left(-\frac{i}{4}(\nu-s)\right).\end{aligned} \tag{29}$$

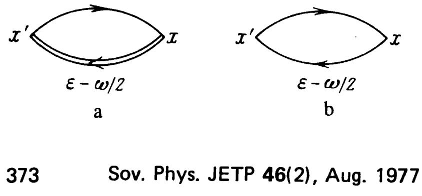

FIG. 5.

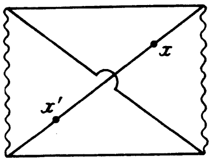

FIG. 6.

The solution of (27) with allowance for (28) is

$$Q^0(p,t)=\frac{G(\sqrt{-2i(p+t)})}{-i(p+t)}\varphi\left(\frac{p-t}{p+t}\right), \tag{30}$$

$$G(z)=I_\lambda(z)\int_z^\infty\xi\,d\xi\,K_\lambda(\xi)K_0(\xi)+K_\lambda(z)\int_0^z\xi\,d\xi\,I_\lambda(\xi)K_0(\xi),\quad \lambda=\sqrt{2i\varkappa}. \tag{31}$$

The solution (30) of the inhomogeneous equation (27) is chosen to satisfy the condition

$$\int_{-\infty}^{\infty}\frac{d\varkappa}{2\pi}Q^a_{m_1m_2}(\nu,\varkappa)=P^a_{m_1m_2}(\nu). \tag{32}$$

The last relation follows from the definition (22) of $Q^a_{m_1m_2}$ and from the boundary condition

$$Z^{m_1'm_2'}_{m_1m_2}(x-0,x)=\delta_{m_1m_1'}\delta_{m_2m_2'}. \tag{33}$$

Formulas (28) and (30) are sufficient for the determination of the density correlator, but contain an unknown function φ. From the course of the solution it is seen that φ does not depend on $\varkappa$, so that the properties of φ which we need can be obtained from the identity that holds at $\varkappa=0$.

The exact solutions of Eqs. (24) at $\varkappa=0$ satisfy the relation

$$(-i\nu)\sum_{m_1,m_2=0}^{\infty}Q^a_{m_1m_2}P^0_{m_1m_2}=\sum_{m_1,m_2=0}^{\infty}P^a_{m_1m_2}P^1_{m_1m_2}. \tag{34}$$

To obtain this relation it is necessary to multiply (24) by $P^1_{m_1m_2}$ and sum over all m_1 and m_2 with allowance for (21). At $a=0$ the identity (34) takes the form

$$(-2i\nu)\sum_{m_1,m_2=0}^{\infty}Q^0_{m_1m_2}P^0_{m_1m_2}=f(s,\nu), \tag{35}$$

$$f(s,\nu)=1+\sum_{m=1}^{\infty}(R_m{}^2(\nu+s)+R_m{}^2(\nu-s)). \tag{36}$$

From (28), (30), and (35) we obtain

$$\int_q^{1/q}dy\,\varphi^2(y)=(-2is)f(s,\nu),\qquad q=(\nu-s)/(\nu+s). \tag{37}$$

This turns out to be sufficient for the calculation of the contribution made to the density correlator by the diagrams of Fig. 5a. The contribution from diagram of the type of Fig. 5b is calculated in perfect analogy. One of these diagrams is shown in Fig. 6. The solution of the corresponding equations leads to expressions that differ from (28) and (30) is that the function $\varphi(y)$ is replaced by the function $\varphi_1(y)$ that satisfies the relation

$$\int_q^{1/q} dy\, \varphi_1^2(y) = (-2is) \sum_{m=0}^{\infty} (R_m^2(s-\nu) - R_m^2(s+\nu)). \tag{38}$$

Ultimately we obtain for the asymptotic form of the correlation function as $\omega \to 0$

$$X^0(s, \omega, \varkappa) = \frac{1}{-i\omega} \frac{\rho(s)}{\rho_0} [f(\varkappa) + f(-\varkappa)], \tag{39}$$

where

$$f(\varkappa) = 4 \int_0^{\infty} z\, dz\, K_0(z) I_\lambda(z) \int_z^{\infty} \xi\, d\xi\, K_\lambda(\xi) K_0(\xi). \tag{40}$$

The expression obtained by us differs from the results from the continual model in the appearance of the common factor $\rho(s)/\rho_0$, which reflects the change in the state density near the center of the band, in the replacement of K_1 and K_0, and in the replacement of $\lambda = (1 + 4i\varkappa)^{1/2}$ by $\lambda = (2i\varkappa)^{1/2}$. Just as before, $f(\varkappa)$ has a branch point, but its position has been shifted from $\varkappa = i/4$[4] to $\varkappa = 0$. This changes the exponential asymptotic form of $X^0(\omega, x)$ into a power-law form. To calculate the form factor of the localization it is necessary as before,[4,13] to displace the contour of the integration with respect to $\varkappa$ to the edges of the cut drawn from the branch point along the imaginary axis. This yields for the density distribution as $t \to \infty$

$$p_\infty(x) = \frac{1}{2\pi^2} \int_0^{\infty} \eta\, d\eta\, e^{-{}^1/_2\eta^2|x|} \left(\frac{\pi\eta}{2 \operatorname{sh} {}^1/_2\pi\eta} \right)^4. \tag{41}$$

A plot of this function is shown in Fig. 7. We point out that $p_\infty(0) = 1/3$ and that at $|x| \gg 1$ the asymptotic form of $p_\infty(x)$ is

$$p_\infty(x) \approx \frac{1}{8\sqrt{\pi}} |x|^{-3/2}, \quad |x| \gg 1. \tag{42}$$

The function $p_\infty(x)$ is normalized to unity. At large $|x| \gg 1$, however, it decreases so slowly that all its moments diverge. This means that the average electron displacements, and consequently the localization region, becomes infinite at the center of the band.

Formulas (40) and (41) were obtained as a result of solving approximate equations which are exact only in the limit s, $\nu \to 0$. Therefore, at small but finite $s \ll 1$ the power-law asymptotic form (42) should go over at sufficiently large x into the exponential law $p_\infty(x) \propto \exp(-|x|/l(s))$, where $l(s) \to \infty$ as $s \to 0$.

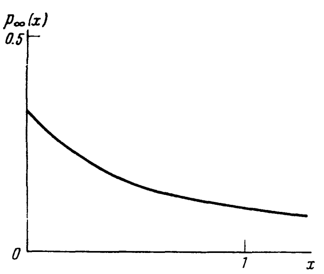

FIG. 7. Asymptotic distribution of the electron density.

4. CONDUCTIVITY AND PERMITTIVITY

The calculation of the conductivity and of the permittivity is a more difficult problem than the calculation of the density correlator.[3,4] In this problem the main difficulty is the absence of an explicit expression for the function $\varphi(y)$ from (28) and (30). In the preceding section this difficulty was overcome because the final answer contained only an integral of φ^2 [Eq. (37)], which could be determined from the identity (34). In this section we shall use a similar device to calculate the the conductivity. We start from expression (23) for the current correlation function at $\varkappa = 0$. From the definition of $P^1_{m_1m_2}$ and formula (28) it follows that at large $m_1, m_2 \gg 1$ we have

$$P^1_{m_1m_2} \approx -\nu \frac{\partial R}{\partial p} = (-i\nu) \left[\varphi\left(\frac{p-t}{p+t}\right) \frac{K_1(\sqrt{-2i(p+t)})}{(-2i(p+t))^{1/2}} - \left(1 - \frac{p-t}{p+t}\right) \varphi'\left(\frac{p-t}{p+t}\right) \frac{K_0(\sqrt{-2i(p+t)})}{-i(p+t)} \right]. \tag{43}$$

From (43) and (27) we obtain for $Q^1(p, t)$

$$Q^1(p,t) = (-i\nu) \left[\varphi\left(\frac{p-t}{p+t}\right) \frac{G_1(\sqrt{-2i(p+t)})}{-i(p+t)} - \left(1 - \frac{p-t}{p+t}\right) \varphi'\left(\frac{p-t}{p+t}\right) \frac{G_2(\sqrt{-2i(p+t)})}{-i(p+t)} \right], \tag{44}$$

where $G_1(z)$ and $G_2(z)$ are given by

$$G_1(z) = I_0(z) \int_z^{\infty} d\xi\, K_0(\xi) K_1(\xi) + K_0(z) \int_0^{z} d\xi\, I_0(\xi) \left(K_1(\xi) - \frac{1}{\xi} e^{-\xi} \right) - K_0(z) \int_z^{\infty} d\xi \frac{1}{\xi} I_0(\xi) e^{-\xi} + C_1 K_0(z), \tag{45}$$

$$G_2(z) = 2I_0(z) \int_z^{\infty} d\xi \frac{1}{\xi} K_0^2(\xi) - 2K_0(z) \int_z^{\infty} d\xi \frac{1}{\xi} I_0(\xi) K_0(\xi) + C_2 K_0(z). \tag{46}$$

Introduction of the term $\xi^{-1}e^{-\xi}$ in the integrand of (45) is necessitated by the redefinition of the integration constant C_1.

In contrast to the density correlator, integrals of the type (40) with respect to z will now diverge logarithmically at small z, because of the additional differentiation in (43). We therefore cut off the integration at a small $z_0 \sim \max(s, \nu)$ and carry out all the subsequent calculations with logarithmic accuracy. We must next multiply expressions (44) and (43) and integrate with respect to the variables p and t. With the aid of (29) and by integrating by parts we can verify that

$$\int_q^{1/q} dy\, \varphi(y) \varphi'(y) (1-y) = 0. \tag{47}$$

Thus, it remains to determine the constants C_1 and C_2 as well as the function $g(s, \nu)$, defined by the expression

$$(-2is) g(s, \nu) = \int_q^{1/q} dy (1-y)^2 (\varphi'(y))^2. \tag{48}$$

To determine the constant C_1 we use the identity

$$\sum_{m_1,m_2=0}^{\infty} Q^0_{m_1m_2}P^1_{m_1m_2}=\sum_{m_1,m_2=0}^{\infty} Q^1_{m_1m_2}P^0_{m_1m_2}, \tag{49}$$

which can be easily obtained by multiplying the equations for $Q^0_{m_1m_2}$ by $Q^1_{m_1m_2}$ and summing over m_1 and m_2. Substituting (28), (30), (43), and (44) in (49) we obtain with logarithmic accuracy

$$C_1\approx-\ln z_0. \tag{50}$$

It is natural to estimate the constant C_2 by using the condition that all of the terms in the right-hand side of (46) have at $z\sim z_0$ the same order of magnitude. Then

$$C_2\sim\ln^2 z_0. \tag{51}$$

As will be shown below, in the principal logarithmic approximation the term with G_2 in (44) makes no contribution to the final results, so that the absence of an exact expression for C_2 does not influence the final formulas.

Substituting (43)–(46) in the identity (34) at $a=1$, we obtain in the principal logarithmic approximation

$$g(s,\nu)\approx\frac{A}{\ln^3 z_0}f(s,\nu), \quad A\sim 1. \tag{52}$$

Thus, g is small in comparison with f and this smallness is not offset by the integral with respect to z in the final expression. Therefore in the principal logarithmic approximation it suffices to retain the first term in (44). Substituting (44) in (23), we get

$$X^1(s,\nu)=l_-v(-2i\nu)f(s,\nu)(-{}^1/{}_3\ln^3 z_0). \tag{53}$$

This formula gives the contribution of the diagrams of type 5a. Taking into account the diagrams of type 5b, we get

$$X^1(s,\nu)=l_-v(-2i\nu)\frac{\rho(s-\nu)}{\rho_0}\left(-\frac{1}{3}\ln^3 z_0\right). \tag{54}$$

To calculate the conductivity we use the Kubo-Greenwood formulas[3]

$$\sigma(\omega)=\frac{e^2}{2\pi iS}\int_{-\infty}^{\infty}\frac{d\omega'}{\omega'-\omega-i0}\frac{1}{\omega'}\int_{-\omega'/2}^{\omega'/2}\frac{2d\varepsilon}{\pi v}(X^1(\varepsilon,\omega')+X^1(\varepsilon,-\omega')). \tag{55}$$

We are interested in two limiting cases. In the first case the Fermi level is close to the center of the band, but does not coincide with it ($|s|\sim|p_F-p_0|l_-\ll 1$), and the frequency $\nu\ll S$. We can then neglect the dependence of X^1 on ε in the region $\Delta\varepsilon\sim\omega'\ll\varepsilon$ and calculate the integral (55) with allowance for the analyticity of $X^1(\omega')$ in the upper half-plane. As a result $\sigma(\omega)$ is proportional to $X^1(\varepsilon,\omega)$ of (45), and the cutoff is carried out at $z_0=|s|$. Separating the real and imaginary parts of this expression, we get

$$\operatorname{Re}\sigma(0)=0, \tag{56}$$

$$\varepsilon'(0)=\frac{16\pi e^2 l_-^2}{3vS|\varepsilon\tau|}, \tag{57}$$

where ε is the distance from the Fermi level to the center of the band.

In the second case the Fermi level coincides with the center of the band. Then the cutoff in (54) must be carried out at $z_0=-i\nu$, and for $\operatorname{Re}\sigma(0)$ we obtain the final expression:

$$\operatorname{Re}\sigma(0)=2\pi e^2 l_-/S. \tag{58}$$

This formula differs by a factor $2\pi^2$ from the results of the solution of the kinetic equation. The dielectric constant in this case is determined by the next term in the expansion of (53) in powers of $\ln z_0$ and increases with decreasing frequency like

$$\varepsilon'(\omega)\approx\frac{8\pi^3e^2l_-^2B}{vS|\omega\tau|\ln^2|2\omega\tau|}, \tag{59}$$

where B is an unknown constant of the order of unity.

The finite conductivity agrees with the statement made above that the electronic states near the center of the band are not localized.

All the calculations were performed for zero temperature. At finite temperature, formulas (58) and (59) are suitable in the case when the temperature is less than the external frequency, and formula (57) is suitable when the temperature is lower than the distance from the Fermi level to the center of the band.

5. CONCLUSION

The influence of disorder on the characteristics of one-dimensional systems, which was first considered by Dyson,[6] has by now become the subject of intensive theoretical and experimental investigations in view of the increase in interest in the properties of quasi-one-dimensional conductors. Bulaevskiĭ, Zvarykina, Karimov, Lyubovskiĭ, and Shchegolev[11] have investigated the temperature dependence of the magnetic susceptibility of the highly conducting TCNQ salts. An analysis of the experimental results has shown that the increase of the susceptibility at low temperatures must be attributed to a singularity in the state density of the disordered one-dimensional systems. For a TCNQ salt with one unpaired electron per molecule (NMP–TCNQ) the singularity in the state density was interpreted[12] on the basis of the model of noninteracting electrons present in the disordered one-dimensional chain.

The disordered character of the well-conducting quasi-one-dimensional TCNQ salts is due predominantly to the random orientation of the asymmetric cations (the only exceptions are salts with symmetrical cations TTF and TTT). For such an internal disorder, as shown by Gor'kov and Dorokhov,[9] the condition that the amplitude for forward scattering by a random potential of an individual cell vanish is satisfied. In those compounds where there is one unpaired electron per molecule, the conduction band is half-filled, so that we must expect the disorder to lead to the appearance of singularities of both the thermodynamic and the kinetic characteristics of these conductors.

In the present paper we investigated a metal model that takes into account all the factors responsible for the peculiar temperature dependence of the magnetic susceptibility of NMP–TCNQ. Namely the electrons were assumed to be non-interacting, the impurities distributed over the lattice sites, the band half-filled, and the amplitude of forward scattering by an individual impurity was assumed equal to zero in the principal part of the article.

Within the framework of this model, it was shown that as the Fermi level approaches the center of the band, the interaction with the impurities alters significantly the state density and the kinetic characteristics of the electrons in comparison with the results obtained with the continuum model.[3] The changes are particularly strong if the forward scattering amplitude by an individual impurity vanishes. For this limiting case we calculated the electron-density correlator, the conductivity, and the permittivity. From the form of the density correlator it follows that the mean squared displacement of the electron increases infinitely at large times if the electron momentum coincides exactly with the center of the band. Thus, the localization length of the electron becomes infinite at the center of the band not only for a model with a strictly non-diagonal disorder,[8,14] but also in the case when the disorder is produced by impurities for which the forward scattering amplitude is equal to zero.

The static conductivity and the permittivity depend on the order in which the frequency and temperature tend to zero and the Fermi level tends to the center of the band. For a half-filled band, i.e., at $\varepsilon = 0$, the conductivity has a finite value in the low-temperature limit, and the permittivity increases infinitely with decreasing frequency. In the case when the Fermi level does not coincide with the center of the band, i.e., at $\varepsilon \neq 0$, the static conductivity is equal to zero and the dielectric constant increases without limit as the center of the band is approached.

If the forward scattering amplitude is finite, then the singularities become smoothed out, but in the case of a metal with a half-filled band, an anomalous temperature dependence of the thermodynamic and kinetic characteristics should be observed. In the model considered we have neglected the interelectron interaction, and therefore the results obtained are valid for temperatures above the phase-transition temperature. Our analysis was carried out for a one-dimensional conductor. The growth of the localization lengths as the Fermi level approaches the center of the band should reinforce the three-dimensionality effects due, for example, to the finite amplitude of the jump of the electron from filament to filament. Even if the indicated amplitude is small, one can expect that at sufficiently low temperatures a quasi-one-dimensional conductor with half-filled band will behave like an anisotropic metal. With increasing temperature, the localization length of the electrons participating in the conductivity will decrease because of the deviation of the electron energy from the center of the band, as a result of which the conductivity of the metal will decrease. This influence can be regarded as a particular case of Anderson localization of the electrons—the localization is the result of competition between the amplitude of the jump from filament to filament and the amplitude of the random potential on the individual filaments. In this case all the electrons should be divided, in accordance with their energy, into delocalized (close to the center of the band) and localized ones. The energy width of the region of the delocalized states should be of the same order as the width of the electron band for motion in transverse directions.

In conclusion, the authors thank L. P. Gor'kov, O. N. Dorokhov, and É. I. Rashba for very useful discussions.

[1)] Another method of calculating the conductivity of a one-dimensional disordered metal was developed by Abrikosov and Ryzhkin.[10]

[2)] A similar equation was obtained by Gor'kov and Dorokhov.[9] The subsequent formulas of the present paper differ from the results of[9] because the integration constant D_1 was incorrectly chosen in[9].

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