Coulomb gap and hopping electric conduction. Computer simulation

E. I. Levin, V. L. Nguen, B. I. Shklovsiĭ, and A. L. Éfros

A. F. Ioffe Physicotechnical Institute, USSR Academy of Sciences

(Submitted 12 October 1986)
Zh. Eksp. Teor. Fiz. **92**, 1499–1511 (April 1987)

Hopping conduction was simulated with a computer, for the first time ever, with allowance for electron-electron interaction. Two- and three-dimensional lattice models were studied with random scatter of the site energies. The density of state is obtained as a function of temperature and energy. It is shown that Coulomb interaction decreases sharply the absolute value of electric conductivity and increases its temperature dependence. The behavior of the conductivity and density of states agrees with the premise of a soft Coulomb gap.

1. INTRODUCTION

The electric conductivity of localized electrons is known to be effected at low temperatures by hopping, with the hop range increasing as the temperature is lowered (variable range hopping, VRH) Mott[1] has shown that for noninteracting electrons the temperature dependence of the electric conductivity is given by

$$\sigma(T) \sim \exp\{-(T_M/T)^{1/(d+1)}\}, \quad T_M = \beta_d{}^M/g_0 a^3, \tag{1}$$

where g_0 is the density of states (DS) on the Fermi level, a is the localization region, $d = 2$ or 3 is the dimensionality of the space, $\beta_3^M = 22.2$ (Ref. 2) and $\beta_2^M = 13.8$ (Ref. 2). Efros and Shkolvskiĭ[3] have shown that electron interaction leads to formation of a soft Coulomb gap, i.e., to a power-law decrease of the DS to zero when the energy tends to the Fermi energy. Consequently, the temperature dependence of the electric conductivity predicted in Ref. 3 is of the form

$$\sigma(T) \sim \exp\{-(T_0/T)^{1/2}\}, \quad T_0 = \beta_d e^2/\varkappa a, \tag{2}$$

where e is the electron charge, $\varkappa$ the dielectric constant, $\beta_3 = 2.8$,[4] and $\beta_2 = 6.5$.[5] In the main, the experimental data for three-dimensional ($3D$) systems confirm Eq. (2) (see Refs. 2 and 6). The available experimental data on MIS structures in the absence of a magnetic field, however, favor more readily Mott's law.[7] Nor is the question quite clear from the theoretical standpoint. A Coulomb gap exists for one-electron excitations that transfer electrons from site (node) to site under the condition that the other electrons are frozen in positions corresponding to the ground state. The initial derivation of (22) corresponded to just this types of electron motion. We shall call this hereafter the one-electron-transport approximation. It does not take into account the possible correlations of the displacements of the various electrons. These correlations can be of two types.[8] First are simultaneous, in the quantum-mechanical sense, hops of several interacting electrons. Second are individual electron hops that take place consecutively in time in such a way that some electrons prepare the path for the others by lowering with their potential the appropriate barriers. One might think that such a motion is capable of lifting the restrictions imposed by the Coulomb gap.

There is at present no theory of multielectron transport, since the interaction in a system of localized electrons is by no means weak. We have therefore decided to simulate electron-field-induced electron motion using a computer and the Monte Carlo method. The simulation does not take multielectron hops into account, i.e., it duplicates only the second type of correlation, which we believed to be the most important during the planning of this study. Our main result is that when account is taken of all the successive hops the temperature dependence of the hopping electric conductivity for $2D$ and $3D$ systems is of the form (2), and that the coefficients β_d do not differ greatly from those obtained above.

Another result of the present study is the temperature-dependent density $g(\varepsilon)$ of the density of one-electron states. In the $3D$ case, ours is the first study of the DS at finite temperatures. At energies $\varepsilon \gg T$ but small compared with the width of the Coulomb gap, our results are well described by the earlier known relations[2]

$$g(\varepsilon) = \begin{cases} \dfrac{3}{\pi}\dfrac{\varkappa^3}{e^6}\varepsilon^2 & \text{if} \quad d=3, \qquad (3a) \\ \dfrac{2}{\pi}\dfrac{\varkappa^2}{e^4}|\varepsilon| & \text{if} \quad d=2, \qquad (3b) \end{cases}$$

where d is the dimensionality of the space and the energy ε is measured from the Fermi level. At nonzero temperatures, the DS on the level is not zero. The reason is that the arguments leading to Eq. (3) are incorrect in an energy band of order T in the vicinity of the Fermi level. We can therefore estimate $g(0)$ by replacing ε in (3) by T. Then

$$g(0) = \begin{cases} G_3 \dfrac{3}{\pi}\dfrac{\varkappa^3}{e^6}T^2 & \text{if} \quad d=3, \qquad (4a) \\ G_2 \dfrac{2}{\pi}\dfrac{\varkappa^2}{e^4}T & \text{if} \quad d=2, \qquad (4b) \end{cases}$$

where G_3 and G_2 are numerical coefficients. The simulation yielded the relation (4) with $G_3 \approx 11$ and $G_2 \approx 2$. It is important to note that we have not observed in the DS any polaron effects[2] which should be manifested by an exponential decrease of $g(0)$ with temperature at $d = 3$.

2. DESCRIPTION OF MODEL

We used for the simulation the so-called lattice model.[2] In this model the electrons can occupy the sites of a simple cubic (or quadratic) lattice, the number of sites being double of the electrons, but not more than one electron can be on each site. Neutrality is achieved by appropriating a charge $e/2$ to each empty site and a charge $-e/2$ to an occupied one. All the charges interact in accordance with Coulomb's law. Each site is assigned a random energy φ_i of non-Coulomb

 0038-5646/87/040842-07$04.00

nature, uniformly distributed in the interval $[-A,A]$. The energies φ_i corresponding to neighboring sites are not correlated. The total system energy can be represented in the form

$$H=\sum_i n_i\varphi_i+\frac{e^2}{2\varkappa}\sum_{i\neq j}\left(n_i-\frac{1}{2}\right)\left(n_j-\frac{1}{2}\right)r_{ij}^{-1}, \quad (5)$$

where i and j number the lattice sites, $n_i=1$ if the site is occupied and $n_i=0$ if it is empty. The single-particle energies φ_i are given by

$$\varepsilon_i=\varphi_i+\frac{e^2}{\varkappa}\sum_j\left(n_j-\frac{1}{2}\right)r_{ij}^{-1}. \quad (6)$$

The Fermi energy E_F is zero in this model at all temperature. The DS $g(\varepsilon)$ of the lattice model was investigated many times for $T=0$ (Refs. 9 and 10), and also for $T\neq 0$ in the $2D$ case.[10] The thermodynamic properties of this and close models were also investigated by the Monte Carlo method.[10,11] Hopping conduction, however, was heretofore investigated by the Monte Carlo method only in systems without Coulomb interaction.[12] In the present paper we simulate, for the first time ever, the electric conductivity of a system, with allowance for Coulomb interaction, by direct calculation of charge carried in an external electric field. To simulate electric conduction, the lattice model must be supplemented by an expression for the frequency of the transitions between two arbitrary sites i and j. In the theory of hopping conduction it is customarily assumed that if an electron is located on site i, while site j is empty, the probability of the electron transition takes the form

$$\gamma_{ij}=\gamma_{ij}^{(0)}\begin{cases}\exp(-\Delta_{ij}/T) & \text{if} \quad \Delta_{ij}>0,\\ 1 & \text{if} \quad \Delta_{ij}<0,\end{cases} \quad (7)$$

where Δ_{ij} is the work needed to transport the electron between sites i and j,

$$\gamma_{ij}^{(0)}=\gamma_0\exp(-2r_{ij}/a), \quad (8)$$

and r_{ij} is the distance between the sites.

Strictly speaking, if the electron transitions were accompanied by phonon absorption and emission, Eq. (7) would have to contain a more complicated equation containing Planck functions. Equation (7) is obtained from this complicated expression at $\Delta_{ij}\gg T$, which holds as a rule under hopping conduction conditions. Expression (8) describes the overlap of the wave functions of sites i and j. the assumption that γ_0 does not depend on r_{ij} and Δ_{ij}, is model-dependent, and does not influence the result, since we are interested mainly in experimental relations.

We have unfortunately arrived at the conclusion that the use of the probability density (8) for the simulation calls for more computer time than available to us. We therefore propose and investigate a model that is simpler in this respect, which we call the R-model. In this model hops are possible only over distance not exceeding R:

$$\gamma_{ij}^{(0)}=\begin{cases}\gamma_0 & \text{if} \quad r_{ij}\leqslant R,\\ 0 & \text{if} \quad r_{ij}>R.\end{cases} \quad (9)$$

The form of the function $\gamma_{ij}^{(0)}(r_{ij})$ does not affect in any way the equilibrium properties of the system, but influence strongly the electric conductivity. Indeed, in the R model the characteristic length of the hop cannot increase monotonically as the temperature is lowered, as is the case in real system, but remains equal to R. Accordingly, the activation energy should not change with temperature, i.e., the temperature dependence of the electric conductivity at low temperatures should be of the form

$$\sigma(R)=\sigma_0(R)\exp\{-\varepsilon_A(R)/T\}, \quad (10)$$

which differs substantially from (1) and (2). We shall show presently, however, that the character of the R-dependence of the activation energy $\varepsilon_A(R)$, obtained within the framework of the R model, explains the role of the Coulomb gap in the hopping conduction. To this end we derive Eq. (10) and an expression for $\varepsilon_A(R)$ within the framework of the one-electron theory of hopping conduction. It is assumed in this theory that all the lattice sites are interconnected by electric impedances Z_{ij} of the form[2]

$$Z_{ij}=T/e^2\langle\gamma_{ij}n_i(1-n_j)\rangle, \quad (11)$$

where $\langle\ldots\rangle$ means averaging over time at fixed occupation of the sites. At low temperatures,[2]

$$Z_{ij}\sim\exp\left(\frac{\varepsilon_{ij}}{T}\right),$$

$$\varepsilon_{ij}=\begin{cases}|\varepsilon_i-\varepsilon_j|-e^2/\varkappa r_{ij} & \text{if} \quad \varepsilon_i\varepsilon_j<0,\\ \max(|\varepsilon_i|,|\varepsilon_j|) & \text{if} \quad \varepsilon_i\varepsilon_j>0.\end{cases}$$

(Recall that the Fermi energy is zero.) The activation energy is determined by solving the percolation-theory problem with the connectivity conditions $\varepsilon_{ij}\leqslant\varepsilon_A(R)$. Neglecting the Coulomb interaction, $\varepsilon_A(R)$ can be estimated from the condition that

$$g_0\varepsilon_A(R)R^d\approx 1. \quad (12)$$

Here $g_0=(2A)^{-1}l^{-d}$ is the density of states, determined by the energy spread φ_i, and l is the lattice constant. Consequently

$$\varepsilon_A(R)=\alpha_d^M(g_0R^d)^{-1}, \quad (13)$$

where α_d^M are numerical coefficients that depend on d. The estimate (13) is made in accordance with Mott's ideas, as emphasized by the superscript M of α_d^M. In the presence of a Coulomb gap, ε_A must be estimated by using the density of states (3) averaged over the ε_A energy band. We then obtain in place of (12), in order of magnitude

$$(\varkappa/e^2)^d\varepsilon_A^{d-1}\,\varepsilon_AR^d\approx 1. \quad (14)$$

This yields

$$\varepsilon_A(R)=\alpha_d^Ce^2/\varkappa R, \quad (15)$$

where α_d^C are numerical coefficients. Thus, the $\varepsilon_A(R)$ dependence with allowance for the Coulomb gap differs greatly from the dependence given by Eq. (13) for the case of a density of states that is constant near the Fermi level.

The numerical coefficients α_d^M and α_d^C must be determined by solving the corresponding percolation-theory problems. We have estimated them by the method of invariants, proposed in Ref. 14. Such an estimate yields for the $3D$ model

$$\alpha_3^M\approx 0.37, \quad \alpha_3^C\approx 0.51, \quad (16)$$

and for the $2D$ model

$$\alpha_2^{M}\approx 0.83, \quad \alpha_2^{C}\approx 1.2. \tag{17}$$

We continue the investigation of $\sigma(R)$ which we need for subsequent comparison with the calculation. Within the context of the one-electron approximation we can obtain also for the pre-exponential factor in (10) an expression valid at $\varepsilon_A(R) \gg T$ (Ref. 2). At $d=3$ we have

$$\sigma_0(R) = C_3\gamma_0 \frac{e^2}{RT}\left(\frac{T}{\varepsilon_A(R)}\right)^{\nu}, \tag{18}$$

and at $d=2$

$$\sigma_0(R) = C_2\gamma_0 e^2/T. \tag{19}$$

Here C_2 and C_3 are unknown numerical coefficients, and ν is the exponent of the percolation-theory correlation radius.

If $T \gg \varepsilon_A(R)$, the electric field in the system can be regarded as uniform and the effective electric conductivity is determined by a simple equation obtained from the expression for the energy dissipated per unit energy. It takes the form

$$\sigma_u(R) = \frac{\gamma_0 e^2}{4dTl^d} \sum_{\substack{j \\ (r_{ij}\leqslant R)}} F(r_{ij}) r_{ij}^2, \tag{20}$$

where

$$F(r_{ij}) = \frac{2}{\gamma_0} \langle\langle n_i(1-n_j)\gamma_{ij}\rangle\rangle. \tag{21}$$

The summation in (20) is over all the lattice sites surrounding the site i. The result is independent of i, since $\langle\langle \ldots \rangle\rangle$ means averaging over the time and over all the sites i. At $T \gg A$ we obtain the simple expression

$$\sigma_u(R) = \frac{\gamma_0 e^2}{8dTl^d} \sum_{\substack{j \\ (r_{ij}\leqslant R)}} r_{ij}^2. \tag{22}$$

Equation (22) is in fact not based on the one-electron approximation and can be used to check on the simulation program.

The electric conductivity $\sigma(R)$ has as a function of temperature a maximum at T of the order of A. At $\varepsilon_A(R) \ll T \ll A$ the conductivity falls off with temperature by a power law. It is easy to verify that in the absence of Coulomb interaction

$$F(r_{ij}) = \left(\frac{T}{A}\right)^2 \frac{\pi^2}{6}. \tag{23}$$

At $A \gg e^2/\varkappa l$ with width Δ of the Coulomb gap is much smaller than A, and there exists a temperature interval $A \gg T \gg \Delta$ in which Eq. (23) is valid also with allowance for the Coulomb interaction. We confine ourselves henceforth to the case when A is of the order of $e^2/\varkappa l$. In this case Eq. (23) cannot be used and $F(r_{ij})$ must be calculated by using with allowance for the Couloamb gap. As a result we find for $\Delta \gg T \gg e^2/\varkappa R$

$$\sigma_u(R) = \frac{D_d \varkappa \gamma_0}{T^{3-d}} \left(\frac{\varkappa RT}{e^2}\right)^{2+d}, \tag{24}$$

where D_d are numerical coefficients. At T of the order of $e^2/\varkappa R$ the electric field can no longer be regarded as uniform, and at even lower temperatures we get the exponential relation (10).

It is not a simple matter to check on the above relations by simulation, since the temperature interval corresponding to (24) is narrow, and it was impossible to use in our computer a temperature low enough to discern an exponential decrease of the conductivity by several orders of magnitude. The checking was facilitated by the following deduction of the one-electron theory. At $T \ll \Delta$ we have

$$\sigma(R) = \varkappa\gamma_0 (e^2/\varkappa T)^{3-d} \Psi_d(\varkappa RT/e^2), \tag{25}$$

where Ψ_d is a certain dimensionless function that decreases exponentially at low values of the arguments. The scaling relation (25) expresses the very essence of the one-electron notions concerning hopping transport in the region of the Coulomb gap. It can be written from dimensionality consideration if it is recognized that the density of state is universal and does not depend on g_0. Its premise is that there is only one significant length R, large enough to make $e^2/\varkappa R \ll \Delta$.

A similar scaling relation can be written also for a system without a Coulomb interaction:

$$\sigma(R) = \varkappa\gamma_0 (e^2/\varkappa T)^{3-d} \varphi_d(g_0 R^d T), \tag{26}$$

where φ_d is a dimensional function. This relation is valid at $T \ll A$. Whereas the verification of (26) is more readily a check on the method, varification of (25) for a system with Coulomb interaction answers the question whether one-electron concepts can be used to calculate the electric conductivity.

The low-temperature expression (10) and Eqs. (13) and (15) obtained within the framework of the R model yield the temperature dependence of variable-range-hopping conductivity, when the transition probability is of the form (8). To this end it must be recognized that the main contribution of the R-model conductivity is made by lengths of order R and the VRH conductivity $\sigma(T)$ must be represented in the form

$$\sigma(T) = \int_l^{\infty} \sigma(R) \exp(-2R/a)\, d\ln R. \tag{27}$$

Evaluating the integral in (17) by the saddle-point method and using (13) and (15), we obtain respectively Eqs. (1) and (2). For the coefficient β_d in (2) we obtain in this manner the expression $\beta_d = 8\alpha_d^C$, which yields, after substitution of the values of α_d^C from (16) and (17), values of β_d that are approximately 1.5 times larger than those that follow from Eq. (2). This should be regarded as satsifactory in view of the fact that Eq. (27) is not exact. In particular, calculation of the pre-exponential factor with its aid would be an exaggeration of the accuracy.

3. DESCRIPTION OF THE SIMULATION PROGRAM

The object of the simulation is a square of cube with side L. The maximum value of L was 18 at $d=3$ and 100 at $d=2$ (in this section we set the lattice constant l, the electron charge e, and the dielectric constant $\varkappa$ equal to unity). Just as in Refs. 10 and 12, we used periodic boundary conditions, viz., the initial cube (square) is periodically continued along each coordinate axis, so that translation of any site by a length L leads to a site having the same values of ε_i and n_i as the initial site.

The values of φ_i were specified for each site, in an interval $[-A, A]$, using a random-number generator. The initial occupation numbers n_i were assumed to be zero for sites with even coordinate along the x axis, and to unity for the remaining sites. The initial placement of the electrons corre-

sponded to alternation of empty and occupied planes or lines (the chosen number L was always even). The site energies were next calculated from Eq. (6), in which the summation was carried out only over the sites of the initial cube. In accordance with the assumed periodic conditions, the distance $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$ between sites i and j of the intial cube we used the distances

$$r_{ij}' = (X_{ij}^2 + Y_{ij}^2 + Z_{ij}^2)^{1/2},$$

where

$$X_{ij} = \min(|x_i - x_j|,\ L - |x_i - x_j|),$$

x_i and x_j are the projections of the radius vectors $\mathbf{r}_i$ and $\mathbf{r}_j$ on the x axis. Similar equations hold for Y_{ij} and Z_{ij}. To permute the electrons, the system recorded all site pairs (i,j) for which the distance r_{ij}' did not exceed R. On going from one site to another, the electron could cross the boundary of the initial cube (square) and land in its periodic continuation. The values of r_{ij}' and also the component x_{ij} of the electron displacement along the direction of the electric field E (the x axis) were recorded in the memory for each pair. The value of x_{ij} was $x_j - x_i$ if the displaced electron did not cross the initial-cube faces perpendicular to the x axis. If these faces were crossed, then

$$\tilde{x}_{ij} = \begin{cases} x_j - x_i + L & \text{if} \quad x_j < x_i, \\ x_j - x_i - L & \text{if} \quad x_j > x_i. \end{cases}$$

After completing the initial placement and recording of the pairs, the program proceeded to simulated electron transitions between sites. One step of the program consisted of the following.

Random and equiprobable choice of one of the registered pairs (i,j). If $n_i = n_j$, the step is regarded as completed and the next one should be taken.

In the opposite case, one calculates the transition energy

$$\Delta_{ij} = \varepsilon_j - \varepsilon_i - (r_{ij}')^{-1} + E\tilde{x}_{ij} \tag{28}$$

and the probability of a transition in the given step

$$p_{ij} = \begin{cases} 1, & \text{if} \quad \Delta_{ij} \leqslant 0, \\ \exp(-\Delta_{ij}/T), & \text{if} \quad \Delta_{ij} > 0. \end{cases} \tag{29}$$

The transition is carried out with probability p_{ij}.

If the transition was effected, the interchange $n_i \rightleftarrows n_j$ is made all values of ε_i are recalculated, and unity is added to the counter of the $i \to j$ transitions.

Every 1000 steps, the sites were ranked by energy and the density of states $g(\varepsilon)$ corresponding to the given instant of time was calculated. Altogether, $M = 10^5 - 3 \cdot 10^7$ steps were taken, depending on the temperature and on the size of the system.

After the end of the simulation, the following quantities were calculated:

a) The system conductivity $\sigma(R)$, defined as the ratio of the total specific dipole moment of the system to the product ME.

b) The number of transitions in pairs of length $r_0 = r$, referred to the number of calls by the program to these pairs. This ratio is the function $F(r)$ defined by Eq. (21).

c) The conductivity $\sigma_u(R)$ of the system, obtained by substituting in (20) the obtained function $F(r)$.

d) The density of states $g(\varepsilon)$ averaged over time. Two variants of averaging were used. In the first the energy was reckoned from zero, and in the second from its mean value at the given instant of time. Following Ref. 10, we have decreased in the second version the influence of the Fermi-level fluctuations on the density of states. No noticeable difference, however was observed between the densities of state calculated by the two methods.

The simulation algorithm chosen by us is simple to implement and effective enough at not too low temperatures. When the temperature is lowered the mean value of the probability p_{ij} decreases exponentially and most steps do not lead to electron transitions. Our algorithm is therefore incapable of handling very low temperatures.

In another method proposed[13,14] for simulation of hopping conduction, the operating speed is practically independent of the temperature of the simulated system. Application of this method to systems with Coulomb interaction, however, leads to an algorithm in which, although accounting for the electron transition in each step, requires $(LR)^d$ arithmetic operations per step, and extensive use of the computer memory. The power of our computer[1)] was at least an order of magnitude too low for low-temperature calculations by this method, this procedure can in principle effected by modern supercomputers.

4. DISCUSSION OF SIMULATION RESULTS

The results of simulation at $A = 1$ are shown in Figs. 1–8. We discuss first the results for the density of states. They were obtained for different values of R, and there was no systematic dependence of the density of states on R. Figures 1 and 2 show the densities of states vs energy at different temperatures for $d = 3$ and $d = 2$, respectively. The energy and temperature are in units of $e^2/\varkappa l$ and the density of states in units of $(e^2 l^{d-1}/\varkappa)^{-1}$. It can be seen that in the region of the Coulomb gap ($\varepsilon < 0.6$) the data for the lowest temperatures are close to the theoretical plots of (3). With increase

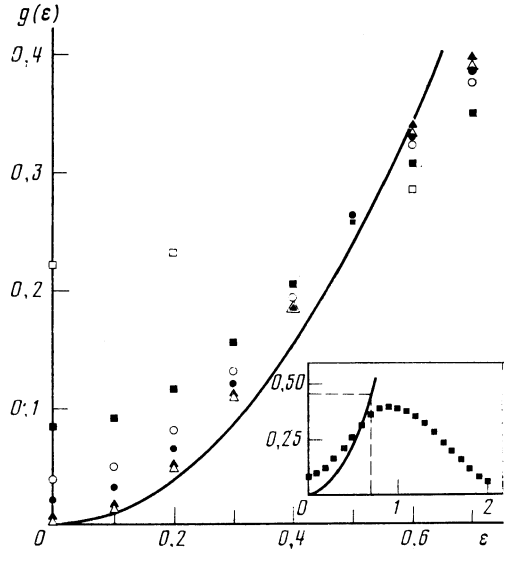

FIG. 1. Density of states in units of $(e^2 l^2/\varkappa)^{-1}$ vs the energy measured in units of $e^2/\varkappa l$ for an $18 \times 18 \times 18$ $3D$ system at the following reciprocal temperature (in units of $l\varkappa/e^2$): □—5, ■—10, ○—15, ●—20, ▲—30, △—40. Solid curve—Eq. (3a). The inset shows the density of states at $T^{-1} = 10$ in a wider energy range. The dashed lines bound the region shown in the main figure.

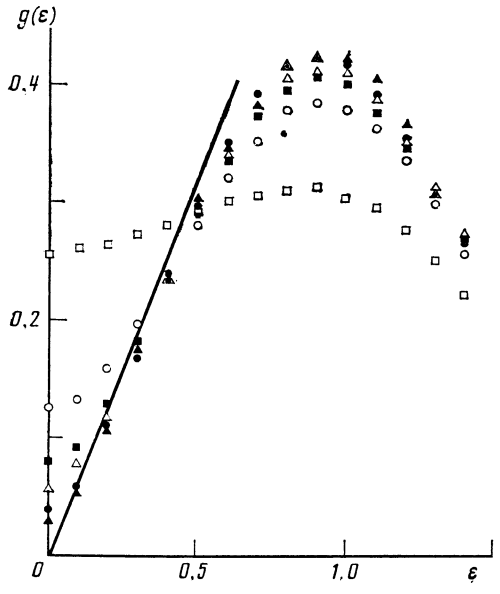

FIG. 2. Density of states in units of $(e^2l/\varkappa)^{-1}$ vs the energy measured in uits of $e^2/\varkappa l$ for a 100×100 $2D$ system at the following values of the reciprocal temperature (in units of $l\varkappa/e^2$): □—5, ○—10, ■—15, △—20, ●—30, ▲—40. The straight line is a plot of Eq. 3b.

of temperatures, the Coulomb gap is gradually "washed away." To verify relation (4), Figs. 3 and 4 show the quantity

$$G(T)=\pi g(0)/T^{d-1}d. \tag{30}$$

The value of $g(0)$ was calculated by averaging the density of states in an energy interval equal to $0.1e^2/\varkappa l$ and with center at the minimum of the density of states. In the large 100×100 and $18\times18\times18$ systems we studied as a rule one realization of the random set $\{\varphi_i\}$. In the small 12×12 and $8\times8\times8$ systems the averaging was over approximately five realizations. In the two-dimensional case (Fig. 3) at $L=100$ the value of $G(T)$ does not depend on temperature at all the investigated temperatures lower than 0.2, as is splendidly confirmed by Eq. (4b). The ensuing constant is $G\approx2$. For $L=20$, it can be seen that $G(T)$ decreases with temperature at lower temperatures. This is a size that manifests itself when T is of the orde of L^{-1}. In the $3D$ case (Fig. 4) the values of L are relatively small, and there is therefore

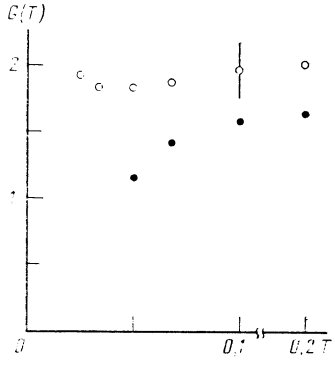

FIG. 3. Check of the theoretical relation (4b). Dimensionless density of states $G(T)$, defined by Eq. (30), vs temperature for a $2D$ system. The values of L are 20 (●) and 100 (○). The vertical stroke shows a typical error. Attention is called to the break in the abscissa axis.

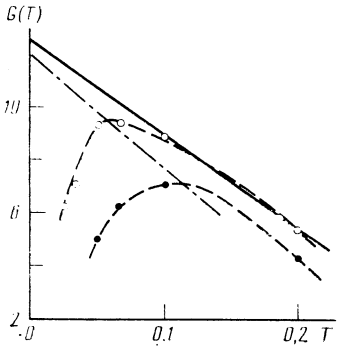

FIG. 4. Determination of the constant G_3 in Eq. (4a). The nondimensional density of states vs temperature for a $3D$ system is represented by the points and the dashed curves drawn through them. The values of L are 8 (●) and 18 (○). The solid and dash-dot straight lines are extrapolations in accordance with Eqs. (31) and (32), respectively.

no such distinct plateau as in the $2D$ case. The smooth decrease of $G(T)$ towards higher temperatures is due to the fact that Eq. (4) for the density of states should be valid only for $T\ll\Delta$, where Δ is the width of the Coulomb gap. As T approaches Δ, the rate of growth of $g(0)$ slows down, since $g(0)$ cannot become substantially larger than 0.5 (see the inset of Fig. 1). Accordingly $G(T)$ decreases with rise of temperature. We propose that at $L=\infty$ and $T/\Delta\ll1$ the decrease follows the law

$$G(T)=G_3(1-qT/\Delta), \tag{31}$$

where q is a numerical factor. The extrapolation shown by the solid line in Fig. 4 yields $G_3\approx11.5$. Approximately the same value is obtained if the aggregate of data on L is extrapolated. The formula used for this purpose is

$$G(T_{max})=G_3(1-q'T_{max}/\Delta), \tag{32}$$

where T_{max} is the temperature at which $G(T)$ reaches its maximum. This temperature decreases with L. Equation (32) is obtained from (31) if it is recognized that the low-temperature decrease is abrupt. The extrapolation in accordance with (32) is shown by the dash-dot curve of Fig. 4. Close values of G_3 are obtained also when the data for $A=2$, which are not presented here, are reduced in accordance with (32).

We proceed now to describe the electric conductivity $\sigma(R)$. As already mentioned, it is determined by dividing the current density by the external electric field. We are interested in ohmic electric conductivity, the determination of which would call for extrapolation of $\sigma(R)$ to zero field. We chose instead the electric field as given by the condition $eER=T$. All the data given here from $\sigma(R)$ pertain precisely to such a field. At $T\geqslant20^{-1}e^2/\varkappa l$ the ohmic character was checked by decreasing the electric field by one-half. No changes of the electric conductivity were oberved at the calculated accuracy 10–15% in this temperature region. We supposed that even at the lowest of the temperatures investigated here the error due to the non-ohmic behavior did not exceed noticeably the error in the calculation of the electric conductivity, which reached 30% here.

The program described above calculates the electric conductivity in units of $\varkappa\gamma_0 l^{3-d}$. It is also plotted in the figures in these units. Figure 5 shows the electric conductiv-

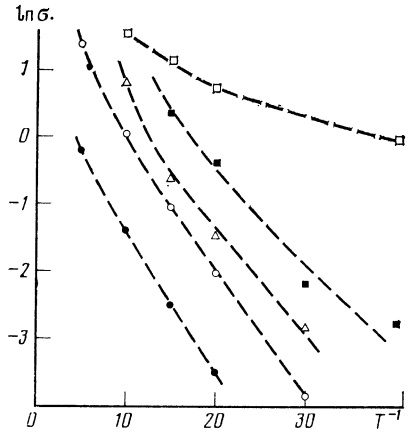

FIG. 5. Electric conductivity $\sigma(R)$ of a $3D$ system in units of $\varkappa\gamma_0$ vs the reciprocal temperature in units of $\varkappa l/e^2$. The points ●,○,△,■ are for an $18\times18\times18$ system with Coulomb interaction, the points □ for an $8\times8\times8$ system without Coulomb interaction. The dashed curves are drawn arbitrarily through the points. The values of R in units of l are: ●—3; ○,□—6; △—3, ■—4.

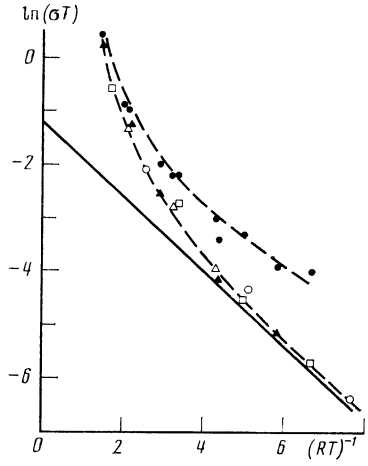

FIG. 7. Dependence of $\ln(\sigma T)$ on $(RT)^{-1}$ for a 100×100 $2D$ system. The values of σT are in units of $\gamma_0 e^2$, and of RT in units of $e^2/\varkappa$. The values of R in units of 1 are: ○—1.94, □—2.98, △—4.65, ▲—6.86. Dark points-values of $\ln(\sigma_u T)$ at different R and T. The dashed curves are drawn arbitrarily through the corresponding points. The straight line determines the activation energy.

ity $\sigma(R)$ of a $3D$ system vs the reciprocal temperature at different values of R. It can be seen that at low temperatures the temperature dependence is of form (10), and the activation energy decreases with increase of R. The same figure shows the electric conductivity for a system without Coulomb interaction for one of the values of R. It can be seen that the Coulomb interaction alters substantially the character of the temperature dependence and decreases the absolute value of the electric conductivity by approximately five orders at the lowest temperature.

To verify the scaling relation (25) for a system with Coulomb interaction, the logarithm of $\sigma(R)$ was plotted in Fig. 6 as a function of $(RT)^{-1}$. To eliminate the nonmonotonicities due to the discrete character of the lattice, the symbol R in this figure, as well as in Figs. 7 and 8, stands not for the maximum length of the transition, but for some other close quantity obtained from the equation $N=\pi R^d(4/3)^{d-2}$, where N is the number of neighbors, for which $\gamma(r_{ij})\neq0$, of an arbitrary site i. These are the values of R indicated in the captions of these figures. It can be seen that the points fit a universal curve, thus verifying relation (25). Figure 6 shows also the electric conductivity σ_u calculated from Eq. (20). This equation was derived under the assumption that the electric field is uniform, and therefore described the electric conductivity $\sigma(R)$ at $T\gtrsim\varepsilon_A(R)$. At low temperatures, the inequality $\sigma_u\gg\sigma(R)$ should hold in the region of the activation conductivity (10). As seen from Fig. 6, in the investigated temperature interval the ratio $\sigma_u/\sigma(R)$ reaches six. This means that at the very lowest temperatures

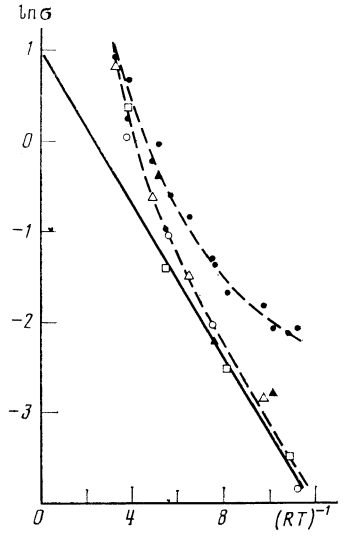

FIG. 6. Dependence of $\ln\sigma$ on $(RT)^{-1}$ for an $18\times18\times18$ $3D$ system. The electric conductivity is units of $\varkappa\gamma_0$, Rt is in units of $e^2/\varkappa$. The values of R in units of l are: □—1.84, ○—2.67, △—3.08, ▲—3.94. Dark points—values of ln at various R and T. The dash-dot curves are drawn arbitrarily through the corresponding points. The straight line determines the activation energy.

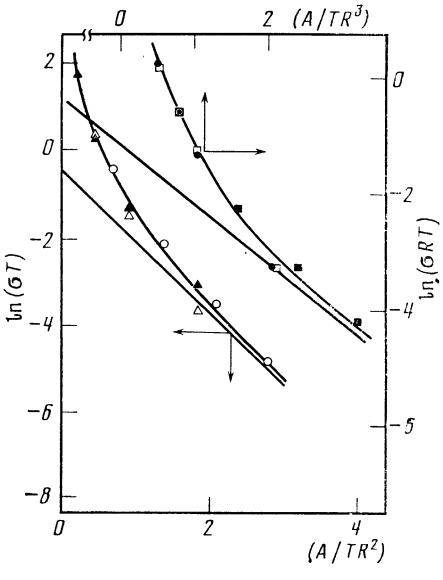

FIG. 8. Verification of the scaling relation for a system without Coulomb interaction. The left and lower scales pertain to a $2D$ system (points ○,▲,△), the right-hand and upper one to a $3D$ one (points ■,●,□). The solid curve are drawn arbitrarily through the points, and the straight lines determine the activation energies. Points ○,▲,■,● correspond to $A=1$, points △,□ to $A=2$. The values of R in units of l are ○—2.76, ▲, △—4.65, ■—1.84, ●, □—2.67.

the simulation results should be described by Eq. (10). The straight line shown in Fig. 6 determines the activation energy. It is described by Eq. (15) with $\alpha_3^C = 0.42$. This value agrees well with the theoretical estimate (15). A check on relation (25) for a $2D$ system is shown in Fig. 7. It can be seen that the points fit well a universal curve. The activation energy determined from the slope of the straight line is described by Eq. (15) with $\alpha_2^C = 0.7$, which differs substantially from the $\alpha_2^C = 1.2$ obtained from the theoretical estimate. By "turning off" in the program the Coulomb interaction, we have also verified the scaling relation at $d = 3$ and $d = 2$. The results are shown in Fig. 8, from which it is seen that the relation is well satisfied. The activation energies are described by Eq. (13), with $\alpha_2{}^M = 0.8$ while $\alpha_3{}^M = 0.5$ in good agreement with the theoretical estimates (16) and (17). We note that the points in Fig. 8 include not only $A = 1$ but also $A = 2$, i.e., the scaling includes three parameters, namely R, T, and A.

5. CONCLUSION

In sum, we list the main deductions of the present paper.

1. At low temperatures, the Coulomb interaction lowers greatly the hopping electric conductivity and strengthens its temperature dependence.

2. The electric conductivity of two-dimensional and three-dimensional systems with Coulomb interactions, calculated in the framework of the R model, satisfies the scaling relation (25) that follows from the premises of the Coulomb gap and the one-electron theory of hopping transport. Note that these premises lead to relation (25) at all values of the scatter of the non-Coulomb part of the energy A, if the temperature is low enough, so that the essential states are inside the Coulomb gap. The width of the Coulomb gap decreases with increase of A, so that it is imore difficult to meet this condition. Figures 6 and 7 show data for $A = 1$, We carried out, however, calculations also for $A = 2$. It was found that $\ln\sigma(R)$ is smaller at $A = 2$ than at $A = 1$ by approximately 1 at $d = 3$ and by 0.7 at $d = 2$. In addition, we have carried out calculations in the classical-impurity-band model,[2] in which the donors and acceptors are located not at the lattice sites but randomly. The degree of compensation was assumed to be 0.5. The characteristic energy scatter in this model is approximately the same as in the lattice model at $A = 2$. Our values of $\sigma(R)$ are in this came aprpoximately the same as in the lattice model for $A = 2$.

We believe that both violations of scaling are due to the fact that the temperatures realized in the simulations were not low enough. The scaling relation (25) obtained for the electric conductivity of the R model is easily generalized to the usual model of hopping electric conductivity with a transition probability of the type (8). For this model we have

$$\sigma = \varkappa\gamma_0(e^2/\varkappa T)^{3-d}\Psi_d(Ta\varkappa/e^2) \qquad (33)$$

at $T \ll \Delta$. At $d = 3$ the relation (33) is met in experiment (sees Ref. 6). If it is assumed, however, that hopping conduction is effected by phonons, it is easy to verify with the aid of the equations of Ref. 2 that γ_0 is, generally speaking, not a constant and depends not only on the product $Ta\varkappa/e^2$. This leads to a contradiction between the contemporary theory, based on hops with emission and absorption of phonons, and the experimental data. It is possible that this contradiction will be resolved by development of a zero-phonon theory in the spirit of Ref. 15.

3. The temperature dependence of the electric conductivity of the R model at the very lowest temperature is descirbed by the Arrhenius law, with the dependence of the activation energy on R described by Eq. (15). It follows from this behavior of $\sigma(R)$ in the R model that in the usual hopping-transport model, which uses the tunnel exponential function (8), the temperature dependence of the electric conductivity should be of the form (2). Note, however, that it is seen from Fig. 6 that the linear dependence of $\ln\sigma(R)$ on $(RT)^{-1}$ sets in only at $(RT)^{-1} \approx 8$, when $(\varepsilon_A/T) \approx 3$. A similar situation obtains also in the $2D$ case. It seems therefore that in the usual hopping-transport model the approach to the relation (2) with decreasing temperature may be delayed. Analysis of the experimental data with the aid of the relation $\sigma \sim \exp[-T_0/T)^s]$ at values of T_0/T that are not large enough $[(T_0/T) \leqslant 6]$ can therefore lead to values of s smaller than 1/2.

The energy and temperature dependences of the one-electron density of states agree with the notions of a soft Coulomb gap, which were advanced in Refs. 2 and 3. We observed no trace of a polaron effect in either the density of states or in the electric conductivity.

It seems to us that computer research into the R model, using a large enough computer, can proceed along the following directions. First, it is necessary to lower the temperature for a more accurate determination of $\varepsilon_A(R)$. Second, the R model can be generalized to take into account simultaneous hops of several electrons. To this end it is necessary to admit of simultaneous hops the sum of whose hops does not exceed R.

The authors thank A. A. Fursenko for organizational help which permitted so large a volume of computer calculations.

[1)]We used a Roberton EC-1055M computer, whose large working memory and reliability compensate to a considerable degree its slow speed (about 0.5 MFLOPS).

[1]N. F. Mott, J. Non-Cryst. Sol. **1**, 1 (1968).
[2]B. I. Shklovskiĭ and A. L. Efros, *Electronic Properties of Doped Semiconductors*, Springer, 1984.
[3]A. L. Efros and B. I. Shklovskiĭ, J. Phys. C8, L49 (1975).
[4]A. L. Efros, V. L. Nguyen, and B. I. Shklovskiĭ, Sol. St. Comm. **32**, 851 (1979).
[5]V. L. Nguyen, Fiz. Tekh. Poluprov. **18**, 335 (1984) [Sov. Phys. Semicond. **18**, 207 (1984)].
[6]A. Möbius, J. Phys. **18**, 4639 (1985).
[7]G. Timp, A. B. Fowler, A. Harstein, and P. N. Butcher, Phys. Rev. **33**, 1499 (1986).
[8]M. Pollak and M. Ortuno, *Electron-Electron Interactions in Disordered Systems*, A. L. Efros and M. Pollak, eds. North-Holland, 1985.
[9]S. D. Baranovskiĭ, A. L. Efros, and B. I. Shklovskiĭ, J. Phys. **C12**, 1023 (1979).
[10]J. H. Davies, P. A. Lee, and T. M. Rice, Phys. Rev. **B49**, 758 (1982).
[11]S. D. Baranovskiĭ, A. A. Uzakov, and A. L. Efros, Zh. Eksp. Teor. Fiz. **83**, 756 (1982) [Sov. Phys. JETP **56**, 422 (1982)].
[12]E. I. Levin, V. L. Nguyen, and A. L. Efros, Fiz. Tekh. Poluprov **16**, 815 (1982) [Sov. Phys. Semicond. **16**, 523 (1982)].
[13]E. I. Levin, V. L. Nguyen, and B. I. Shklovskiĭ, Zh. Eksp. Teor Fiz. **82**, 1591 (1982) [Sov. Phys. JETP **55**, 921 (1982)].
[14]E. I. Levin, Candidate's dissertation, Leningrad Physicotech. Inst., 1984.
[15]L. Fleishman, D. C. Licciardello, and P. W. Anderson, Phys. Rev. Lett. **40**, 1340 (1978).

Translated by J. G. Adashko