Singularities of the localization length and of the dielectric constant near the band center in one-dimensional metals with strong disorder

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The Berezinskiĭ diagram technique is used to investigate singularities of the localization length l_{loc} and of the static dielectric constant ε' in one-dimensional metals with strong disorder in the presence of commensurability effects. The character of the singularity of l_{loc} and ε' at the center of the band is obtained: $l_{\text{loc}}(\varepsilon) \propto \ln^2\varepsilon, \varepsilon'(\varepsilon) \propto |\varepsilon|^{-1}$, $\varepsilon \to 0$. It is proved that in the case of sufficiently strong scattering the characteristic maxima of $\varepsilon'(\varepsilon)$ and of $l_{\text{loc}}(\varepsilon)$ occur at all rational points of the band. It is shown that the singularity of $l_{\text{loc}}(\varepsilon)$ near the center of the band jointly with the Dyson singularity of the density of states leads to a power-law decrease of the Mott hopping conductivity at low temperatures.

1. INTRODUCTION

In view of the current extensive investigations of quasi-one-dimensional organic conductors (see the reviews[1,2]), interest has noticeably increased in the theory of Mott localization of electrons in one-dimensional ($1D$) disordered systems (see the reviews[3–6]). A characteristic property of many quasi-$1D$ organic conductors, such as TCNQ salts with asymmetric cations, is a strong structural disorder.[1,3] This disorder is due to the random orientations of the asymmetric cations, which produce a strong random potential $\overline{V} \sim 0.1$ eV,[7,8] but do not disturb the spatial structure of the crystal, since they are located at the sites of the initial lattice.[1] It is known that the placement of the impurities in the lattice sites calls for taking into account the commensurability of the electron wavelength λ with the crystal period a_0.[3,9] This gives rise to a number of new effects in the system, particularly to delocalized electron states near the center of the band[3,9] as well as to the Dyson singularity of the density of states.[9] The cited papers, however, consider only weak disorder, and their results can therefore not be applied directly to an analysis of experimental data.

The present paper deals with the role of the commensurability of λ and a_0 in $1D$ crystals with strong disorder. We show that the delocalization of the electron states, which leads to the onset of significant singularities of the localization length l_{loc} and of the static dielectric constant ε', is preserved in such systems. It turns out, in particular, that in the absence of a phase shift and for forward scattering by impurities, we have $\varepsilon'(\varepsilon) \propto |\varepsilon|^{-1}$ and $l_{\text{loc}}(\varepsilon) \propto \ln^2\varepsilon$, where the energy ε is reckoned from the center of the band. This situation occurs in a large number of one-dimensional systems, e.g., in the case of purely nondiagonal disorder.[3,10] These include also the well-conducting TCNQ salts with asymmetric cations, as shown by Gor'kov and Dorokhov.[11] It is interesting to note that such systems are also always subject to the Dyson instability of the density of states: $\rho(\varepsilon) \propto |\varepsilon \ln^3\varepsilon|^{-1}$ (Refs. 9–11). It is curious that in the case of scattering by impurities this singularity is preserved even if the electron spectrum has a Peierls gap.[11–13]

The singularities of the localization length $l_{\text{loc}}(\varepsilon)$, of the dielectric constant $\varepsilon'(\varepsilon)$, and of the density of states $\rho(\varepsilon)$ lead to a substantial change of the character of the hopping conduction in the system; in particular, they transform Mott's exponential laws into power laws. To calculate l_{loc} and ε' we use a generalized variant, which I developed earlier,[3,10,15] of the Berezinskiĭ diagram technique. Note that this method is now used in many $1D$ problems, particularly for the calculation of the density of states, as well as to calculate the hopping mobility of classical particles.[17] Its use in the present paper allows us to take into account simultaneously the effects of commensurability and the effects of strong scattering by impurities. A similar approach, which I developed in a preceding paper[10] for the calculation of the density of states $\rho(\varepsilon)$, has made it possible to demonstrate the existence of a Dyson singularity even in the case of very strong scattering by impurities.

We note that by assuming that the interaction with the impurities is strong enough we imply that their density is low, $c \ll \lambda^{-1}$, so that $p_F l \gg 1$.[3,10] We assume also that the average distance c^{-1} between impurities is small compared with their characteristic dimension b. The condition $p_F l \gg 1$ makes it necessary to discard all diagrams containing rapidly oscillating factors such as $\exp(ip_F x)$, $x = na_0$ (Refs. 3, 10). We must retain here diagrams that contain large contributions of the type

$$\sum_n \exp(2is_0 p_F n a_0) \gg 1$$

if the electron momentum p_F turns out to be close to one of the rational values[10]

$$p_F = \pi k_0/s_0 a_0, \quad k_0 = \pm 1; \ldots; \pm(s_0-1), \quad s_0 > 1.$$

2. DERIVATION OF THE BASIC EQUATIONS

To calculate l_{loc} and ε' it is necessary to find the asymptotic low-frequency correlators of the density ($a = 0$) and of the current ($a = 1$). In diagram language these correlators $X^a(\varepsilon,\omega,k)$ take the form of a polarization loop with density and current operators $j^a(x), j^a(x')$ in the input vertices x and x'.[3,14,15] To calculate these correlators in the coordinate-energy representation we use the Berezinskiĭ diagram technique[14] generalized in my earlier papers[3,10,15] to include the case of strong interaction with the impurities.

According to this method, allowance for the strong interaction with the impurities leads to connecting individual crosses corresponding to the Born scattering amplitude α into clusters corresponding to scattering by an individual

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impurity. The diagrams must then summed in two stages. The first is summation over all crosses that enter in a single act of scattering by an impurity, so that the Born amplitude α is replaced by the total forward- and backward-scattering amplitudes f_+ and f_-, respectively. It is next necessary to sum over these clusters; this summation corresponds to allowance for multiple scattering by an individual impurity. The integration over the positions of the individual clusters is carried out over a scale on the order of the mean free path $l\sim c^{-1}$, and the integration within clusters over a scale $x\sim b\ll l$.

Since we are interested in the singularities of l_{loc} and near the center of the band ($p(\varepsilon)\approx p_0\approx\pi/2a_0$), we should take into account impurity vertices that contain factors of the type $e^{\pm 4ipx}$, $x=na_0$. We note that such factors are encountered, in particular, in impurity vertices that contain only single lines, i.e., retarded Green's functions

$$G_0^+(\varepsilon,\ x,\ x')=-i\exp(ip(\varepsilon)|x-x'|)/v(\varepsilon),$$

or only double lines, i.e., advanced Green's functions

$$G_0^-(\varepsilon,\ x,\ x')=i\exp(-ip(\varepsilon)|x-x'|)/v(\varepsilon).$$

Therefore changes in the numbers of pairs of single and double lines in section of each diagram can take place independently and these numbers, m_1 and m_2, are now unequal.

Subdividing now the polarization loop for the correlators $X^a(\varepsilon,\omega,k)$, in accord with the Berenzinskiĭ method, into right-hand, left-hand, and central parts and considering their changes as the point x is displaced, we obtain the following equation for the right-hand parts $R_{m_1m_2}(x)$:

$$-\frac{d}{dx}R_{m_1m_2}=c\sum_{s_1,s_2}v_{m_1s_1}v^*_{m_2s_2}R_{m_1+s_1,m_2+s_2}\times\exp\{2ix[(p_0-p_1)s_1-(p_0-p_2)s_2]\}$$
$$-cR_{m_1m_2}+cR_{00}(f_-)^{m_1}(f_-^*)^{m_2}\times\exp\{2ix[(p_1-p_0)m_1-(p_2-p_0)m_2]\},\qquad(1)$$

where $p_{1,2}=p(\varepsilon\pm\omega/2)$,

$$v_{ms}=\sum_k C_m^k C_{m+s-1}^{k+s}(f_-)^{2k+s}(1+f_+)^{2m-2k},\qquad(2)$$

and the summation over s_1 and s_2 includes only terms with even values of the difference s_1-s_2. Here m_1 and m_2 denote respectively the number of pairs of single and double lines in the section $x+0$, while s_1 and s_2 are their changes due to insertion of clusters of impurity lines. The binomial coefficients correspond to the number of methods of connecting the cluster to the diagram. The second term in (1) corresponds to exclusion, from the sum over s_1 and s_2, of terms with $s_i=k_i=0$, and the third to allowance for terms with $s_i=-m_i$ ($i=1;2$). Equation (1) must be solved with the boundary condition $R_{00}=1$.

It is similarly possible to obtain also equations for the central parts $Z^{m_1'm_2'}_{m_1m_2}(x',x)$:

$$\frac{d}{dx}Z^{m_1'm_2'}_{m_1m_2}=c\sum_{s_1,s_2}w_{m_1s_1}w_{m_2s_2}Z^{m_1'm_2'}_{m_1+s_1,m_2+s_2}\exp\{-2ix[(p_0-p_1)s_1-(p_0-p_2)s_2]\}-cZ^{m_1'm_2'}_{m_1m_2}+i(p_1-p_2)Z^{m_1'm_2'}_{m_1m_2},\qquad(3)$$

where

$$w_{ms}=\sum_k C_m^k C_{m+s}^{k+s}(f_-)^{2k+s}(1+f_+)^{2m-2k+1}.\qquad(4)$$

The substitution

$$R_{m_1m_2}(x)=(-1)^{(m_1-m_2)/2}R_{m_1m_2}\times\exp\{-2ix[m_1(p_0-p_1)-m_2(p_0-p_2)]\}\qquad(5)$$

leads to the following equation for the quantities $R_{m_1m_2}$:

$$2i[m_1(p_0-p_1)-m_2(p_0-p_2)]R_{m_1m_2}=c\sum_{s_1,s_2}v_{m_1s_1}v_{m_2s_2}R_{m_1+s_1,m_2+s_2}-cR_{m_1m_2}+cR_{00}(f_-)^{m_1}(f_-^*)^{m_2},\quad R_{00}=1,\qquad(6)$$

where the v_{ms} are defined in Eq. (2).

The correlation functions $\tilde{X}^a(\varepsilon,\omega,k)$ are expressed in this case in terms of the quantities $P^a_{m_1m_2}$ and $Q^a_{m_1m_2}$ that are defined by the expressions[3,9,15]

$$P^0_{m_1m_2}=\tfrac{1}{2}(R_{m_1m_2}+R_{m_1+1,m_2+1}),\quad P^1_{m_1m_2}=R_{m_1m_2}-R_{m_1+1,m_2+1},$$
$$Q^a_{m_1m_2}=(-1)^{(m_1-m_2)/2}\sum_{m_1',m_2'=0}^{\infty}\frac{1}{l}\int_{x'}^{\infty}dx\times e^{ik(x'-x)}Z^{m_1'm_2'}_{m_1m_2}(x',x)P^a_{m_1'm_2'}(-1)^{(m_1'-m_2')/2}\times\exp\{2i[(p_1-p_0)(m_1x-m_1'x')+(p_0-p_2)(m_2x-m_2'x')]\}\qquad(7,8)$$

according to the formula[3,9,15]

$$\tilde{X}^a(\varepsilon,\omega,k)=\frac{2l}{v}\left[\frac{v}{2}\right]^{2a}\sum_{m_1,m_2=0}^{\infty}P^a_{m_1m_2}(\omega)[Q^a_{m_1m_2}(\omega,k)+Q^a_{m_1m_2}(\omega,-k)],\qquad(9)$$

where l is the mean free path relative to the backscattering. The quantity $l=(c\gamma)^{-1}$ is determined by the coefficient $\gamma=|f_-|^2$ of reflection from individual impurities.

Equations for $Q^a_{m_1m_2}$ can be easily obtained from (3) and are of the form

$$i[(2m_1+1)(p_0-p_1)-(2m_2+1)(p_0-p_2)]Q^a_{m_1m_2}=cP^a_{m_1m_2}-ikQ^a_{m_1m_2}-cQ^a_{m_1m_2}+c\sum_{s_1,s_2}w_{m_1s_1}w^*_{m_2s_2}Q^a_{m_1+s_1,m_2+s_2},\qquad(10)$$

where the w_{ms} are defined in Eq. (4).

The derived expressions (6) and (10) allow us to investigate the characteristics of the electron states near the center of the band. As indicated in the earlier Refs. 3, 9, and 10, the most interesting situation arises when the forward-scattering amplitude f_+ is a real quantity and consequently the phase shift φ_0 for forward scattering is zero. The unitarity relation for the dimensionless quantities $f_\pm$ are of the usual form[3,10]:

$$-(f_++f_+^*)=|f_+|^2+|f_-|^2,\qquad(11)$$
$$-(f_-+f_-^*)=f_+f_-^*+f_-f_+^*.\qquad(12)$$

It follows therefore from (11) that

$$|1+f_+|^2=1-\gamma, \tag{13}$$

and from (12) we get the equality

$$f_-(1+f_+^*)=-f_-^*(1+f_+). \tag{14}$$

The value of φ_0 is determined in this case from the relation

$$1+f_+=(1-\gamma)^{1/2}e^{i\varphi_0}, \tag{15}$$

and real values of f_+ correspond to the condition $\varphi_0=0$.

The expressions for v_{ms} and w_{ms} take in this notation the form

$$v_{ms}=\sum_k C_m^k C_{m+s-1}^{k+s}(-1)^s(-\gamma)^{k+s/2}(1-\gamma)^{m-k}e^{i\varphi_0(2m+s)} \tag{16}$$

$$w_{ms}=\sum_k C_m^k C_{m+s}^{k+s}(-1)^s(-\gamma)^{k+s/2}(1-\gamma)^{m-k+1/2}e^{i\varphi_0(2m+s+1)}. \tag{17}$$

The reflection coefficient γ in (16) and (17) varies in the range $0\leqslant\gamma\leqslant 1$ and determines the character of the interaction of the electrons with the impurities. Very strong scattering corresponds to $\gamma\to 1$, and the Born approximation to $\gamma\ll 1$.

We note in conclusion that at $m_1=0$ or $m_2=0$ Eq. (6) describes averaging of an individual Green's function $G^+(\varepsilon,x,x)$ or $G^-(\varepsilon,x,x)$, and yields known[10] results for the density of states $\rho(\varepsilon)$. In particular, at $\varphi_0=0$ the Dyson singularity of $\rho(\varepsilon)$ appears near the center of the band at all values of γ.[10]

We note that the correlation functions $\tilde{X}^a$ (9) correspond to averaging of the product G^+G^- (Refs. 3, 9, 15). The contribution of products of the type G^+G^+ to the static characteristics vanishes by virtue of its even dependence on the frequency ω (Refs. 9 and 15).

3. LOCALIZATION OF ELECTRON STATES

We shall be interested hereafter in the static characteristics l_{loc} and ε' of the electron states. We should therefore investigate the low-frequency asymptotic forms of the correlation functions $\tilde{X}^a(\varepsilon,\omega,k)$ as $\omega\to 0$. This calls for solving Eqs. (6) and (10) at $\omega\ll\tau^{-1}$. We know[3,9,10,15] that in this limit the significant terms in the sums (9) over m_1 and m_2 are the large $m_1, m_2\sim(\omega\tau)^{-1}\gg 1$. Thus, expanding Eqs. (6) and (10) in terms the small m_1^{-1}, m_2^{-1}, we can transform from the discrete variables m_1 and m_2 to the continuous variable $q=-i\omega\tau(m_1+m_2)=-2i\omega\tau M\sim 1$ and the continuous one $m=1/2(m_1-m_2)\sim 1$. Similarly, summation over m_1 and m_2 in (9) can be replaced by integration with respect to q and summation over m.

To carry out the expansions with respect to $m_1^{-1}, m_2^{-1}\ll 1$ we shall find it convenient to introduce in the sums (6) and (10) over s_1 and s_2 the variables $S=1/2(s_1+s_2)$ and $s=1/2(s_1-s_2)$. We can now substitute the quantities $R_{M+S,m+s}$ in the form of series in powers of S:

$$R_{M+S,m+s}=\sum_{v=0}^{\infty}\frac{1}{v!}S^v\left(\frac{d}{dM}\right)^v R_{m+s}. \tag{18}$$

Using the known integral representation for the binomial coefficients

$$C_{m_j+s_j}^{k_j+s_j}=\frac{1}{2\pi i}\oint\frac{dz_j}{z_j^{k_j+s_j+1}(1-z_j)^{m_j-k_j}}, \quad j=1;2, \tag{19}$$

where the integration is over a circle of radius $\rho<1$ centered at zero,[3,10,15] we obtain for the quantities $v_{m_js_j}$ the following expression:

$$v_{m_j\,s_j}=\gamma^{1/2s_j}\exp[i\varphi_0(2m_j+s_j)]\frac{i^{s_j}}{2\pi i}\oint\frac{dz_j}{z_j^{m_j+s_j+1}}\left(\frac{z_j-\gamma}{1-z_j}\right)^{m_j}. \tag{20}$$

Representing the factor S^v in (18) in the form

$$S^v=\left(a\frac{d}{da}\right)^v\Big|_{a=1}a^S \tag{21}$$

and using the representation (20) for the quantities $v_{m_js_j}$, we obtain. After summing over S and integrating with respect to z_2, an equation for $R_m(M)$ at large $M\gg 1$:

$$(q-imt_0)R_m=\frac{1}{\gamma}\sum_{v,s}\frac{1}{v!}V_v(M,s,m)\left(\frac{d}{dM}\right)^v R_m-\frac{1}{\gamma}R_m, \tag{22}$$

where

$$V_v(M,s,m)=\left(a\frac{d}{da}\right)^v\Big|_{a=1}\frac{(-1)^s}{2\pi i}\oint\frac{dz}{z}\left(\frac{\gamma^{1/2}}{z}\right)^{2(m+s)}\times\left[\frac{z-\gamma}{\gamma^{1/2}(1-z)}\right]^{2m}\left(\frac{z-\gamma}{1-z}\frac{z-a}{z-\gamma a}\frac{1}{a}\right)^M e^{2i\varphi_0(2m+s)}. \tag{23}$$

Here $t_0=4l(p-p_0)$, and the integration with respect to z in (13) is along a circle of radius $\gamma<\rho<1$ around zero. At large $M\gg 1$ the quantities $V_v(M,s,m)$ assume in principal order in M^{-1} the form

$$V_v(M,s,m)\approx\frac{M^v(-1)^s}{2\pi i}\oint\frac{dz}{z}\left(\frac{\gamma^{1/2}}{z}\right)^{2(m+s)}\left[\frac{z-\gamma}{\gamma^{1/2}(1-z)}\right]^{2m}\times\left(\frac{z}{1-z}+\frac{\gamma}{z-\gamma}\right)^v e^{2i\varphi_0(2m+s)}. \tag{24}$$

In terms of the continuous variable $q=-2i\omega\tau M=-iv_1M$, the equation for $R_m(q)$ take therefore the form

$$(q-imt_0)R_m=\sum_{v,s}\frac{1}{v!}\varphi_v(s,m,q)q^v\left(\frac{d}{dq}\right)^v R_{m+s}-\frac{1}{\gamma}R_m, \tag{25}$$

where

$$\varphi_v(s,m,q)=\frac{(-1)^s}{2\pi i\gamma}\oint\frac{dz}{z}\left(\frac{\gamma^{1/2}}{z}\right)^{2(m+s)}\left[\frac{z-\gamma}{\gamma^{1/2}(1-z)}\right]^{2m}\times\left(\frac{z}{1-z}+\frac{\gamma}{z-\gamma}\right)^v e^{2i\varphi_0(2m+s)}. \tag{26}$$

We can similarly obtain equations for $Q_m^a(q,\varkappa)$, viz.,

$$(q-imt_0)Q_m^a=P_m^a-i\varkappa Q_m^a-\frac{1}{\gamma}Q_m^a+\sum_{v,s}\frac{1}{v!}\psi_v(s,m,q)q^v\left(\frac{d}{dq}\right)^v Q_{m+s}^a, \tag{27}$$

where $\varkappa=kl$,

$$\psi_v(s,m,q)=\frac{1-\gamma}{2\pi i\gamma}(-1)^s\oint\frac{dz}{(1-z)(z-\gamma)}\left(\frac{\gamma^{1/2}}{z}\right)^{2(m+s)}$$

$$\times\left[\frac{z-\gamma}{\gamma^{1/2}(1-z)}\right]^{2m}\left(\frac{z}{1-z}+\frac{\gamma}{z-\gamma}\right)^{v}e^{2i\varphi_0(2m+s)}. \quad (28)$$

The integrals with respect to z in (26) and (28) are along a circle of radius $\gamma<\rho<1$ around zero. The most convenient integration contour is a circle of radius $\rho=\gamma^{1/2}$.

The expression for the correlation functions $\tilde{x}^a$ in terms of R_m and Q^a_m takes as $\omega\to 0$ the form

$$\tilde{X}^a(\varepsilon,\omega,k)\approx\frac{2l}{-iv_1v}\left[\frac{v}{2}\right]^{2a}$$

$$\times\int_0^\infty dq\sum_m P_m{}^a(q)\,[Q_m{}^a(q,\varkappa)+Q_m{}^a(q,-\varkappa)], \quad (29)$$

where

$$P_m{}^0(q)=R_m(q),\quad P_m{}^1(q)=iv_1(dR_m/dq). \quad (30)$$

Equations (25) and (27) yield the low-frequency asymptotic forms of the density and current correlators. It follows from them in particular, when (29) and (30) are taken into account, that as $\omega\to 0$ we get

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

The density correlator $\tilde{x}^0$ has thus at long times $t\to\infty$ a stationary asymptotic form that determines the spatial distribution $p_\infty(x)$ of the electron density for localized states, while the conductivity $\sigma(\omega)$ defined in accord with the Kubo formula in terms of the quantity $\tilde{x}_1(\omega)$ vanishes at $\omega=0$.

The coefficient of the linear term in the low-frequency asymptotic form of the complex conductivity $\sigma(\omega)$ determines the static dielectric constant ε':

$$\varepsilon'=\lim_{\omega\to 0}4\pi\sigma(\omega)/(-i\omega), \quad (31)$$

while the spatial asymptotic value $p_\infty(x)$ determines the localization length:

$$l_{loc}^{-1}=\lim_{|x|\to\infty}|\ln p_\infty(x)/x|. \quad (32)$$

Equations (25) and (27) thus enable us to find the values of $l_{\rm loc}$ and ε' and to investigate their singularities near the center of the band as $\varepsilon\to 0$. The most interesting results occur in the case $\varphi_0=0$ (Ref. 10), which we shall in fact consider hereafter.

4. LOCALIZATION LENGTH

To calculate the localization length $l_{\rm loc}$ we must find the asymptotic density correlator $\tilde{x}_0(\varepsilon,t,x)$ for long times $t\to\infty$ and large distances $|x|\to\infty$. As shown in the preceding section, the limit

$$\lim_{t\to\infty}\tilde{X}^0(\varepsilon,t,x)=p_\infty(x)$$

determines the spatial distribution of the electron density. The asymptotic form of $p_\infty(x)$ as $|x|\to\infty$ is determined in this case by the branch point of the quantities $Q^0_m(q,\varkappa)$ with respect to $\varkappa$ (Refs. 3, 9, 15). The position of the branch point can be easily obtained from the asymptotic values of $Q^0_m(q,\varkappa)$ at $q\ll 1$.[3,15]

Indeed, substituting in the homogeneous part of (27) the quantities $Q^0_m(q,\varkappa)$ at $q\ll 1$ in the form $Q^0_m(q,\varkappa)=a_m q^\lambda$, we obtain for the a_m the equation

$$(imt_0-i\varkappa-1/\gamma)a_m+\sum_s f_{ms}(\lambda)a_{m+s}=0, \quad (33)$$

where

$$f_{ms}(\lambda)=\frac{1-\gamma}{2\pi i\gamma}\oint\frac{dz(-1)^s}{(1-z)(z-\gamma)}\left(\frac{\gamma^{1/2}}{z}\right)^{2(m+s)}$$

$$\times\left[\frac{z-\gamma}{\gamma^{1/2}(1-z)}\right]^{2m}\left[\frac{z(1-\gamma)}{(1-z)(z-\gamma)}\right]^{\lambda}e^{2i\varphi_0(2m+s)}. \quad (34)$$

The most convenient contour of integration with respect to z in (34) is a circle of radius $\rho=\gamma^{1/2}$. Using the known integral representation of the hypergeometric function $F(\alpha,\beta,\delta,y)$,[18] we easily obtain the expression

$$f_{ms}(\lambda)=(-1)^s e^{2i\varphi_0(2m+s)}(1-\gamma)^{1+\lambda}\gamma^{2m-2-\lambda+s}$$

$$\times\frac{\Gamma(2m-\lambda)}{\Gamma(1-2s)\Gamma(2m+2s-\lambda)}F(\lambda+1-2(m+s),$$

$$\lambda+1-2m,\ 1-2s,\ 1/\gamma). \quad (35)$$

We shall be interested hereafter in the singularities of $l_{\rm loc}$ near the center of the band, and consider therefore the case of small $|t_0|\ll 1$.

We consider first the case of weak disorder $\gamma\ll 1$. Expanding Eqs. (33) in powers of the small γ and retaining only the principal terms, we obtain the following equations for the values of a_m:

$$0=a_m[\lambda(\lambda+1)-4m^2+imt_0-i\varkappa]+a_{m-1}[{}^1/_2\lambda(\lambda+1)$$
$$+\lambda(1-2m)+2m^2-3m+1]+a_{m+1}[{}^1/_2\lambda(\lambda+1)$$
$$+\lambda(1+2m)+2m^2+3m+1]. \quad (36)$$

It follows from the structure of (36) that small $|t_0|\ll 1$ correspond to large $m\sim|t_0|^{-1}\gg 1$. We can therefore transform from difference to differential equations. Introducing the continuous variable $p=-imt_0$, we obtain for the function $a(p)$ the equation

$$p^2\frac{d^2a}{dp^2}+(2\lambda+3)p\frac{da}{dp}+a\left[\frac{1}{2}p+(\lambda+1)^2-\frac{1}{2}i\varkappa\right]=0. \quad (37)$$

This equation reduces to the Bessel equation,[19] and its general solution that decreases at infinity is of the form

$$a(p)=Cp^{-(\lambda+1)}K_{2\nu}(\sqrt{2p}),\quad \nu=(i\varkappa/2)^{1/2}, \quad (38)$$

where K is a modified Bessel function and C an arbitrary constant. It follows from (38) that at $t_0=0$ the quantities Q^0_m have a branch point at $\varkappa_c=0$. Thus, at large distances $|x|\gg l$ the electron density $p_\infty(x)$ decreases as a power law and the localization length $l_{\rm loc}\to\infty$.[3,9]

This result can be obtained directly from Eq. (37). Indeed, as follows from (37), $a(p)$ is a power-law function at small $p\ll 1$. Therefore, rewriting $a(p)$ in (37) at $p\ll 1$ in the form Cp^η, we obtain for η the simple equation

$$\eta^2+2\eta(\lambda+1)+(\lambda+1)^2-{}^1/_2i\varkappa=0,\quad \eta=-(\lambda+1)\pm({}^1/_2i\varkappa)^{1/2}. \quad (39)$$

This method can be used in the case of strong scattering,

when $\gamma \sim 1$. Indeed, using the fact that small $|t_0|$ correspond to large $m \sim |t_0|^{-1}$, we can transform from the difference equations (33) to continuous ones. To this end we represent a_{m+s} from (33) in the series form

$$a_{m+s} = \sum_{u=0}^{\infty} \frac{s^u}{u!} \left(\frac{d}{dm}\right)^u a_m. \tag{40}$$

Substituting next s^u in the form

$$s^u = \left(a \frac{d}{da}\right)^u a^s|_{a=1} \tag{41}$$

and summing over s and integrating with respect to z in (33) and (34), we obtain an equation for the function $a(p)$ in the principal order in $m^{-1} \ll 1$:

$$\left(i\varkappa + p + \frac{1}{\gamma} - 1\right) a = \sum_{u=0}^{\infty} \frac{1}{u!} f(u) p^u \left(\frac{d}{dp}\right)^u a, \tag{42}$$

where

$$f(u) = \frac{1-\gamma}{2\gamma}\left[\left(\frac{2\gamma^{1/2}}{1-\gamma^{1/2}}\right)^u \left(\frac{1+\gamma^{1/2}}{1-\gamma^{1/2}}\right)^{\lambda+1} + \left(\frac{-2\gamma^{1/2}}{1+\gamma^{1/2}}\right)^u \left(\frac{1-\gamma^{1/2}}{1+\gamma^{1/2}}\right)^{\lambda+1}\right]. \tag{43}$$

It follows from (42) that as $p \to 0$ the function $a(p)$ has a power-law asymptotic form Cp^{η}. Substituting $a(p)$ in such a form in (42), we obtain an equation for the exponent η:

$$i\varkappa + \frac{1}{\gamma} - 1 = \frac{1-\gamma}{2\gamma}\left[\left(\frac{1+\gamma^{1/2}}{1-\gamma^{1/2}}\right)^{1+\lambda+\eta} + \left(\frac{1-\gamma^{1/2}}{1+\gamma^{1/2}}\right)^{1+\lambda+\eta}\right]. \tag{44}$$

Introducing new variables

$$\tilde{z} = \left(\frac{1+\gamma^{1/2}}{1-\gamma^{1/2}}\right)^{1+\lambda+\eta}, \quad \tilde{\varkappa} = \frac{\varkappa}{1-\gamma} \tag{45}$$

and solving the equation for z, we get

$$\tilde{z} = 1 + i\gamma\tilde{\varkappa} \pm [i\gamma\tilde{\varkappa}(2+i\gamma\tilde{\varkappa})]^{1/2}. \tag{46}$$

It follows therefore that at an arbitrary $\gamma < 1$ the position of the branch point $t_0 = 0$ is determined by the condition $\varkappa = \varkappa_c = 0$, so that the localization length l_{loc} becomes infinite near the center of the band in the absence of a phase shift for forward scattering by the impurities. This singularity vanishes only in the case $\gamma = 1$, which corresponds to infinitely strong scattering by the impurities.

5. CHARACTER OF THE SINGULARITY

To determine the character of the singularity of l_{loc} as $\varepsilon \to 0$, we must analyze Eqs. (33) in greater detail. We consider first the case of weak disorder, $\gamma \ll 1$, which is described by Eq. (36).

Introducing the continuous function

$$a(\varphi) = \sum_m e^{im\varphi} a_m, \tag{47}$$

we obtain the following differential equation

$$0 = 4\frac{d^2a}{d\varphi^2}(1-\cos\varphi) + \frac{da}{d\varphi}[t_0 + (1-2\lambda)2\sin\varphi] + a[\lambda(\lambda+1) - i\varkappa + \lambda(\lambda-1)\cos\varphi]. \tag{48}$$

We are interested in the asymptotic form of the dependence of l_{loc} on t_0 as $t_0 \to 0$, and consider therefore the case $|t_0| \ll 1$. In this limit we can solve (48) by perturbation theory in the small t_0. It must be noted, however, that the term $t_0 da/d\varphi$ in (48) turns out to be small only at $\varphi \sim 1$, but in the region of small $\varphi \sim t_0$ it is predominant. At small $\varphi \sim t_0$ we must therefore solve Eq. (48) with this term taken into account, and obtain the effective boundary condition for $a(\varphi)$ as $\varphi \to 0$.

We construct first the zeroth approximation for $a(\varphi)$ as $t_0 \to 0$. To this end we must solve Eq. (48) at $t_0 = 0$. Simple transformations[19] yield for it two linearly independent solutions:

$$a_{\pm}(\varphi) = C_{\pm}\left(1+\cos\frac{\varphi}{2}\right)^{(\lambda\pm\nu)/2}\left(1-\cos\frac{\varphi}{2}\right)^{(\lambda\mp\nu)/2}, \quad \nu = \left(\frac{1}{2} - i\varkappa\right)^{1/2}, \tag{49}$$

where $C_{\pm}$ are unknown constants of the order of unity. It follows hence that $\varkappa_c(t_0)$ vanishes at $t_0 = 0$. To determine the manner in which $\varkappa_c(t_0) \to 0$ as $t_0 \to 0$, we must solve Eq. (48) for small $\varphi \sim t_0$.

Expanding (38) in powers of $\varphi \ll 1$ and making the substitution

$$a(\varphi) = a_1(2t_0/\varphi)\,(\varphi/2t_0)^{\lambda\pm\nu},$$

we obtain for $a_1(2t_0/\varphi)$ a confluent hypergeometric function.[18,19] Choosing for this equation a solution that is bounded as $\varphi \to 0$, we obtain for $a(\varphi)$ at $\varphi \sim t_0$

$$a(\varphi) = C(\varphi/2t_0)^{\lambda\pm\nu}\Psi(\pm\nu-\lambda,\ 1\pm 2\nu,\ 2t_0/\varphi), \tag{50}$$

where Ψ is a confluent hypergeometric function[18,20] and C is an arbitrary constant of the order of unity.

Expanding the solution (49) in powers of the small $\varphi \ll 1$ and using the known asymptotic form of Ψ at $t_0/\varphi \ll 1$ (Ref. 20), we obtain, by matching these solutions in the region $t_0 \ll \varphi \ll 1$ the following expression for the ratio of the constants C_+ and C_- in (49) at $t_0 \ll 1$:

$$C_+/C_- \approx -(2t_0)^{2\nu}. \tag{51}$$

It follows hence that for a finite limit $\lim_{t_0 \to 0}(C_+/C_-)$ to exist it is necessary that the characteristic value $\nu_c(t_0)$ vanish as $t \to 0$ like

$$\nu_c(t_0) \propto (\ln|t_0|)^{-1}.$$

This means that the value of $\varkappa_c$, which determines the position of the branch point, vanishes as $t_0 \to 0$ like $(\ln|t_0|)^{-2}$, while the localization length l_{loc} is found to be proportional to $\ln^2|t_0|$:

$$l_{\text{loc}}(t_0) \approx \beta l \ln^2|t_0|, \quad |t_0| \ll 1. \tag{52}$$

A more detailed analysis of this asymptotic form by numerical methods shows that the coefficient β in (52) is close to 0.5.

It can be seen from (52) that the localization length has at $\varphi_0 = 0$ a logarithmic singularity at the center of the band. The dependence $l_{\text{loc}}(\varepsilon) \propto \ln^2\varepsilon$ obtained by us is substantially stronger than the result $l_{\text{loc}}(\varepsilon) \propto \ln\varepsilon$ of Eggarter and Riedinger,[21] which they obtained for one-dimensional systems with purely nondiagonal disorder by averaging localized wave functions. The reason for this difference is that direct

averaging of the wave functions affects the corresponding oscillating factors and leads to a faster decrease at long distances and to underestimates of l_{loc}.[3]

The asymptotic expression (52) indicated above can be obtained also by a simpler method from the continuous equation (37) with allowance for the correction terms of first order in the small t_0. Indeed, expanding the difference equation (36) to the next term in powers of m^{-1}, we obtain the correction

$$(\lambda+1)\left(\frac{1}{2}\lambda+1\right)\frac{d^2a}{dm^2}=-(\lambda+1)\left(\frac{1}{2}\lambda+1\right)t_0^2\frac{d^2a}{dp^2}. \qquad (53)$$

This correction, however, plays a dominant role at small $p\sim t_0\ll 1$, where it determines completely the structure of the solution $a(p)$. It can be easily seen that the power-law asymptotic relation (38) is replaced by an exponential one: $\ln a(p)\propto p/t_0$. These solutions should be matched in a region where both are of the same order of magnitude, i.e., at $p\sim t_0\ln t_0$. It follows therefore that in this region of p the correction terms (53) yield a shift $\delta\varkappa_c(t_0)\sim(\ln t_0)^{-2}$, in agreement with (52). This reasoning can be used also in the case $\gamma\sim 1$. Indeed, simple calculations show that the structure of the correction terms in powers of m^{-1} is similar in form and starts with terms $\sim m^{-2}$. The reason is that the difference operators (33) and (36) are even with respect to replacement of m by $-m$. Since the location of the matching region depends little on γ, the correction to the zero value $\varkappa_c=0$ will be of the order of $(\ln t_0)^{-2}$ and the localization length will have the singularity

$$l_{\text{loc}}(t_0)\infty\ln^2|t_0|$$

as $t_0\to 0$ and at arbitrary values of $\gamma<1$. The proportionality coefficient β turns out to depend substantially on the value of γ. This conclusion is incorrect only at $\gamma=1$. It follows from (34) that as $\gamma\to 1$ all the f_{ms} vanish, so that only the diagonal terms remain in (33), and the minimum eigenvalue is $\varkappa_c=1$. This result is valid only at $\gamma=1$. At $\gamma<1$ and small $t_0\lesssim(1-\gamma)^{1/2}$ large $m\sim t_0^{-1}$ become significant and this factor compensates for the small quantity of the type $1-\gamma$ in the matrix elements f_{ms}. Therefore the logarithmic singularity of the localization length is always preserved in a narrow vicinity of $|t_0|\lesssim(1-\gamma)^{1/2}$ near zero.

The situation considered by us pertained to the case $\varphi_0=0$. At nonzero values of φ_0 the singularity of l at the band center vanishes and is transformed into a characteristic maximum of finite height that tends to infinity as $\varphi_0\to 0$. We note that at finite values $\gamma\sim 1$ similar peaks of $l_{\text{loc}}(\varepsilon)$ appear also at all other rational points of the band near the values

$$p_F=p_0=\pi k_0/s_0a_0, \qquad k_0=\pm 1;\ldots;\pm(s_0-1), \qquad s_0>1,$$

in analogy with their appearance in the density $\rho(\varepsilon)$ of the electron states.[10] For numerical reasons, however, their height is relatively small and reaches only several percent of the initial value of l_{loc}. The corresponding equations are easily obtained from (25), (27), and (33) by replacing $2m$ and $2s$ in (26), (28), and (34) by s_0m and s_0s, and can be solved by numerical methods.

In the limit of very strong scattering, as $\gamma\to 1$, all the singularities vanish, for in this limit the electron becomes locked-in between two neighboring impurities and the length l_{loc} is determined only by the average distance between them. In the weak-scattering limit, only the singularities near the center of the band are preserved.

6. DIELECTRIC CONSTANT

To investigate the singularities of the static dielectric constant ε' near the center of the band it is necessary to analyze the structure of the continuous equations (25) and (27) in the region of small $|t_0|\ll 1$. As shown in Sec. 4, in this limit large values $m\sim t_0^{-1}$ become significant in Eqs. (25) and (27). We can therefore transform from the difference equations (25) and (27) to differential ones, and from summation over m in (29) to integration. Going to the corresponding limit in accord with Sec. 4, we obtain in terms of the continuous variables q and p the following equations for the functions $R(q,p)$ and $Q^a(q,p)$ at $|t_0|\ll 1$:

$$\left(q+p+\frac{1}{\gamma}\right)R=\frac{1}{2\gamma}\sum_{u,v=0}^{\infty}\frac{1}{u!v!}\left[\left(\frac{2\gamma^{1/2}}{1-\gamma^{1/2}}\right)^{u+v}+\left(\frac{-2\gamma^{1/2}}{1+\gamma^{1/2}}\right)^{u+v}\right]p^u\left(\frac{\partial}{\partial p}\right)^u q^v\left(\frac{\partial}{\partial q}\right)^v R, \qquad (54)$$

$$\left(q+p+i\varkappa+\frac{1}{\gamma}-1\right)Q^a$$

$$=P^a+\frac{1-\gamma}{2\gamma}\sum_{u,v=0}\frac{1}{u!v!}\left[\frac{1+\gamma^{1/2}}{1-\gamma^{1/2}}\left(\frac{2\gamma^{1/2}}{1-\gamma^{1/2}}\right)^{u+v}+\frac{1-\gamma^{1/2}}{1+\gamma^{1/2}}\left(\frac{-2\gamma^{1/2}}{1+\gamma^{1/2}}\right)^{u+v}\right]p^u\left(\frac{\partial}{\partial p}\right)^u q^v\left(\frac{\partial}{\partial q}\right)^v Q^a, \qquad (55)$$

where

$$P^a=\left(-iv_1\frac{\partial}{\partial q}\right)^a R. \qquad (56)$$

The general expression (29) for the correlation functions $\tilde{X}^a(\varepsilon,\omega,k)$ takes in this limit the form

$$\tilde{X}^a(\varepsilon,\omega,k)\approx\frac{2\tau}{-v_1t_0}\left[\frac{v}{2}\right]^{2a}\times\int_{-\infty}^{\infty}dp\int_0^{\infty}dq\,P^a(p,q)\,[Q^a(p,q,\varkappa)+Q^a(p,q,-\varkappa)]. \qquad (57)$$

From (57) follows the existence of an energy singularity near the band center:

$$\tilde{X}^a(\varepsilon,\omega,k)\infty|\varepsilon\tau|^{-1}, \qquad |\varepsilon\tau|\ll 1. \qquad (58)$$

Such a singularity in the current correlator corresponds to the static dielectric constant going to infinity:

$$\varepsilon'(\varepsilon)\infty|\varepsilon\tau|^{-1}, \qquad |\varepsilon\tau|\ll 1. \qquad (59)$$

The absolute-value signs in (58) and (59) are due to the general analytic structure of (57). This structure was investigated in the limit of weak scattering $\gamma\ll 1$ in Ref. 9.

In the small-γ limit there remain in Eqs. (54) and (55) in the lowest order only first- and second-derivative terms that coincide with the equations of Ref. 9. In these equations the

radial and angle variables $q+p$ and $(q-p)/(q+p)$ separate, and as a result the radial dependences are determined by the Bessel equation, and the necessary integrals with respect to the angle variables are obtained directly from the boundary conditions and from elementary identities of the form

$$(-i\nu_1)\sum_{m_1,m_2=0}^{\infty} Q^a_{m_1m_2}P^0_{m_1m_2}=\sum_{m_1,m_2=0}^{\infty} P^a_{m_1m_2}P^1_{m_1m_2}, \tag{60}$$

$$\sum_{m_1,m_2=0}^{\infty} Q^0_{m_1m_2}P^1_{m_1m_2}=\sum_{m_1,m_2=0}^{\infty} Q^1_{m_1m_2}P^0_{m_1m_2}. \tag{61}$$

In the case $\gamma\sim 1$ the identities (60) and (61) can be made valid by multiplying Eqs. (10) at $a=0$ and 1 by $P^1_{m_1m_2}$ or at $a=0$ by $Q^1_{m_1m_2}$ and summing over m_1 and m_2 with allowance for (6). In addition, by virtue of the obvious symmetry of Eqs. (54) and (55) they admit also of separation of the radial and angular variables $q+p$ and $(q-p)(q+p)$. The equation for the radial function $R_{\rm rad}(q+p)$ takes then the form

$$t_1R_{rad}=\frac{1}{2\gamma}\sum_{v=1}^{\infty}\frac{1}{v!}\left[\left(\frac{\gamma^{1/2}}{1-\gamma^{1/2}}\right)^v+\left(\frac{-\gamma^{1/2}}{1+\gamma^{1/2}}\right)^v\right]\times(2t_1)^v\left(\frac{d}{dt_1}\right)^v R_{rad},\quad t_1=q+p. \tag{62}$$

This equation coincides with the one that determines the character of the singularity of the density of states $\rho(\varepsilon)$ near the center of the band.[10] The solution (62) can be obtained in the form of a series in powers of t_1.[10] To investigate the character of the singularity of ε' we need only the asymptotic form of $R_{\rm rad}(t_1)$ as $t_1\to 0$, viz.,

$$R_{rad}(t_1)\approx A\ln t_1,\quad |t_1|\ll 1, \tag{63}$$

where A is a constant that does not depend on the radial variable t_1. With allowance for the angular dependences, the expressions for the quantities P^a take now the form[9]

$$P^0(q,p)=\varphi\left(\frac{q-p}{q+p}\right)R_{rad}(q+p), \tag{64}$$

$$P^1(q,p)=(-i\nu_1)\left[\varphi\left(\frac{q-p}{q+p}\right)R'_{rad}(q+p)-\left(1-\frac{q-p}{q+p}\right)\varphi'\left(\frac{q-p}{q+p}\right)R_{rad}(q+p)\right], \tag{65}$$

where $\varphi(y)$ is the angular part of the function $R(q,p)$. We note that the constant factor A in the asymptotic relation (63) can be included in the angular dependence. We therefore put hereafter $A=-1/2$ to conform with the notation of Ref. 9.

We shall be interested hereafter only in static characteristics, so that we can put $\nu_1\to 0$ and neglect this quantity together with t_0. The boundary conditions for the angular function $\varphi(y)$, whose structure is determined from the solution of Eqs. (6) and (10) at $m_1\sim 1$ and $m_2\sim 1$, is obtained from the solutions (6) and (10) with $m_1=0$ or $m_2=0$:

$$R_{m_10}=R_{m_1}(t_0),\quad R_{0m_2}=R_{m_2}(t_0), \tag{66}$$

where the functions $R_m(t_0)$ are obtained from the equation that determines the distribution of the density $\rho(\varepsilon)$ of the electron states,[9,10] and are connected with this equation by the relation

$$\rho(\varepsilon)=\rho_0\left[1+2\,\mathrm{Re}\sum_{m=1}^{\infty}R_m^2(t_0)\right]. \tag{67}$$

Going to the continuous limit $m_1,m_2\gg 1$ in (66) and using the known asymptotic form for $R_m(t_0)$ at $|t_0|\ll 1$ and $1\ll m\ll t_0^{-1}$ (Ref. 10),

$$R_m(t_0)\approx\ln p/\ln(-it_0),\quad |p|\ll 1, \tag{68}$$

we obtain in the principal logarithmic approximation

$$\varphi(1)\approx 2/\ln(-it_0),\quad \varphi(-1)\approx 2/\ln(it_0),\quad |t_0|\ll 1. \tag{69}$$

The integrals of the function $\varphi^2(y)$ with respect to the angle varaibles can be obtained from the identity (60) at $a=0$ and are of the form

$$\int_{-1}^{1} dy\,\varphi^2(y)=-2it_0\rho(t_0)/\rho_0. \tag{70}$$

A simple analysis of the integrals with respect to the angle variables[9] shows that in the principal logarithmic approximation in t_0 the main contribution to the current correlator $\tilde{X}^1(\varepsilon,\omega)$ is made by the first term of (65). We note further that it proves also the smallness of the contribution made to the correlator by the product $G^+(\varepsilon+\omega/2)G^+(\varepsilon-\omega/2)$, of the electron Green's function, which is an even function of ω and therefore contains an extra power of ω as $\omega\to 0$ (Ref. 9). We can therefore omit henceforth the tilde from the correlators $X^a(\varepsilon,\omega,k)$.

It can be easily seen that the radial dependences of $Q^1(q+p)$ at small $|q+p|\ll 1$, with allowance for the first term of (65), is of the form

$$Q^1_{rad}(t_1)\approx(-i\nu_1)(4t_1)^{-1}\ln^2 t_1,\quad |t_1|\ll 1. \tag{71}$$

The angular dependences of $Q^1(q+p)$ is described in this case by the same function $\varphi(y)$. Substituting the asymptotic relations (63) and (71) in the integral of (57), we find, cutting off the divergence at the lower limit in the region $t_1\sim(-it_0)$, the following expression for $\tilde{X}^1(\varepsilon,\omega)$ in the principal logarithmic approximation in $|t_0|\ll 1$:

$$X^1(\varepsilon,\omega)\approx vl(-2i\nu_1)\frac{\rho(\varepsilon)}{\rho_0}\left(-\frac{1}{24}\ln^3|t_0|\right). \tag{72}$$

It follows from this equation, in particular, that the contribution to the static dielectric constant ε' from electrons of energy ε is

$$\varepsilon'(\varepsilon)\approx\varepsilon_0\frac{\rho(\varepsilon)}{\rho_0}\left(-\frac{1}{24}\ln^3|\varepsilon\tau|\right),\quad |\varepsilon\tau|\ll 1, \tag{73}$$

where

$$\varepsilon_0=16e^2l^2/vS, \tag{74}$$

and S is the cross section area per conducting filament.

To obtain the total dielectric constant ε' it is necessary to integrate expression (73) for $\varepsilon'(\varepsilon)$ with respect to ε with an additional factor $(-\partial n/\partial\varepsilon)$, where $n(\varepsilon)$ is the Fermi distribution function. We note that in this case two most interesting situations are possible: the Fermi level is either within

the small distance $\varepsilon \ll \tau^{-1}$ from the center of the band or exactly at the center.

In the first case the dielectric constant ε' at $T=0$ is determined directly by Eq. (73), in which ε_0 is determined by the values of the velocity v and of the mean free path l on the Fermi level, while $\rho(\varepsilon)$ is given by the equation obtained in Ref. 10:

$$\rho(\varepsilon) \approx \rho_0 \frac{2\pi B(\gamma)}{|4\varepsilon\tau \ln^3(\varepsilon\tau)|}, \quad |\varepsilon\tau| \ll 1. \tag{75}$$

Here $B(\gamma)$ is a numerical coefficient of the order of unity and depends on γ. A plot obtained for $B(\gamma)$ by numerical methods is given in Ref. 10. $B(\gamma) \to 2$ at small $\gamma \ll 1$, while $B(\gamma) \to \infty$ like $B(\gamma) \approx 1/4\ln^2(1-\gamma)$ as $(1 \to \gamma)$. With allowance for (75), Eq. (73) for the static dielectric constant ε' takes the final form

$$\varepsilon' \approx \varepsilon_0 \pi B(\gamma)/48|\varepsilon\tau|, \quad |\varepsilon\tau| \ll 1. \tag{76}$$

In the limit $\gamma \ll 1$ Eq. (76) goes over into the corresponding result for weak scattering,[9] multiplied by the factor 1/8 that was omitted in the cited reference.

In the second case the static dielectric constant ε' becomes infinite as $T \to 0$. To determine the manner in which $\varepsilon' \to \infty$ it suffices to integrate (76) with respect to ε with a weight $(\partial n/\partial\varepsilon)$. The corresponding logarithmic divergences are cut off at $\varepsilon \sim T$ and at $\varepsilon \sim \tau_{in}^{-1}(T)$, where $\tau_{in}^{-1}(T)$ is the electron inelastic-scattering probability and determines the corresponding damping of the localized electron states and the probability of inelastic transitions between them.[3,22] Integrating (76) with respect to ε with weight $(-\partial n/\partial\varepsilon)$ we obtain ultimately at $T\tau \ll 1$ and $T\tau_{in} \gg 1$, $\tau_{in}^{-1} \ll \tau^{-1}$ the asymptotic relation

$$\varepsilon'(T) \approx \varepsilon_0 \frac{\pi B(\gamma)}{96 T\tau} \ln(T\tau_{in}), \quad T \to 0. \tag{77}$$

Since the phonon spectrum in quasi-1D organic conductors is usually three-dimensional,[1,2] the temperature dependence of $\tau_{in}^{-1}(T)$, determined by the scattering by acoustic phonons, takes the power-law form

$$\tau_{in}^{-1}(T) \propto T^3, \quad T \to 0. \tag{78}$$

Therefore as $T \to 0$ we have

$$\varepsilon'(T) \propto T^{-1} \ln T. \tag{79}$$

The dielectric constant of a one-dimensional disordered metal with half-filled band, in the absence of forward scattering, has thus at low temperatures the singularity (79). A similar singularity occurs in the frequency dependence of $\varepsilon'(\omega)$ as $\omega \to 0$. Indeed, as follows from the symmetry of Eqs. (54) and (55) to permutation of the variables p and q, in the limit $t_0 \ll \nu_1 \ll 1$ the cutoff of the logarithmic divergences (72) should occur not at $(p+q) \sim (-it_0)$ but at $(p+q) \sim (-i\nu_1)$ (Ref. 9), and corresponds to replacing ε by ω in Eq. (72). The detailed analysis carried out in the preceding paper[9] for the general Kubo-Greenwood formula for complex conductivity can be repeated also in the case considered here, since this analysis was based only on the general structure of expression (72), which retains the same form for strong scattering. The final result for the asymptotic form of $\varepsilon'(\omega)$ as $\omega \to 0$ is[9]

$$\varepsilon'(\omega) \propto |\omega\tau \ln^2(\omega\tau)|^{-1}. \tag{80}$$

We note that all the singularities (73), (79), (80) of the dielectric constant near the center of the band are due mainly to the Dyson singularity (75) of the electron density of states $\rho(\varepsilon)$. As shown in my preceding paper,[10] in the presence of sufficiently strong scattering, when $\gamma \sim 1$, large peaks of $\rho(\varepsilon)$ occur at all rational points of the electron band, i.e., near the values

$$p_F = p_0 = \pi k_0/s_0 a_0, \quad k_0 = \pm 1; \ldots; \pm(s_0-1); \quad s_0 > 1.$$

As $\gamma \to 1$ these peaks are transformed into δ functions, and at all irrational points of the band the density of states vanishes, for in this limit of infinitely strong scattering the electron becomes locked-in between two nearest impurities and only states with rational values of the wavelength $\lambda/2 = a_0 s_0/k_0$ are preserved in the system.[10] Since the dielectric constant is determined to a considerable degree by the density of the electron states, similar peaks should be observed also in the $\varepsilon'(\varepsilon)$ dependence.

To obtain the equations that describe the localization of the electron states near an arbitrary rational point of the band it suffices, as already shown earlier,[10] to replace $2m$ and $2s$ in (25) and (27) by $s_0 m$ and $s_0 s$. The equations obtained in this manner can be solved by numerical methods. Plots of $\varepsilon'(\varepsilon)$ at $\varphi_0 = 0$ and $\gamma = 0.5$, 0.7, and 0.9 for a quarter-filled electron band (this corresponds to $s_0 = 4$) are shown in Fig. 1. We note that the peaks of ε' are quite large even at values not too close to unity. It is curious that near the maximum there appear relatively deep minima that cause ε' to seem smaller than ε_0 if $p_F \neq p_0$ but is in a close vicinity of this point. As $\gamma \to 1$ these minima sink deeper to zero in accord with a law that can be easily obtained directly by solving the initial equations (6) and (10) at $\gamma = 1$. Indeed, retaining in these equations only terms of lowest order in the small parameter $(1-\gamma) \ll 1$, we easily obtain the following expression for the quantities $R_{m_1 m_2}$ and $Q^a_{m_1 m_2}$:

$$R_{m_1 m_2} = [1 + 2il(m_2(p_2 - p_0) - m_1(p_1 - p_0))]^{-1}, \tag{81}$$

$$Q^a_{m_1 m_2} = P^a_{m_1 m_2}[1 + i\chi + il((2m_2+1)(p_2-p_0) - (2m_1+1)(p_1-p_0))]^{-1}. \tag{82}$$

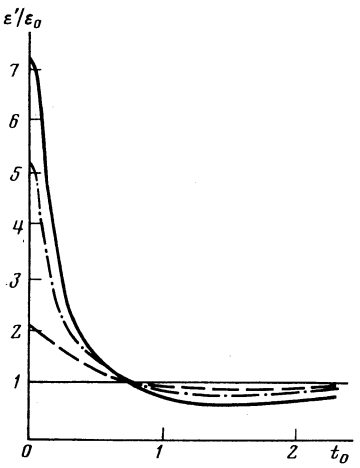

FIG. 1. Dependence of the static dielectric constant ε' on the dimensionless electron energy t_0 near 1/4 of the band at $\varphi_0 = 0$ and $\gamma = 0.5$ (dashed line), $\gamma = 0.7$ (dash-dot), and $\gamma = 0.9$ (solid).

Transforming the continuous variable q as $\omega \to 0$, we get

$$R_m(q) = (1+q-imt_2)^{-1}, \tag{83}$$

$$Q_m{}^a(q, \varkappa) = P_m{}^a(1+i\varkappa+q-imt_2)^{-1}, \tag{84}$$

where $t_2 = t_0 s_0/2$. Substituting Eqs. (83) and (84) in (29) and taking (30) into account with $\varkappa = 0$ and $a = 1$, we easily obtain, after integrating with respect to q and summing over m, the following expression for the static dielectric constant:

$$\varepsilon'(\varepsilon) = \varepsilon_0 \left(\frac{\pi}{t_2 \operatorname{sh}(\pi/t_2)}\right)^2 \times \left[1 + \frac{1}{12}\left(\frac{\pi}{t_2 \operatorname{sh}(\pi/t_2)}\right)^2 \left(1 + 2\operatorname{ch}^2 \frac{\pi}{t_2}\right)\right]. \tag{85}$$

It follows from this equation, in particular, that at $|t_2| \ll 1$

$$\varepsilon'(\varepsilon) \approx \varepsilon_0 \frac{1}{6}\left(\frac{\pi}{t_2}\right)^4 \exp\left(-\frac{2\pi}{|t_2|}\right). \tag{86}$$

We see hence that at small t_2 the dielectric constant goes to zero exponentially because of the vanishing of the density of the electron states.[10] At $\gamma < 1$ there is no dip to zero, but the value of the dielectric constant at the minimum can be quite small, at least as $\gamma \to 1$. Thus, allowance for effects of strong scattering by impurities leads to formation of sharp maxima and minima of $\varepsilon'(\varepsilon)$ near all the rational points of the band. We note that all these singularities, except those at the center, vanish in the case of weak scattering, when $\gamma \ll 1$.

7. HOPPING CONDUCTIVITY

As shown in the preceding section, effects of commensurability of the electron wavelength λ and the lattice period a_0 in one-dimensional metals with strong disorder lead to strong singularities of the localization length l_{loc} and the static dielectric constant ε'. These singularities, as well as the corresponding singularities of the electron density of states,[10] lead to substantial changes in the hopping conductivity σ_{hopp} in $1D$ metals and influence noticeably, in particular, its temperature dependence.

Indeed, as shown in earlier papers,[3,22] at not too low temperatures the hopping conduction is the result of electron hops between neighboring localized states, due to inelastic scattering by phonons, and the temperature dependence of $\sigma_{\text{hopp}}(T)$ is given by

$$\sigma_{hopp}(T) = \frac{1}{4\pi}\varepsilon'\tau_{in}^{-1}(T). \tag{87}$$

In the case of a half-filled band and in the absence of forward scattering by the impurities, the temperature dependence of $\varepsilon'(T)$ is given by (77) and causes a noticeable change of $\sigma_{\text{hopp}}(T)$. If the Fermi level is close to but does not coincide with the center of the band, ε' is determined by Eq. (76), so that σ_{hopp} depends substantially on the distance to the center of the band. In a quasi-$1D$ organic metal ε can be altered by many factors and, in particular, depends strongly on the external pressure P.[2] This leads to substantial maxima of the $\sigma_{\text{hopp}}(P)$ dependence as the Fermi level ε_F passes through the center of the band $\varepsilon_F = 0$. We note that in the case of sufficiently strong scattering by the impurities the $\varepsilon'(\varepsilon)$ dependence is determined at $\varepsilon \neq 0$ by Eq. (85) and corresponds to the presence of deep minima that precede a narrow maximum at the band center. The plot of σ_{hopp} has therefore besides the sharp maxima also deep minima at values of ε_F close to the center of the band.

We point out that on passing through the center of the band were observed already at $P \sim 10$ kbar by Jerome *et al.* (see the review[2]), who investigated the pressure dependence of the conductivity of the quasi-$1D$ organic conductor TTF-TCNQ. It was assumed in these studies that the strong influence of the commensurability of λ_F and a_0 on the conductivity is an exclusive attribute of the charge-density wave (CDW). It follows from our present results that similar effects occur also in localization theory, where they are due to a specific quantum interference between scattered electron waves.

In the limit of very low temperatures, the hopping conductivity is determined by hops between localized states that are spatially far from one another but have close energy; it is described then by the Mott theory.[23] In the usual situation, when $\rho(\varepsilon)$ and l_{loc} have no singularities, this theory predicts an exponential decrease of $\sigma_{\text{hopp}}(T)$ as $T \to 0$:

$$\ln \sigma_{hopp} \propto -(T_0/T)^{1/2}, \quad T_0 \sim (\rho l_{loc})^{-1}.$$

In the presence of the singularities (52) and (57), the corresponding estimate yields as $\varepsilon \to 0$ the following asymptotic behavior of T_0:

$$T_0 \propto |\varepsilon \ln \varepsilon|. \tag{88}$$

At low temperatures this singularity is cut off at $\varepsilon \sim T$, so that the exponential singularity of $\sigma_{\text{hopp}}(T)$ as $T \to 0$ vanishes. We note that this general fact is not connected with the details of the derivation of the equations for $\sigma_{\text{hopp}}(T)$,[23–25] since they contain in all cases exponentials of different powers of T_0/T. Therefore different methods of calculating $\sigma_{\text{hopp}}(T)$ can lead only to different exponents α in the asymptotic relation $\sigma_{\text{hopp}}(T) \propto T^{\alpha}$ as $T \to 0$. It must be noted that the low-temperature behavior of the conductivity in quasi-$1D$ organic conductors based on the TCNQ molecule is well described by Mott's relations.[1] We therefore confine ourselves here to this case.

According to Mott's theory, the low-temperature asymptotic value of $\sigma_{\text{hopp}}(T)$ is determined by the extremum of a product of the small wave-function overlap factor $\exp(-2R/l_{\text{loc}})$ and the activation factor $\exp(-\Delta\varepsilon(R)/T)$, where R is the mean spatial distance between localized states that have an energy difference $\Delta\varepsilon(R)$. In the absence of $\rho(\varepsilon)$ singularities, the value lf $\Delta\varepsilon$ is estimated at $(\rho R)^{-1}$ (Ref. 23). In the case considered here, where ρ depends substantially on ε, this relation gives a self-consistent equation for the $\Delta\varepsilon(R)$ dependence:

$$\Delta\varepsilon \sim [\rho(\Delta\varepsilon)R]^{-1}. \tag{89}$$

Substituting $\rho(\Delta\varepsilon)$ in the form (75) in (89) we get

$$\Delta\varepsilon(R) \sim \tau^{-1} \exp\{-[2R/lB(\gamma)]^{1/4}\}. \tag{90}$$

Minimizing now the product

$$\exp(-2R/l_{loc}(\Delta\varepsilon) - \Delta\varepsilon/T) \tag{91}$$

with respect to R and taking (90) and (52) into account, we readily find, after simple transformations, that as $T\to 0$ we have

$$\sigma_{hopp}(T)\propto(T\tau)^{\alpha},\quad \alpha=B/\beta. \tag{92}$$

We note that in the weak-scattering limit, when $\gamma\ll 1$, we have $\alpha\approx 4$. Thus, the singularities of the localization length and of the density of states near the center of the band cause the exponential asymptotic dependence of $\sigma_{\text{hopp}}(T)$ as $T\to 0$ to be replaced by a power-law dependence.

8. CONCLUSION

We have investigated the influence of effects of commensurability of the electron wavelength λ and of the lattice period a_0 on the characteristics of localized states in a $1D$ metal. We have shown that in the absence of forward scattering from impurities, substantial singularities of the localization length and of the static dielectric constant appear near the center of the band:

$$l_{loc}(\varepsilon)\propto\ln^2\varepsilon,\quad \varepsilon'(\varepsilon)\propto|\varepsilon|^{-1}\quad \text{as}\quad \varepsilon\to 0.$$

In the presence of sufficiently strong scattering, charcteristic maxima of $\varepsilon'(\varepsilon)$ and $l_{\text{loc}}(\varepsilon)$ occur at all rational points of the band. Sharp maxima of $\varepsilon'(\varepsilon)$ near these points should lead to a substantial increase of ε' with decreasing temperature. We note however, that just such an $\varepsilon'(T)$ dependence is observed at present, at not too low temperatures, in the quasi-$1D$ organic conductors $Qn(TCNQ)_2$ and $Adz(TCNQ)_2$.[3,7] As shown in a large number of studies,[1,3,15,8] the electrons are strongly scattered in these substances, therefore the noticeable decrease of ε' with increasing T can be explained with the aid of the results of the present paper. We note that, as shown by Gor'kov and Dorokhov,[11] the condition that there be no forward scattering by the impurities is satisfied just in such compounds with disordered orientation of the asymmetric cations. Satisfaction of this condition, however, is not essential for the analysis of the experimental data for $Qn(TCNQ)_2$ and $Adz(TCNQ)_2$, since the high peaks of $\varepsilon'(\varepsilon)$ near 1/4 of the band appear in the case scattering also when $\varphi_0\neq 0$.

We note in conclusion that the real density c, per site, of the structure defects in these substances, which is governed by the random orientation of the asymmetric cations in two opposite directions, is not small and is equal to 1/2. Therefore the mean free path l estimated from the value of ε' at $T\approx 100$ K is found to be (3–4) a_0 and $p_F l\approx 3$, since $p_F\approx\pi/4a_0$. Thus, the condition $p_F l\gg 1$ is satisfied with some difficulty. We note, however, that the expansion in powers of $(p_F l)^{-1}$ contains only even powers,[15] so that the model considered can describe a real situation. This pertains also to the condition $c\ll 1$. In $Qn(TCNQ)_2$ and $Adz(TCNQ)_2$ we have $c=1/2$, but it is well known[11,21] that the effective density c_{eff} that determines the mean free path $l=(\gamma c_{\text{eff}})^{-1}$ is equal in this case to $c(1-c)=1/4$, meaning that configurations at which two defects land on one site are excluded. Therefore the effective defect density is low, and the reflection coefficient γ is close to unity.

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