Low-temperature conductivity of highly disordered Coulomb systems

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A new mechanism, involving electron-electron interactions, is proposed for the conductivity of highly disordered systems. The conductivity has a power-law, rather than exponential, low-temperature behavior. The results give a qualitative explanation of experimental data on the conductivity of doped semiconductors.

1. INTRODUCTION

The electronic properties of highly disordered systems such as doped semiconductors, solid solutions and amorphous and liquid semiconductors are of current interest in research in solid state physics. The theoretical analysis of such systems is based on the concept of Anderson localization.[1] When applied to a system of noninteracting electrons, this concept means[2] that at absolute zero the electrical conductivity of the system vanishes if the Fermi energy μ lies below the mobility threshold E_c (states with energies below E_c are localized, while those above E_c are delocalized). At a nonzero temperature, the conductivity mechanism may involve tunneling between localized states as a result of an interaction with phonons[2–8] and also an electron-electron interaction.[9]

As was shown in Ref. 2, the following relation holds in the case of a phonon-supported conductivity of noninteracting electrons at low temperatures:

$$\sigma \propto \exp\left[-(T_0/T)^{1/4}\right]. \tag{1}$$

A similar behavior was found in Ref. 9 on the basis of a mechanism involving tunneling due to an electron-electron interaction. However, temporal fluctuations of the energies of the localized states due to the diffusion of electrons were ignored in that paper, as was the resulting possibility of correlated motion (more on this below). It was shown in Refs. 3 and 4 that the long-range nature of Coulomb forces should give rise to a pseudogap at the Fermi level, with the result that the Mott decay of the electrical conductivity described by (1) should give way to a faster decay with decreasing temperature:

$$\sigma \propto \exp\left[-(T_1/T)^{1/2}\right]. \tag{2}$$

A conductivity mechanism involving many-particle (cascaded) excitations accompanied by involving the emission or absorption of a phonon was proposed in Refs. 7 and 8. That mechanism leads to a power-law temperature dependence of the conductivity.

The operation of a hopping conductivity at zero frequency means that a macroscopic diffusion of electrons is occurring in the system. The corresponding coefficients are related to each other by the Einstein relation

$$\sigma = e^2 |\partial n/\partial \mu| D,$$

where $|\partial n/\partial \mu|$ is the compressibility of the electron subsystem. The diffusion of electrons gives rise to a temporal fluctuation of the energy of a one-particle state, ε, in an energy region on the order of the Coulomb gap Δ (we should actually be speaking about the energies of dipole excitations: ω_β^α, $E_{\beta\delta}^{\alpha\gamma}$; see the discussion below). If the value of ε initially lies in the interval $(-\Delta, 0)$, and if the state of interest is filled by an electron, then a fluctuation in ε with a transition in the interval $(0, \Delta)$ should lead to a transition of the electron from the given localization center to a vacant center. These fluctuations thus cause a new mechanism for electron transitions—a mechanism distinct from the Mott mechanism. In the latter, the energies of the one-particle states are assumed to be fixed. This new process does not require the participation of phonons with an energy $\omega \gg T$, as in the Mott mechanism does.

Using this new mechanism, we can describe the overall electron hopping frequency τ_{tot}^{-1} by

$$\tau_{tot}^{-1} = \tau_{ph}^{-1} + \dot{W}(\tau_{tot}^{-1}), \tag{3}$$

where τ_{ph}^{-1} is the frequency of the hops caused by phonons, and $\dot{W}$ is the frequency of the hops caused by this new mechanism. For $\dot{W} \ll \tau_{\text{ph}}^{-1}$, the contribution of this new diffusion channel reduces to an insignificant increase in the coefficients of the exponential functions in (1) and (2). In the case

$$\dot{W} \gg \tau_{ph}^{-1} \tag{4}$$

the fluctuational hopping mechanism should play an independent role.

In this paper we adopt the hypothesis that the fluctuational mechanism for hopping diffusion (zero-frequency hopping conductivity) does not disappear when all electron-phonon interactions are turned off. Setting $\tau_{ph}^{-1} = 0$ in (3), we can evaluate the non phonon hopping frequency. We find an approximately quadratic temperature dependence for the diffusion coefficient.

In this paper we take the approach which was pointed out in Refs. 10 and 11, for the case of the diffusion of impurity particles in quantum crystals, and also in Refs. 12 and 13, for the propagation of spin excitations.

As a rule, the experimental data on the electrical conductivity of doped semiconductors confirm expressions (1) and (2). On the other hand, there are reports[14–17] that in certain materials the exponential decay of the conductivity softens at low temperatures, becoming a power law. Such a behavior of the conductivity can be explained by the mechanism proposed in the present paper.

2. RESONANT CLUSTERS

We consider a system of electrons in a highly disordered medium in which the mobility threshold E_c lies well above

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the Fermi level μ. Among the one-particle localized states, the only ones which play a decisive role are those whose energies lie in the Coulomb gap[4]:

$$-\Delta<\Phi_\alpha<\Delta. \tag{5}$$

Here Φ_α is a seed energy of state α with respect to μ. We assume that the random quantity Φ_α is distributed uniformly over the interval (5) with a density $g_0[g_0=(2\Delta)^{-1}]$. We assume that the localization centers are positioned randomly with a density a_0^{-3} but that the smallest separation of adjacent centers which satisfy (5) is larger than a_0. This restriction simplifies the percolation problem in such a system.

The magnitude of the Coulomb gap is found from the condition that the sign of the energy of the state corresponding to any center [see (10) below] can vary when the occupation of neighboring center changes.[7] It follows that we have

$$\Delta=\gamma_0 e^2/a_0, \qquad \gamma_0\approx 1. \tag{6}$$

In general, centers for which the seed energy of the corresponding states does not belong to the interval (5) are either always filled or always empty at sufficiently low temperatures. The Hamiltonian of the model in the basis of states α is

$$\begin{aligned}
&\hat{H}=\hat{H}_0+\hat{V}_1+\hat{V}_2,\\
&\hat{H}_0=\sum \Phi_\alpha(n_\alpha-{}^1/_2)+{}^1/_2\sum U_{\alpha\beta}(n_\alpha-{}^1/_2)(n_\beta-{}^1/_2),\\
&\hat{V}_1={}^1/_2\sum A_\alpha{}^\beta c_\beta{}^+c_\alpha, \qquad \hat{V}_2={}^1/_2\sum U_{\alpha\gamma}{}^{\beta\delta}c_\beta{}^+c_\delta{}^+c_\gamma c_\alpha,\\
&A_\alpha{}^\beta=\sum U_{\alpha\gamma}{}^\beta n_\gamma, \qquad n_\alpha=c_\alpha{}^+c_\alpha, \qquad \langle n_\alpha\rangle={}^1/_2.
\end{aligned} \tag{7}$$

The term $\hat{V}_1$ describes hops of electrons which are induced by surrounding electrons; $\hat{V}_2$ describes two-electron transitions. We will use the following estimates of the matrix elements of the Coulomb interaction:

$$\begin{aligned}
&U_{\alpha\beta}=\Delta/r_{\alpha\beta}, \qquad |U_{\alpha\gamma}{}^\beta|\approx|A_\alpha{}^\beta|(a_0/r_{\alpha\gamma})^2,\\
&|U_{\alpha\gamma}{}^{\beta\delta}|\approx\Delta^{-1}|A_\alpha{}^\beta|\,|A_\gamma{}^\delta|(a_0/r_{\alpha\gamma})^3,\\
&|A_\alpha{}^\beta|\approx A(r_{\alpha\beta})=\Delta\exp(-r_{\alpha\beta}/l), \qquad \mathbf{r}_{\alpha\beta}=\mathbf{r}_\alpha-\mathbf{r}_\beta.
\end{aligned} \tag{8}$$

We assume that the localization radius l of the one-particle states is small in comparison with the distance a_0 between localization centers ($l\ll a_0$). Here and below, we assume $a_0=1$.

The Coulomb repulsion of the particles in one state is assumed to be the largest of the energy parameters of the system, so there is a filling in which there is a single particle per state. We are thereby ignoring the role played by the spin.

The ground state and elementary excitations of Hamilton $\hat{H}_0$ were described in Refs. 3 and 4. We are interested in the properties of the model at low but nonzero temperatures. In describing a state of the system which is close to the ground state, we use the self-consistent method of Ref. 4. For $T\neq 0$, the centers α are filled with a probability

$$[1+\exp(\beta\varepsilon_\alpha)]^{-1}, \qquad \beta=T^{-1}, \tag{9}$$

where ε_α is the self-consistent energy of a localized state:

$$\varepsilon_\alpha=\Phi_\alpha+\sum_\beta U_{\alpha\beta}(n_\beta-{}^1/_2). \tag{10}$$

In the approximation of a soft Coulomb gap,[3] the distribution of energies (10) is

$$g(\varepsilon)=g_0\begin{cases}1, & |\varepsilon|\geqslant\Delta,\\ (\varepsilon/\Delta)^2, & |\varepsilon|<\Delta.\end{cases} \tag{11}$$

The perturbation $\hat{V}_1$ in (7) causes an electron to hop from center α to center β. The change in $\hat{H}_0$ in the course of this transition is

$$\omega_\alpha{}^\beta=\varepsilon_\alpha-\varepsilon_\beta-\Delta/r, \qquad r=r_{\alpha\beta}. \tag{12}$$

We are interested in pairs with $r\gtrsim 1$ and $\omega<\Delta$. At $T=0$, in the soft-Coulomb-gap approximation, such pairs have a distribution[4]

$$F_1(\omega, r)=g_0 r^{-5}\theta(\omega)\theta(r-1) \tag{13}$$

[a soft gap arises from the requirement that the ground state be stable with respect to perturbations (12)]. A deeper analysis of the ground state of Hamiltonian $\hat{H}_0$ (Ref. 4) strengthens the singularities of distribution (13) at large r and small ω [a hard Coulomb gap[4] arises from the additional requirement of stability against the excitations (18)]:

$$\begin{aligned}
&F(\omega, r)=F_1\exp[-G(\omega, r)],\\
&G(\omega, r)=\alpha r(\ln(\Delta/\omega))^{1/4}, \qquad \alpha\approx 1.
\end{aligned} \tag{14}$$

The perturbation $\hat{V}_1$ in (7) reconstructs (hybridizes) the eigenstates of Hamiltonian $\hat{H}_0$. The effect is basically a renormalization of the transition energy:

$$\tilde{\omega}_\alpha{}^\beta=[(\omega_\alpha{}^\beta)^2+(A_\alpha{}^\beta)^2]^{1/2}\operatorname{sign}(\omega_\alpha{}^\beta). \tag{15}$$

This level of repulsion is important under the resonance condition

$$|\omega_\alpha{}^\beta|<|A_\alpha{}^\beta|. \tag{16}$$

A more important point for our purposes is that in a resonant pair an electron is at centers α and β simultaneously, although with different probability amplitudes. Using (13) and (14), we find that the probability for an electron to belong to a resonant pair of size r is

$$P_r\approx A(r)F(A(r), r). \tag{17}$$

The perturbation $\hat{V}$ in (7) causes two electrons to hop simultaneously ($\alpha, \nabla\to\beta, \delta$), with a change in the energy $\hat{H}_0$ (the transition energy):

$$\begin{aligned}
&E_{\alpha\gamma}{}^{\beta\delta}=\omega_1+\omega_2-E_d, \quad \omega_1=\omega_\alpha{}^\beta, \quad \omega_2=\omega_\gamma{}^\circ,\\
&E_d=U_{\alpha\delta}+U_{\beta\gamma}-U_{\beta\delta}-U_{\alpha\gamma}.
\end{aligned} \tag{18}$$

For $R\gg r_1, r_2$ ($R=r_{\alpha\gamma}$, $r_1=r_{\alpha\beta}$, $r_2=r_{\gamma\delta}$) the quantity E_d is equal to the interaction energy of two dipoles:

$$E_d\simeq\Delta r_1 r_2/R^3. \tag{19}$$

If one or both pairs of the 4-cluster $\nu(\nu=\alpha,\beta,\gamma,\delta)$ are close to resonance, we should use normalized values (15) in (18):

$$E_\nu=\tilde{E}_{\alpha\gamma}{}^{\beta\delta}=\tilde{\omega}_1+\tilde{\omega}_2-E_d. \tag{20}$$

An important point for the discussion below is that in

this case the amplitude for a transition of a 4-cluster from a ground state to an excited state increases substantially by virtue of the hybridization:

$$B_\nu = \tilde{U}_{\alpha\gamma}^{\beta\delta} = U_{\alpha\gamma}^{\beta\delta} + E_d A_\alpha^\beta A_\gamma^\delta (\tilde{\omega}_1 \tilde{\omega}_2)^{-1}. \quad (21)$$

Actually, the last term in (21) always dominates. The 4-clusters are resonant under the condition

$$|E_\nu| < |B_\nu|. \quad (22)$$

In a resonant 4-cluster, both of the electrons are "smeared" within the corresonding pairs, even if these pairs are not themselves resonant.

The distribution of 4-clusters can be approximated as a product of the pair distributions (14). The probability that a given electron belongs to a resonant 4-cluster of a given configuration (with fixed values of ω_1, r_1, ω_2, r_2, and R) is then

$$P_\nu \approx B_\nu F(\omega_1, r_1) F(\omega_2, r_2) \delta(\tilde{\omega}_1 + \tilde{\omega}_2 - E_d). \quad (23)$$

At a nonzero but low temperature $T \ll \Delta$ the state of the system can be described approximately as a set of neutral m-clusters ($m = 2,4,...$) whose energies are set by the fixed occupation numbers of the surrounding one-particle states. Most such m-clusters are, as before, in the ground state, but a small fraction are in an excited state and thus have a negative transition energy. From this standpoint, the m-clusters constitute two-level systems of a sort. In particular, at the temperature $T = \beta^{-1}$ the numbers of pairs in the ground and excited states are, respectively,

$$F(|\omega|, r)\,[1+\exp(-\beta|\tilde{\omega}|)]^{-1},\ F(|\omega|, r)\,[1+\exp(\beta|\tilde{\omega}|)]^{-1}. \quad (24)$$

As a result we can say that at $T \neq 0$ the pairs have a distribution

$$F(|\omega|, r)\,[1+\exp(-\beta\tilde{\omega})]^{-1}. \quad (25)$$

We will not consider clusters with $m \geqslant 6$ in the present paper.

3. LOW-TEMPERATURE DIFFUSION NOT INVOLVING PHONONS

In the Introduction we described a fluctuational mechanism for hopping diffusion which we believe may operate in the absence of an interaction with phonons. Let us examine this mechanism in more detail. We assume that most of the electrons belonging to an energy layer of width Δ near the Fermi surface are participating in a diffusion process. The diffusing electrons create an irreversible fluctuation of the Coulomb part of the energy over a length scale Δ. As a result, nearly every electron in the layer (5) which is initially at the center α will sooner or later be part of the resonant cluster ν and will belong to two centers (α,β) simultaneously. Over a time t_ν the resonant conditions will be violated, and an electron will be at the center β with a finite probability. After a certain time τ_*, the center α becomes part of a new resonant cluster; after the latter breaks up, the electron moves to the center β. Over a time t, the repetition of this process moves an electron a distance

$$r_n = r_* n^{1/2}, \quad n = t/\tau_*, \quad (26)$$

where r_* is a length scale of the pair which determines the hopping length. Expressions (26) determine a diffusion coefficient

$$D \approx r_*^2/\tau_*. \quad (27)$$

Since the space in a disordered Coulomb system is inhomogeneous, there is the possibility in principle that as this process takes place an electron will remain at all times in a bounded region of size R_x. This is a bounded diffusion, which corresponds to a high-frequency conductivity $\sigma(\omega)$, where

$$\omega > \tau_*^{-1} (r_*/R_x)^2. \quad (28)$$

In the present paper we adopt the hypothesis that this nonphonon diffusion is unbounded ($R_x = \infty$), so we have

$$\sigma(0) \neq 0.$$

In order to find the hopping frequency τ_*^{-1} we need to solve a self-consistent problem: Starting from a given τ_*^{-1}, we are to find the temporal fluctuation of the energy of one-particle states, which in turn determines the hopping frequency.

In the steady state, tunneling in a highly inhomogeneous medium smears the wave function over several sites, but the state remains local. The motion of an electron becomes irreversible only if the resonant conditions are satisfied temporarily. Let us find the lifetime of a resonant cluster. We assume that a single electron undergoes on the average a single irreversible hop over a time τ_*. Such a hop creates a fluctuation in the transition energy of a resonant cluster at a distance R from the electron:

$$\delta E_\nu \approx \Delta r_* r_\nu R^{-3}, \quad (29)$$

where r_ν is the length scale over which the wave function of an electron belonging to resonant cluster ν is localized. If

$$|\delta E_\nu| > |C_\nu| \quad (30)$$

[C_ν is $A(r)$ from (8) for pairs or B_ν from (21) for 4-clusters], such a jump drives cluster ν from resonance. Condition (30) holds if the distance between cluster ν and the electron which is hopping is less than

$$R_\nu = (\Delta r_\nu r_*/C_\nu)^{1/3}. \quad (31)$$

For $R > R_\nu$, many hops would be required to drive a cluster from resonance. It can be shown that this mechanism is not very effective.

In a sphere of radius R_ν around cluster ν there are $(r\pi/3)R_\nu^3$ electrons, which generate one jump of the cluster energy over a time

$$t_\nu \approx \tau_* R_\nu^{-3} = \tau_* |C_\nu| (\Delta r_\nu r_*)^{-1}, \quad (32)$$

which is the lifetime of cluster ν. Correspondingly, t_ν^{-1} is the probability for the decay of this cluster per unit time.

We can speak in terms of the existence of a resonant clusters and electron hopping in it only if

$$t_\nu > \tau_\nu \approx |C_\nu|^{-1}, \quad (33)$$

where τ_ν is a typical period of the beats in cluster ν. In other words, if the inequality (33) is violated, an electron cannot

undergo a transition to a new state. Using (32), we can rewrite (33) as

$$|C_\nu|(r_\nu r_*)^{-1/2}>C_*, \quad C_*=(\Delta/\tau_*)^{1/2}. \tag{34}$$

We assume that at the time $t=0$ a given electron is at the localization center α and belongs to the resonant cluster ν. This electron executes beats with a period τ_ν, and at the time t_ν when the resonant cluster breaks up, the electron has a probability of order 1/2 to be at center β of the same cluster. The probability for such a transition per unit time is $(1/2)t_\nu^{-1}$. Since the probability for an electron to belong to the given cluster is $P_\nu d\nu$ [see (23) and (25)], the total probability for an irreversible hop of an electron per unit time is, in order of magnitude,

$$W=\sum P_\nu t_\nu^{-1}\theta(|C_\nu|(r_\nu r_*)^{-1/2}-C_*). \tag{35}$$

The inverse of W is the average time per hop, i.e., τ_*. As a result we find a self-consistent equation for τ_*:

$$W(\tau_*)=\int_0^{\tau_*} W\,dt=1,$$

$$W(\tau_*)=\tau_*\sum P_\nu t_\nu^{-1}\theta(|C_\nu|(r_\nu r_*)^{-1/2}-C_*). \tag{36}$$

The 4-clusters actually cause simultaneous hopping of two electrons. This circumstance does not, however, affect the form of Eq. (36). Equation (36) should be supplemented with an expression which gives the hopping length scale over a time τ_*:

$$r_*^2=\tau_*\sum P_\nu r_\nu^2 t_\nu^{-1}\theta(|C_\nu|(r_\nu r_*)^{-1/2}-C_*). \tag{37}$$

We first assume that the sums in (36) and (37) are dominated by 2-clusters. In this case, (36) takes the following form at $T=0$:

$$W_2=\int_1 d^3\mathbf{r}\, r^{-4}\exp(-G)\theta[A(r)(rr_*)^{-1/2}-C_*], \tag{38}$$

where $A(r)$ and G are defined by (8) and (14). In the approximation of a soft gap ($G=0$) this integral is determined by small values of r. In order of magnitude we have $W_2\approx r$. The right side of (37) differs from (38) by a factor of r^2. In the approximation of a soft Coulomb gap, the corresponding integral is determined by values of r of order

$$r_{max}=1/2\ln(\Delta\tau_*)$$

and is equal to $r_* r_{\max}$. As a result we find from (36) and (37)

$$r_*\approx 1, \quad \tau_*^{-1}\approx\Delta\exp(-2/l), \tag{39}$$

and, according to (27), $D\neq 0$. We see that in the soft-Coulomb-gap approximation, (11), (13), a disordered electron system is delocalized even in its ground state. Incorporating the hardness factor of the Coulomb gap, $\exp(-G)$ [see (14)], leads to a substantial decrease in the corresponding integrals in (36) and (37), and the system of self-consistent equations does not have a solution. An important point is that for $T<\Delta$ the contribution of 2-clusters to (36) and (37) depends only weakly on the temperature, so we will ignore resonant pairs in the discussion below.

Let us examine the contribution to Eqs. (36) and (37) from 4-clusters. The gap hardness factor $\exp(-G)$ [see (14)] and hopping amplitudes (8) fall off exponentially with increasing hop length. In the coefficient of the exponential function we can thus set the dimensions r_* and r_ν equal to unity. In this approximation, Eq. (37) becomes extraneous. We will ignore the factors which vary logarithmically slowly with the temperature.

Substituting expressions (21) and (23) into the right side of (36), we find

$$W_4\approx\int_1^\infty dr_1\int_1^\infty dr_2\int_1^\infty d^3\mathbf{R}\int_{-\Delta}^{\Delta}d\omega_1\int_{-\Delta}^{\Delta}d\omega_2\Delta^{-1}$$
$$\times\exp(-G_1-G_2)[1+\exp(-\beta\tilde\omega_1)]^{-1}$$
$$\times[1+\exp(-\beta\tilde\omega_2)]^{-1}\delta(\tilde\omega_1+\tilde\omega_2-E_d)\theta$$
$$\times\{E_d-C_*\tilde\omega_1\tilde\omega_2[A(r_1)A(r_2)]^{-1}\}. \tag{40}$$

Expression (40) contains the three energy parameters T, $A_1=\Delta\exp(-1/l)$, and $C_*=(\Delta/\tau_*)^{1/2}$. The last is always smaller than the first two, by a factor of order of the gap hardness parameter $\exp(-G)$ [see (41) and (44) below]. In the integration over the size of a 4-cluster, R, the dimensions corresponding to $E_d\approx C_*$ play the major role. We can thus discard E_d from the δ-function. In the integration in (40), we can ignore the dependence of G on ω and r.

For $A_1<T$, the values ω_1, $\omega_2<T$ and $r_1\approx r_2\approx r_*\approx 1$. are important for the integration. We find

$$W_4\approx l^2(A_1/C_*)\exp[-2G(A_1,1)]. \tag{41}$$

For $T<A_1$, we conclude that (40) is dominated by hops of electrons over a distance $r_*\approx r_1\approx r_2$, for which we have

$$A(r_*)=T. \tag{42}$$

This equation determines a characteristic hopping distance

$$r_*(T)=1+l\ln(A_1/T)=l\ln(\Delta/T). \tag{43}$$

In this case we have

$$W_4\approx l^2(T/C_*)\exp\{-2G[T,r_*(T)]\}. \tag{44}$$

Equating (41) or (44) to unity, we find the temperature dependence of diffusion coefficient (28):

$$D=\Delta l^4\begin{cases}(T/\Delta)^{2+\lambda(T)}, & T<A_1,\\ (A_1/\Delta)^{2+\lambda(A_1)}, & T>A_1,\end{cases} \tag{45}$$
$$\lambda(E)=4\alpha l[\ln(\Delta/E)]^{1/4}.$$

For $T<T_\lambda$, at which we have $T_\lambda=\Delta\exp[-(4\alpha l)^{-4}]$, the parameter $\lambda(T)$ is greater than unity, and the diffusion coefficient is very small. Since the relation $l\ll 1$ holds, there is a comparatively wide temperature interval,

$$T_\lambda<T<A_1,$$

in which the parameter λ is small in comparison with unity and in which the diffusion coefficient depends on the temperature in accordance with

$$D\propto T^2. \tag{46}$$

For $T>A_1$ the diffusion coefficient does not depend on the temperature.

The condition $l \ll 1$ does not mean that the factor $\exp(-G)$ plays no role. This point can be seen clearly by rewriting result (45) in the form

$$D=\Delta l^4[E(T)/\Delta]^2 \exp\{-\bar{G}[E, r_*(E)]\},$$
$$E(T)=\begin{cases} T, & T<A_1, \\ A_1, & T>A_1. \end{cases} \quad (47)$$

We see that at all temperatures (but with $T < T_m$; Sec. 4) the decrease in the state density near the Fermi level determined by the hard Coulomb gap (a factor $G \gg 1$) shows the diffusion process down substantially.

4. MOTT LAW; ROLE OF PHONONS

In the model of electrons in a highly disordered medium which was proposed in Ref. 4, the scatter in the bare values of the energy is significantly larger than Δ, and the concentration of centers is significantly larger than a_0^{-3}. At low temperature $T < T_m$ [see (53) below], centers with $\Phi_\alpha < -\Delta$ are always filled, while those with $\Phi_\alpha > \Delta$ are always empty.[7] The numerical value of the parameter γ_0, which determines the size of Coulomb gap (6), should be found from the condition that all of the centers which satisfy condition (5) belong to some resonant cluster from time to time. This assumption allows electrons to escape to infinity and thus diffuse.

With increasing temperature, the number of electrons participating in the diffusive motion should increase. Let us assume $A_1 < T < \Delta$. Corresponding to center 1 is a potential energy $\Phi_1 = \xi\Delta$ $(1 < \xi < 2)$ in the external field. Because of the interaction with neighboring electrons, this center has an energy (10) in the interval $((\xi-1)\Delta, (\xi+1)\Delta)$. By virtue of the thermal motion of the surroundings, the energy takes on all values in this interval alternately. The intervals $(-\Delta,\Delta)$ and $((\xi-1)\Delta, (\xi+1)\Delta)$ overlap, so an electron from layer $(-\Delta,\Delta)$ may hop to center 1 resonantly in a process which does not involve phonons. The probability for finding an electron at center 1 is proportional to

$$\exp[-(\xi-1)\Delta/T].$$

The probability that there is no electron at center 2, for which we have $\Phi_2 = -\xi\Delta$, is proportional to the same exponential function. With increasing temperature there is accordingly an increase in the number of centers for which the occupation numbers fluctuate significantly. Correspondingly, there is an increase in the density of electrons participating in the diffusive motion, and the effective hopping length decreases.

Let us find the characteristic layer width $(-\xi\Delta,\xi\Delta)$ and the density of centers which form an infinite cluster at $T \neq 0$:

$$[a(T)]^{-3}=\xi(T)a_0^{-3}.$$

In an inhomogeneous medium, the diffusion is determined by the rate of passage through a "bottleneck." The bottleneck of a new cluster would be centers of type 1 or 2. Let us estimate the probability [see (40)] for an electron to escape from center 2. For definiteness we assume that center 2 is part of that pair of the resonant 4-cluster for which the transition energy ω is positive. For it we find

$$F(\omega, r, T) \propto \theta(r-r_{min})\theta(\omega-\omega_{min}),$$
$$r_{min} \approx \xi^{-1/3}a_0. \quad (48)$$

The first factor incorporates the circumstance that in an expanded system of clusters the minimum distance between clusters decreases. In the second factor, $\omega_{\min}$ is the lowest energy [see (12)] for a transition of an electron from the upper state of center 2, $\varepsilon_2 = (\xi-1)\Delta$, to the closest center, $\varepsilon_1 = (\xi-1)\Delta$:

$$\omega_{min} \approx (\xi-1-\xi^{1/3})\Delta. \quad (49)$$

The second pair of a resonant 4-cluster should have a negative transition energy, so we can write

$$F(-\omega_{\min}, r_2, T) \propto \exp(-\beta\omega_{min}). \quad (50)$$

In place of (41), (44) we thus have

$$W_4 = \frac{1}{C_*}\exp\left[-\frac{2r_{min}}{l}-\beta\omega_{min}\right]. \quad (51)$$

Substituting in expressions from (48) and (49), we find

$$W_4 = \frac{1}{C_*}\exp\left[-\frac{2a_0}{l\xi^{1/3}}-\beta\Delta(\xi-1-\xi^{1/3})\right]. \quad (52)$$

The value of the parameter ξ, which determines the effective density of centers which form an infinite cluster, should be found from the requirement that the bottleneck be traversed as fast as possible. The minimum value of (52) does not depend on the temperature for

$$T<T_m,\ T_m=\Delta l/a_0. \quad (53)$$

For $T > T_m$ the maximum value of (52) corresponds to $\xi \sim t^{3/4}$, and the electrical conductivity is described by a Mott law

$$\sigma \propto \exp[-(T_0/T)^{1/4}],\ T_0=\Delta(a_0/l)^3. \quad (54)$$

The values of T_0 in (1) and (54) are the same in order of magnitude. Consequently, the Coulomb interaction makes the electrical conductivity relatively independent of the temperature [see (45)] at very low temperatures; as the temperature is increased, the conductivity begins to increase in accordance with the Mott law (54). The overall behavior is shown schematically by the solid trace in Fig. 1. When the phonon mechanism and the nonphonon mechanism for hopping diffusion are taken into account simultaneously, the former may predominate over a wide temperature range and may convert directly into a T^2 law (the dashed line in Fig. 1) as the temperature is lowered.

According to Ref. 3, expression (53) determines the temperature of the transition from regime (1) to (2), so for $T < T_m$ the phonon conductivity decreases with decreasing

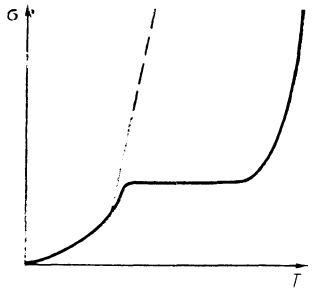

FIG. 1. Temperature dependence of the electrical conductivity.

temperature more rapidly than for $T > T_m$. According to (45), in contrast, below T_m the temperature dependence of σ should become smoother. The observation of this transition regime could tell us which of the diffusion mechanisms predominates. Doped semiconductors exhibiting T^2 behavior for the conductivity were discussed in Refs. 14 and 15. As a rule, the behavior of the conductivity in these materials is described well by a functional dependence similar to that shown by the solid curve in Fig. 1.

The T^2 law observed in doped semiconductors is sometimes explained on the basis of the cascade conductivity mechanism proposed in Refs. 7 and 8. However, the power to which the temperature is raised in the case of that mechanism should be substantially greater than 2 (Ref. 7).

We have not analyzed the role played by multicenter resonant clusters, with $m \geqslant 6$. We believe that they would give rise to unbounded motion of the electrons, since a hard Coulomb gap would have less effect on them than on pairs and 4-clusters.

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