The resistor network model in the theory of hopping conductivity

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The existing theory of hopping conductivity is based on Miller and Abrahams's equivalent-resistor-network concept, which is a result of the mean-field approximation. In fact, the forbidding of two electrons to occupy the same site leads to the Hubbard current correlations, the description of which falls outside the limits of the mean-field method. It is well known that the Hubbard current correlations alter significantly the hopping-electrical-conduction activation energy for classical periodic systems, e.g., superionic crystals. In the present paper the role of the Hubbard current correlations in disordered sytems, such as lightly doped crystalline and amorphous semiconductors, is investigated. The hopping conductivity of such a system is calculated with the aid of a computer in two ways: from first principles by the Monte-Carlo method and with the aid of the Miller-Abrahams network in accordance with Kirchhoff's rules. A comparison of the results of these calculations reveals the effects of the Hubbard current correlations. But it turns out that these effects are relatively weak, and cannot significantly affect the exponential dependences found through the use of the Miller-Abrahams network for the hopping conductivity. The weakness of the effects of the Hubbard current correlations in a disordered system is explained on the basis of the exact description of the Hubbard current correlations for four-impurity chains.

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1. INTRODUCTION

The electrons in lightly doped semiconductors are localized on the individual donors (we are, for definiteness, discussing n-type semiconductors), and the low-temperature conduction has a hopping character. The repulsion energy for two electrons on the same donor (the Hubbard energy) is usually very high. Therefore, if the semiconductor is compensated, i.e., if it contains a certain number of acceptors and the same number of unoccupied donors, then at low temperatures the electrons largely hop from the occupied to the unoccupied donors, and the large Hubbard energy merely forbids two electrons to be on the same donor. With allowance for this exclusion, the current flowing between the donors i and j has the form

$$I_{ij}=-e[\gamma_{ij}\langle n_i(1-n_j)\rangle-\gamma_{ji}\langle n_j(1-n_i)\rangle]=I_{ij}^{MF}+I_{ij}^{c}, \tag{1}$$

$$I_{ij}^{MF}=-e[\gamma_{ij}f_i(1-f_j)-\gamma_{ji}f_j(1-f_i)], \tag{2}$$

$$I_{ij}^{c}=-e(\gamma_{ji}-\gamma_{ij})(\langle n_in_j\rangle-f_if_j). \tag{3}$$

The occupation number n_i has the value 1 if the donor i is occupied and 0 if it is vacant; the angle brackets denote averaging over the time; $f_i=\langle n_i\rangle$ is the mean population of the i-th donor; γ_{ij} is the probability for transition of an electron from the i-th to the j-th donor in unit time (i.e., $\gamma_{ij}dt$ is the probability for transition in the time dt); e is the absolute value of the electron charge. For simplicity, we neglect the interaction between electrons on different donors. Under such conditions the electron energies ε_i and ε_j on the i-th and j-th donors do not depend on the occupation numbers of the other donors, and, consequently, γ_{ij} and γ_{ji} do not depend on the time. A customary approximation made in the theory of hopping conductivity, which may be called the mean field approximation, consists in the replacement of the quantities n_i by the f_i, i.e., the neglect of the occupation-number correlations. Then the current is given by the formula (2). Within the framework of this approximation, we can, as is well known,[1] associate with the pair of donors i and j the resistance

$$R_{ij}=kT/e^2\Gamma_{ij}, \tag{4}$$

Here

$$\Gamma_{ij}=\gamma_{ij}^0f_i^0(1-f_j^0)=\gamma_{ji}^0f_j^0(1-f_i^0),$$

(γ_{ij}^0 is the $i\to j$ transition probability in the absence of an electric field and f_i^0 is the equilibrium Fermi population function) is the equilibrium rate of $i\to j$ and $j\to i$ transitions. After this, the problem reduces to the problem of computing the conductivity of an equivalent resistance (R_{ij}) network, which was first introduced by Miller and Abrahams (MA). This is done either by percolation-theory methods,[1] or by a direct computer calculation with the Kirchhoff laws.[2]

But what is the effect of the correlation correction to the current I_{ij}^c on the hopping conductivity? At equilibrium n_i and n_j fluctuate independently ($\langle n_in_j\rangle=f_if_j$), and the correlation correction to the current is equal to zero. But if there is an external electric field, and a current flows through the pair (i,j), then the correlator $\langle n_in_j\rangle$ should not, generally speaking, split up. The difference $\langle n_in_j\rangle-f_if_j$ may turn out to be proportional to the external field, and then the term I_{ij}^c may not be less important than I_{ij}^{MF}. The presence of the current I_{ij}^c is clearly due to the fact that the motion of each electron is correlated with the motion of the others owing to the fact that it is forbidden for two electrons to be on the same donor. Therefore, we call such correlations the Hubbard current correlations (HCC). It follows from the expressions (1)–(3) that the HCC are unimportant in the presence of strong or weak compensation, when the overwhelming majority of the numbers n_i are each equal to zero or unity. Finally, it is clear that, when the temperature is so high that we have, on the basis of the detailed-balance relation

$$\gamma_{ji}=\gamma_{ij}\exp[(\varepsilon_j-\varepsilon_i)/kT]$$

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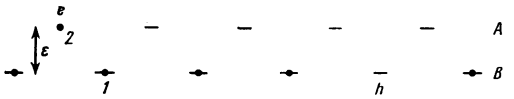

FIG. 1. Richards' AB model (e is an "electron"; h, a "hole").

$\gamma_{ij} \approx \gamma_{ji}$, the correction I_{ij}^C is equal to zero, and the HCC are unimportant. But they can play an important role at intermediate levels of compensation and at sufficiently low temperatures.

The HCC problem for ordered systems has been considered before in connection with the question of the ionic-electrical-conduction activation energy for superionic crystals.[3,4] The problem is especially clearly formulated by Richards.[4] He considers a chain of two sublattices, A and B (Fig. 1), differing in their site energies: $\varepsilon_A + \varepsilon_B + \varepsilon$ (we shall assume that $\varepsilon \gg kT$). A charged classical particle can hop from one site of the chain to the next one, the hopping probabilities γ_{AB} and γ_{BA} being connected by the relation $\gamma_{AB} = \gamma_{BA} \exp(\varepsilon/kT)$. The interparticle interaction is taken into account only in terms of the exclusion of two particles from simultaneously occupying the same site. For this problem, the self-consistent field approximation, which is equivalent to the use of the formulas (2) and (4), clearly yields $\sigma \propto \exp(-\varepsilon/kT)$. Richards, however, shows that, when allowance is made for the HCC, and the number of particles is equal to half the number of sites, so that all the type-B sites are occupied in the ground state, the electrical conductivity of the chain is much lower, it having the form

$$\sigma \propto \exp(-3\varepsilon/2kT). \tag{5}$$

Physically, the decrease in the electrical conductivity is due to the fact that, at low temperatures, a particle that has moved, say to the right, from a B site to an A site cannot, as a rule, move further to the right because the next B site is occupied, and should return to the original B site (a "traffic-jam" effect). Let us give a simple explanation of the result (5)—one very close to Richards'. The simplest charged excitations of Richards' AB chain are the "electron" and the "hole" (Fig. 1). Let us consider the contribution of the electrons to the conductivity $\sigma = ne\mu_e$, where n is the concentration of the electrons and μ_e is their mobility. It is clear that $n \propto \exp(-\varepsilon/2kT)$ in the intrinsic semiconductor. On the other hand, for the electron to move to the right, the particle 1 should rise from the B site to the A site and the particle 2 should drop into its place. Therefore, $\mu_e \propto \exp(-\varepsilon/kT)$, and we arrive at the formula (5). From these same arguments it appears that the result (5) is valid also for two- and three-dimensional lattices.[5]

The formula (5) demonstrates that the effect of the HCC on the electrical conductivity can be very strong. The object of the present paper is to investigate this effect for donors randomly disposed in space in the case of some prescribed distribution of their energies ε_i, i.e., for the hopping conductivity of lightly-doped and amorphous semiconductors. In this case the quantities γ_{ij} have the form

$$\gamma_{ij} = \gamma_0 \exp\left(-\frac{2r_{ij}}{a}\right) \begin{cases} N\left(\frac{\tilde{\varepsilon}_i - \tilde{\varepsilon}_j}{kT}\right) + 1, & \tilde{\varepsilon}_j < \tilde{\varepsilon}_i \\ N\left(\frac{\tilde{\varepsilon}_j - \tilde{\varepsilon}_i}{kT}\right), & \tilde{\varepsilon}_i < \tilde{\varepsilon}_j \end{cases}, \tag{6}$$

while the resistance R_{ij} for $kT \ll \varepsilon_{ij}$ is, according to (4), equal to

$$\begin{aligned} R_{ij} &= R_0 \exp \xi_{ij}; \\ \xi_{ij} &= 2r_{ij}/a + \varepsilon_{ij}/kT, \ R_0 = kT/\gamma_0 e^2, \\ \varepsilon_{ij} &= {}^1/_2(|\varepsilon_i - \mu| + |\varepsilon_j - \mu| + |\varepsilon_i - \varepsilon_j|). \end{aligned} \tag{7}$$

Here r_{ij} is the distance between the i-th and j-th donors; a is the Bohr radius, which is much smaller than the characteristic r_{ij} values; $N(x) = (e^x - 1)^{-1}$ is the Planck distribution function; $\tilde{\varepsilon}_i = \varepsilon_i + e\mathbf{E} \cdot \mathbf{r}_i$ is the energy of the i-th site in the electric field E; and μ is the Fermi level at $T = 0$. According to (6) and (7), the quantities γ_{ij} and R_{ij} fluctuate strongly from donor pair to donor pair. The HCC problem for such systems was first formulated by one of the present authors (B.I.S.) and Efros.[1] But the results obtained by Richards[4] could not be generalized to the case of disordered systems, since the method proposed by him is very complicated. To find the stationary current in a constant electric field, we must write down the stationarity conditions for the multinode distribution function $F\{n_i\}$, which is the probability for realizing a given set $\{n_i\}$ of occupation numbers.

This infinite set of equations becomes greatly simplified when we go over to the case of the AB chain. This simplification is due not only to the periodicity of the chain, but also to the invariance of the chain under reversal of the external field. Disordered systems, which are of interest to us here, do not possess this symmetry, and we could not make way in the investigation of the infinite chain of equations. Therefore, we undertook to study analytically the HCC in very short chains, specifically, in four-donor chains, where the investigation of the system of stationarity equations can easily be carried out to the end. The study shows that, because of the disordered state of the system, the HCC should have a slight effect on the electrical conductivity. Since the investigation of short chains does not have a strong demonstrative force, we performed, using the Monte Carlo method, a computer simulation of the hopping conduction of a cube containing 800 donors. Random donor-to-donor transitions of the electrons in the electric field were "tossed" in accord with the probabilities (6) and with allowance for the fact that two electrons are not allowed to occupy the same donor. On the other hand, using the Kirchhoff laws, we calculated the electrical conductivity of the MA resistor network for exactly the same system with the aid of a computer. The difference between the results of these calculations is, by definition, due to the effect of the HCC. We were able to find the effect of the HCC on the hopping conductivity, but it turned out that even at the lowest temperatures investigated by us the HCC decrease the electrical conductivity by roughly a factor of two, with the argument of the exponential hopping-conductivity function changing by only 3%. This means that we can, in the theory of the exponential hopping-conductivity functions, neglect the HCC and use the MA network.

2. THE FOUR-DONOR CHAIN

Let us consider a linear chain consisting of four donors, 1, 2, 3, and 4, in which transitions can occur only between neighboring impurities. We shall assume that an electrochemical potential difference exists across the chain, i.e., between the end donors 1 and 4. We shall also assume that the occupation numbers of the end donors 1 and 4 do not fluctuate, and are equal to their mean values. This assumption corresponds to the fact that these donors very often exchange electrons with the metallic contacts. We can also imagine that, for example, instead of the donor 1, we have many entirely identical donors located close to each other. Then the mean occupation number of these donors, which determines the $1 \to 2$ transition rate, will not fluctuate. In both interpretations it is clear that the donors 1 and 4 in the chain under consideration play the role of contacts. The chain is completely described by the probabilities $F(n_2, n_3)$ for the four combinations of the occupation numbers of the impurities 2 and 3: $F(0,0)$, $F(1,0)$, $F(0,1)$, and $F(1,1)$. The sum of these probabilities is equal to unity, so that there are three independent quantities, as which we can choose the single-node distribution functions

$$f_2 = F(1,0) + F(1,1), \quad f_3 = F(0,1) + F(1,1)$$

and the quantity $F(1,1)$. The stationarity conditions for these quantities give three equations for their determination:

$$I_{12}^{MF} = I_{23}^{MF} + I_{23}^{C} = I_{34}^{MF}, \tag{8}$$

$$\frac{dF(1,1)}{dt} = -[\gamma_{21}(1-f_1) + \gamma_{34}(1-f_4)]F(1,1) + \gamma_{12} f_1 [f_3 - F(1,1)] + \gamma_{43} f_4 [f_2 - F(1,1)] = 0. \tag{9}$$

Under steady-state conditions $F(1,1) = \langle n_2 n_3 \rangle$, and Eq. (9) yields the relation

$$\langle n_2 n_3 \rangle - f_2 f_3 = (f_3^0 - f_2^0) I_{12}^{MF} \Omega^{-1}, \tag{10}$$

where

$$\Omega = \gamma_{21}^0 (1-f_1^0) + \gamma_{34}^0 (1-f_4^0) + \gamma_{12}^0 f_1^0 + \gamma_{43}^0 f_4^0. \tag{11}$$

Substituting (10) into (3), we obtain

$$I_{23}^{C} = -C I_{12}^{MF}, \tag{12}$$

where

$$C = (\gamma_{23}^0 - \gamma_{32}^0)(f_3^0 - f_2^0)\Omega^{-1}. \tag{13}$$

Since we are interested in the ohmic current, we have written the formulas (11) and (13) in the zeroth order in E, i.e., we have replaced the quantities f_i and γ_{ij} by their values f_i^0 and γ_{ij}^0 in zero field. At the same time, the expressions for the currents I^{MF} in (8), (10), and (12) contain the values of these quantities in the electric field, and, what is more, the functions f_i are not equal to the values that they would have in the mean field approximation, but are given by the solution to the system (8) and (9). It can be seen from (11) and (13) that $C \geq 0$, so that the HCC can only increase the resistance. Substituting (12) into (8), we find that

$$I_{23} = I_{23}^{MF} + I_{23}^{C} = I_{12}^{MF} = I_{23}^{MF}(1+C)^{-1} = U_{23}/R_{23}(1+C), \tag{14}$$

where U_{23} is the electrochemical potential difference between the donors 2 and 3.

Thus, with allowance for the HCC, the resistance of the entire network is equal to

$$R_{12} + R_{23}(1+C) + R_{34}, \tag{15}$$

and not $R_{12} + R_{23} + R_{34}$, as obtains in the mean field approximation. To estimate the importance of the HCC, let us compute the quantity C in some examples. Let us first consider the tetrad, for which

$$r_{12} = r_{23} = r_{34} = r; \quad \varepsilon_1 = \varepsilon_3 = \mu - \varepsilon/2; \quad \varepsilon_2 = \varepsilon_4 = \mu + \varepsilon/2, \tag{16}$$

and, consequently, for $kT \ll \varepsilon$

$$\gamma_{21} = \gamma_{23} = \gamma_{43} = \gamma_0 \exp(-2r/a), \quad \gamma_{12} = \gamma_{32} = \gamma_{34} = \gamma_0 \exp(-2r/a - \varepsilon/kT), \tag{17}$$

$$R_{12} = R_{23} = R_{34} = R = (kT/\gamma_0 e^2) \exp(2r/a + \varepsilon/kT). \tag{18}$$

Substituting (17) into (11) and (13), we find that $C = \frac{1}{2}\exp(\varepsilon/2kT)$. Thus, the resistance of the chain is equal to $R(3 + \frac{1}{2}\exp \varepsilon/2kT)$, i.e., for $T \to 0$ it, like (5), has an activation energy equal to $\frac{3}{2}\varepsilon$. This coincidence is not surprising, since we are dealing in this example with a portion of the AB chain.

For hopping conduction in a system of randomly disposed donors, it is interesting to consider a tetrad in which r_{12}, r_{23}, and r_{34} are different. Of special interest in this case is the investigation of tetrads in which the resistance $R_{23} \gg R_{12}, R_{34}$. The point is that in the theory based on the MA network and the percolation method the hopping conductivity is determined by the percolation-ensuring critical resistor network, whose electrical conductivity is, in its turn, determined by the relatively widely spaced "critical" resistors having the highest resistances in the network.[1] Therefore, of greatest interest in connection with the computation of the resistivity of the whole network is the effect of the HCC on the critical resistance.

Let us first consider the case of relatively high temperatures, when $\varepsilon_{ij}/kT \ll 2r_{ij}/a$ for typical pairs, and the conductivity possesses an activation energy of ε_3. In this case the length of a critical resistor is close to the percolation radius $r_c \approx 0.87 N^{-1/3}$ (N is the donor concentration), and the resistors on both sides of it have smaller lengths r_{ij}. In order to simulate such a situation, we can consider a set of four donors in which $r_{23} > r_{12}, r_{34}$, with $R_{23} \geq R_{12}, R_{34}$ at the same time. Substituting the corresponding γ_{ij} into (11), and using the inequality $\varepsilon_{ij}/kT \ll 2r_{ij}/a$, we easily verify that in this case

$$C \propto \exp[-(2/a)(r_{23} - \max\{r_{12}, r_{34}\})] \ll 1.$$

Thus, in such a situation the role of the HCC is very minor. The physical cause of this lies in the fact, because of the inequalities

$$\gamma_{12}, \gamma_{21}, \gamma_{34}, \gamma_{43} \gg \gamma_{23}, \gamma_{32}$$

the deviation of the correlator $\langle n_2 n_3 \rangle$ from $f_2 f_3$ is actively disrupted by the transitions $1 \rightleftarrows 2$ and $3 \rightleftarrows 4$. It can be said that in this case the metallic contacts are, as it were, drawn out to the donors 2 and 3, and liquidate all the correlation effects.

In the present critical network, there are, of course, no metallic contacts, i.e., donors on which the number n_i does not fluctuate at all. But the critical resis-

tors are separated by clusters of relatively highly conducting resistors, that contain donors with energies close to the Fermi level. The transitions from a critical resistor to such a cluster should destroy the correlation for this resistor. Thus, the role of the HCC can be expected to be minor in the ε_3-conduction region.

In the region of lower temperatures where $\varepsilon_{ij}/kT \gg 2r_{ij}/a$ for typical neighbors, only the states with energy in the band close to the Fermi energies participate in the electrical conduction. The temperature dependence of this electrical conductivity (without allowance for the electron–electron interaction on the various donors) is given by the Mott law:

$$\sigma=\sigma_0 \exp\{-(T_0/T)^{1/4}\}, \quad T_0=\beta/ga^3, \tag{19}$$

where g is the density of states at the Fermi level and β is a numerical coefficient. In the region of the Mott law a critical resistor can differ from its neighbors by having a large r_{ij} value. Then, as in the ε_3 region, the HCC do not change the magnitude of the critical resistance. There is, in principle, another possibility which can be simulated on a set of four impurities. Let, for example,

$$\varepsilon_1=\varepsilon_4=\mu, \quad \varepsilon_2=\mu+\varepsilon/2, \quad \varepsilon_3=\mu-\varepsilon/2, \quad r_{23}<\min\{r_{12}, r_{34}\},$$

but $R_{23}>R_{12},R_{34}$, so that R_{23} plays the role of a critical resistance. Substituting these parameter values into (13) and (15), we find that the resistance of such a chain is

$$R_{12}+R_{34}+R_{23}(1+{}^1/_2 \exp[(2/a)(\min\{r_{12}, r_{34}\}-r_{23})]),$$

i.e., in this case the HCC sharply increases the resistance. This occurs because the correlations are produced by the transitions occurring at the rate γ_{23}^0, which does not contain an energy factor, and is much higher than the rate $\Omega \approx \gamma_{43}^0+\gamma_{21}^0$ at which the correlations are resolved. It is clear that such tetrads appear around critical resistors as a result of the simultaneous fulfillment of several requirements, so that the fraction of critical resistors for which the HCC are important is apparently small. To estimate the role of the tetrads that cause an increase in the resistance, we simulated on a computer tetrads having a critical resistance at their center and lower resistances at their ends.

In order to simulate the situation obtaining in the region of action of the law (19), we generated the energies of each of the four donors in such a way that they were uniformly distributed in the interval from $-\xi_c kT$ to $\xi_c kT$; and the distances r_{12}, r_{23}, and r_{34}, in such a way that they were uniformly distributed in the range from 0 to $\frac{1}{2}a\xi_c$ (Ref. 1), where ξ_c is the index of the exponential function (7) for the critical resistance. Then out of these tetrads were chosen only those for which ξ_{23} is close to ξ_c and ξ_{12}, $\xi_{34}<\xi_{23}$ (there were 5000 of them). Using (13), we computed the quantity C for them, and averaged the quantity $\ln(1+C)$ with the weight $(r_{12}r_{23}r_{34})^2$ on the lines of the percolation theory of perturbations.[1] It turned out that

$$\langle \ln(1+C)\rangle \approx 0.01\xi_c,$$

i.e., on the basis of the analysis of the tetrads, the effect of the HCC should be weak. But, bearing in mind the importance, in principle, of the question of the HCC, we could not be satisfied with the tetrad simulation, and performed hopping-conductivity calculations for a large block of donors, using the Monte Carlo method and Kirchhoff's laws.

3. HOPPING-CONDUCTION SIMULATION BY THE MONTE CARLO METHOD

The idea of the simulation of hopping conduction by the Monte Carlo method is this: Taking a specific realization of the randomly distributed donors, and prescribing a value for the field E, we "toss," during a certain period of time, random electron transitions between the donors in accordance with the probabilities (6). Then the current density $j(t)$, averaged over a time interval $(t, t+\delta t)$ covering many transitions, can be computed from the formula $j=\delta P/\delta t$, where δP is the change that occurs in the dipole moment of a unit volume of the system during this time. As for the electrical conductivity of the system, it is found as the ratio of the time-averaged value of $j(t)$ to E in the limit $E \to 0$.

The simulation of the hopping conduction in a system of randomly disposed donors by the Monte Carlo method has been performed by Marshall[6] and Imgrund and Overhof[7] for the situation in which the electrons are so few that each electron moves independently of the others. In our previous paper[8] we proposed a simulation procedure for a system in which the fact that two electrons cannot simultaneously occupy one donor is important. In the present investigation we used the same formulation of the problem and the same model used in Ref. 8, but we considered lower temperatures and used a different random-tossing algorithm for the electron transitions.

The program ran as follows. First, with the aid of a random-number generator we assigned the coordinates of $M=800$ donors uniformly distributed in a cube of volume $V=MN^{-1}$ (N is the donor density). Then we generated random energies ε_i lying in the interval from $-\Delta/2$ to $\Delta/2$ (Δ is the impurity-band width). The initial occupation numbers n_i were randomly chosen such that the number of donors occupied by electrons was equal to $(1-K)M$ (K is the degree of compensation), while the probability for realization of the set $\{n_i\}$ was proportional to $\exp\{-(1/kT)\Sigma n_i\varepsilon_i\}$. We assumed the presence of an electric field E applied perpendicularly to one of the cube faces along the x axis, and computed the energies of the donor levels in the field from the formula $\bar{\varepsilon}_i=\varepsilon_i+eEx_i$. We assumed periodic boundary conditions along the x axis, i.e., we assumed that the cube has through the gluing together of the faces $x=0$ and $x=L$ (L is the length of the cube edge) been transformed into a torus in which an eddy electric field and, consequently, an eddy electric current exist (for details see Ref. 8).

For the "tossing" of the random donor-to-donor electron jumps, the program first chose pairs of donors, the transitions between which were to be considered. For this purpose, the resistances (7) of all the donor pairs in the cube were computed, and $Q=4096$ pairs

with the lowest resistance were chosen, which corresponds to roughly 10 bonds per donor. Since percolation occurs in a three-dimensional random system when the average number of bonds per site is roughly equal to 2.7 (Ref. 1), and the spread in the resistance values is very large, the highest resistance computed turned out to be two-three orders of magnitude higher than the critical resistance. For this reason, a further increase in Q should not lead to a change in the electrical conductivity of the whole system. The probabilities γ_{ij} and γ_{ji} for each selected pair l consisting of the donors i and j were computed from the formulas (6) and stored, and the quantity

$$\gamma_l(t)=\begin{cases}0, & n_i=n_j\\ \gamma_{ij}, & n_i=1,\ n_j=0,\\ \gamma_{ji}, & n_i=0,\ n_j=1,\end{cases} \tag{20}$$

which has the meaning of the probability per unit time for transition in the l-th pair of donors with occupation numbers corresponding to the given moment of time t, was introduced. The quantity

$$W(t)=\sum_{l=1}^{Q}\gamma_l(t), \tag{21}$$

which has the meaning of the probability for the occurrence in unit time of some transition in the whole system, was also computed.

Further, the program repeated many times the following operations which we call the "program step:" 1) one of the Q pairs was selected in such a way that the probability of "hitting" the pair l was equal to $\gamma_l(t)W^{-1}(t)$; 2) an electron was transferred from the unoccupied to the occupied donor in the pair l [according to (20), the situation in which $n_i=n_j$ is excluded]; 3) the change δP_x occurring in the dipole moment of the cube as a result of the electron transfer was computed and stored (see Ref. 8); 4) the time spent by the system in making this transition was computed from the formula $\delta t=W^{-1}(t)$, and the time that had passed since the beginning of the calculation was increased by δt[1]; 5) the set of $\gamma_l(t)$ values and the quantity $W(t)$ were recalculated with allowance for the changed occupation numbers, and the program proceeded to the next step.

This is a standard scheme for the simulation of a Markov process with continuous time, and is widely used in the simulation of hot-electron kinetics,[9] the passage of radiation through matter,[10] and in other problems. Let us note that the realization of this algorithm as applied to our problem meets with serious computational difficulties connected with the large value of Q.

The simulation of the current should be sufficiently prolonged in order, on the one hand, for the transient process following the switching on of the field to end[8] and, on the other, for the effect of the thermal noise on the computed mean-current strength to be slight. For the lowest of the fields used in this investigation, the second requirement was significantly stricter. It can be shown that, in order for the error due to the noise in these fields to be less than 5%, the simulation time τ should be of the order of $1000\,\Gamma_c^{-1}$, where Γ_c is the equilibrium transition rate in the critical resistors.

The time required for the execution of one step of the program on the computer was roughly equal to 1.5 msec; therefore, during a reasonable time of about one hour the program was able to carry out $m\approx 3\times 10^6$ steps, which corresponds to a physical time of $T=m\langle W^{-1}(t)\rangle$. We can, by estimating the ratio T/τ, show that for typical data of our problem T is significantly shorter than τ. This is due to the fact that there exist in the cube fast pairs with an arm of the order of a and energies of the order of kT. For such pairs $\gamma_{ij}\sim\gamma_{ji}\sim\gamma_0\gg\Gamma_c$, and it is precisely these pairs that make the dominant contribution to the sum (21). Thus, the direct application of the above-expounded algorithm does not yet allow us to study the static conductivity of the system.

We found that a way out of this situation was to sharply "slow down" all the fast pairs. We chose some frequency Γ_{sup}, such that $\gamma_0\gg\Gamma_{sup}\gg\Gamma_c$, and reduced the probabilities γ_{ij} and γ_{ji} for all the pairs in which the equilibrium transition rate Γ_{ij} was higher than Γ_{sup} by the same factor, chosen such that Γ_{ij} became equal to Γ_{sup}. The resistance of the pairs that had been subjected to this procedure increased to $kT/e^2\Gamma_{sup}$, i.e., by several orders of magnitude, but this increase should not, on account of the inequality $\Gamma_{sup}\gg\Gamma_c$, affect the value of the resistance of the system as a whole. On the other hand, the sharp decrease of the transition rate in the fast pairs, which earlier made the dominant contribution to (21), enabled us to increase $\langle W^{-1}(t)\rangle$ very significantly, and thus achieve a satisfactorily fast run of the program. This method of cutting off the fast pairs relative to the equilibrium transition rate or, in other words, with the resistances, is a generalization of the cutoff used in Ref. 8 in the high-temperature case, relative to the pair arm. As for the reduction of the error in the result, it is advantageous to choose the smallest possible values for Γ_{sup}, but a further decrease of Γ_{sup} when it is close to Γ_c leads to an increase in the resistance of the system as a whole, i.e., to a distortion of the physical results. We regarded as optimum that value of $\Gamma_{sup}\equiv\Gamma_{opt}$ at which the resistance of the system as computed within the framework of the MA equivalent network model (see Sec. 4) differed from its value in the limit $\Gamma_{sup}\to\infty$ roughly by 5%.

The abandonment of the simple algorithm used in Ref. 8 is due to specific difficulties encountered in the simulation of hopping conduction at low temperatures. The step of the program of the old algorithm consisted in the following: one of the Q pairs was chosen randomly and with equal probability, after which either a transition was produced with probability γ_l/γ_{max} in this pair, or nothing was done with probability equal to $(1-\gamma_l)/\gamma_{max}$, and the program proceeded to the next step. Here $\gamma_{max}=\max_{ij}\{\gamma_{ij}\}$. The overwhelming majority of the steps of this program turned out to be empty, since even after the cutoff with respect to the resistances the frequency γ_{max} was very high in comparison with the majority of the γ_l. The point is that at low temperatures the system is in a state close to the ground state, and the majority of the γ_l contain very small activation exponentials whereas γ_{max} is determined by the fastest downward transition. As a result, the number of steps needed in the old program to transfer one electron in-

creased exponentially with decreasing temperature. At the same time, the new algorithm transfers one electron in each step. Therefore, even though the processing time spent on one step in the new algorithm is approximately 20 times longer than the corresponding time for the old algorithm, at low temperatures the relative effectiveness of the new algorithm increases exponentially with decreasing temperature. For example, at $kT=\Delta/16$ (this case was investigated in both programs) the new algorithm runs 15 times faster.

4. COMPUTATION OF THE CONDUCTIVITY OF THE SYSTEM WITHIN THE FRAMEWORK OF THE MILLER-ABRAHAMS EQUIVALENT-NETWORK MODEL

For comparison with the Monte Carlo calculation, we computed the resistance of the MA network for exactly the same set of donor coordinates and energies ε_i, using the Kirchhoff laws. The computation was performed according to the Gauss-Seidel iterative scheme, and the main difference between our computation and the usual computations performed by this method (see, for example, Ref. 11) lies in the fact that, to get the system to be entirely identical with the one investigated by the Monte Carlo method, we assumed the same periodic boundary conditions, i.e., we introduced resistances connecting the donors located near the opposite faces of the cube. We assumed, for the same purpose, that the current could flow through only the $Q=4096$ lowest resistances, the higher resistances being broken, and that all the resistances R_{ij} lower than $kT/e^2\Gamma_{sup}$ had been replaced by resistances equal to $kT/e^2\Gamma_{sup}$. Thus, the difference between the σ values computed by the Monte Carlo method and the values computed with the aid of the MA network (we shall denote them by σ_{MA}) should be related only to the HCC.

To find the electrical conductivity of the system with the aid of the Kirchhoff equations, we usually (see, for example, Ref. 11) prescribe the applied voltage in the form of boundary conditions on the potential (at one contact all the potentials are equal to zero; at the other, to unity), and solve the Kirchhoff equations only for the inner sites. In the case of periodic boundary conditions such a formulation of the problem is not possible, and therefore we solved the Kirchhoff equations for a closed circuit of 4096 resistances, assuming that each resistance R_{ij} joining the donors i and j has series-connected to it an external-electric-field (E) produced emf

$$\varepsilon_{ij}=Ex_{ij}, \quad x_{ij}=x_j-x_i+\eta L,$$

where $\eta=0$ if the resistor does not intersect the face $x=L$, $\eta=1$ if the resistor intersects this face in the positive direction, $\eta=-1$ if the face is intersected in the negative direction. In an inhomogeneous system there arise additional potentials V_i on the donors as a reaction to the uniform external field E. Using the expression for the current flowing from i to j:

$$I_{ij}=(V_i-V_j+\varepsilon_{ij})R_{ij}^{-1}, \tag{22}$$

we find for the V_i from Kirchhoff's first law the expression

$$V_i=\sum_j (V_j-\varepsilon_{ij})R_{ij}^{-1}\Big/\sum_j R_{ij}^{-1}, \tag{23}$$

where the summation is performed over all the neighbors of the i-th donor, that are connected with it by unbroken resistances. The formula (23) served as the basis of the iterative procedure for finding the potentials V_i, starting from the values $V_i=0$. Otherwise, we entirely followed the algorithm of Ref. 11.

After determining all the potentials V_i, we found the averaged—over the cube—current density j and the conductivity $\sigma=j/E$. Since in the case of highly inhomogeneous systems the iterations converge slowly, we began the procedure with small Γ_{sup} values (a small Γ_{sup} makes the system artificially more homogeneous). When the iterations for the given Γ_{sup} converged, we went over to a higher Γ_{sup} value, using the already computed V_i values as the initial approximation. The value of Γ_{sup} was increased until the conductivity ceased to depend on it. The thus obtained Γ_{sup} dependence of the conductivity was used to select the optimal value of $\Gamma_{sup}\equiv\Gamma_{opt}$ for the simulation program using the Monte Carlo method (see Sec. 3). A comparison of the calculation by the Monte Carlo method and the calculation with the aid of the Kirchhoff laws was carried out for $\Gamma_{sup}=\Gamma_{opt}$.

5. RESULTS OF THE CALCULATIONS AND DISCUSSION

The calculations were performed largely for one random set of coordinates and energies of the 800 donors with the parameter values $K=0.5$ and 0.05 and $2r_c/a=8$ and 15. Several values of the temperature in the region $\Delta\geq kT\geq\Delta/50$ were investigated. After determining by the Monte Carlo method the mean value of the current for fixed T and E, we computed $\sigma(T,E)=j(T,E)/E$. To find the dc value of $\sigma(T)\equiv\sigma(T,0)$, we computed $\sigma(T,E)$ for several E values satisfying the condition $e|E|N^{-1/3}\leq kT$. In an infinite block $\sigma(E)=\sigma(-E)$, and it

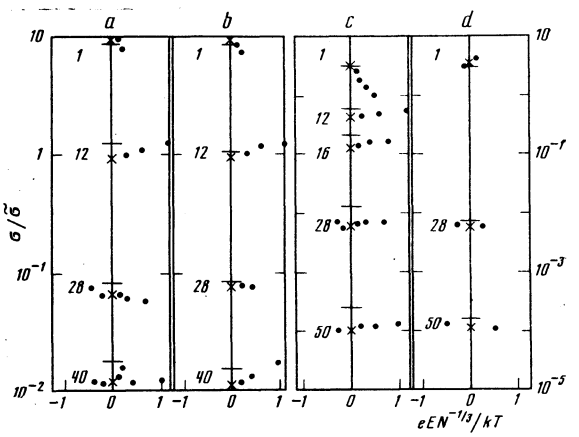

FIG. 2. Dependence of the conductivity (in units of $\tilde{\sigma}$) on the parameter $eEN^{-1/3}/kT$ for different values of T, K, and $2r_c/a$: a) $2r_c/a=8$, $K=0.5$; b) $2r_c/a=8$, $K=0.05$; c) $2r_c/a=15$, $K=0.5$; d) $2r_c/a=15$, $K=0.05$. The points represent the data obtained by the Monte Carlo method; the crosses represent the extrapolations of the data to $E=0$; the horizontal dashes at $E=0$ indicate the values of $\tilde{\sigma}_{MA}$. The value of the parameter Δ/kT is indicated on the graph near each set of points. The scale marked on the left pertains to the graphs a) and b); the scale on the right, to c) and d).

would not have been necessary to perform calculations for negative E values. A finite sufficiently small block does not possess such a symmetry, and the calculations for negative E values enable us to find the dc value of the electrical conductivity more accurately. Figure 2 shows the dependence of $\sigma(T,E)/\tilde{\sigma}$ on the parameter $eEN^{-1/3}/kT$ for different temperatures. The dashes on the ordinate axis, i.e., at $E=0$, indicate the values of $\sigma_{MA}(T)/\tilde{\sigma}$, where $\sigma_{MA}(T)$ is the value of the electrical conductivity for the same temperature in exactly the same object, but computed with the Kirchhoff laws for the MA network. Here

$$\tilde{\sigma}\left(K,\frac{2r_c}{a}\right)=K(1-K)\left(\frac{2r_c}{a}\right)^{-\nu}\frac{e^2N^{1/3}}{\Delta}\gamma_0\exp(-2r_c/a) \qquad (24)$$

is the characteristic electrical conductivity and $\nu\approx 0.9$ is the critical exponent of the correlation length. The use of the quantity $\tilde{\sigma}$ to normalize the electrical conductivities $\sigma(T,E)$ and $\sigma_{MA}(T)$ is convenient because, according to percolation theory (see Refs. 1 and 8), for the hopping conductivity with the probabilities (6) the electrical conductivity at $kT\gg\Delta$ is equal to $4.48\tilde{\sigma}$, where A is a number of the order of unity.

The error in the data shown in Fig. 2 does not, according to our estimates, exceed 10%. We could not advance into the region of low fields with the aid of the Monte Carlo method, since the error increased in the process on account of the thermal noise. To find $\sigma(T)=\sigma(T,0)$, we must interpolate $\sigma(T,E)$ between the available values of E. In Fig. 2 the most probable—from our point of view—values of $\sigma(T)$ are indicated by crosses at $E=0$. The ratio $\sigma_{MA}/\sigma(T)$ as a function of Δ/kT is shown in Fig. 3.

Let us first consider the data for $K=0.5$ [Figs. 2(a) and 2(c)]. At high temperatures the HCC are, as they should be, entirely insignificant. When the temperature is lowered, the HCC decrease the conductivity, but not more than 2.3 times. Against the background of the exponential decrease of the electrical conductivity, this, of course, is very small, so that it can be stated that no significant changes similar to the results for the Richards AB model occur in the index of the exponential electrical-conductivity function.

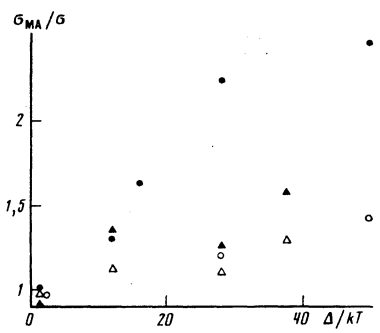

FIG. 3. Dependence of the ratio σ_{MA}/σ on the parameter Δ/kT for different values of K and $2r_c/a$: ▲) $2r_c/a=8$, $K=0.5$; △) $2r_c/a=8$, $K=0.05$; ●) $2r_c/a=15$, $K=0.5$; ○) $2r_c/a=15$, $K=0.05$.

It should be borne in mind that, for the energy distribution assumed in the present paper, the temperature starting from which the Mott law (19) should be applicable has, according to Ref. 1, the form

$$kT_c=0.29\frac{\Delta}{2}N^{1/3}a=0.25\Delta\left(\frac{2r_c}{a}\right)^{-1}, \qquad (25)$$

so that, for $2r_c/a=15$ and 8, the ratio $\Delta/kT_c=60$ and 32 respectively. This means that the point with $\Delta/kT=40$ and in practice the point with $\Delta/kT=28$ for $2r_c/a=8$ belong to the region of applicability of the Mott law. Thus, the HCC play a minor role in the Mott-law region as well. As we saw in Sec. 2, this is due to the fact that the system is disordered.

It can be seen from Figs. 2 and 3 that the effect of the HCC is stronger at $2r_c/a=15$ than at $2r_c/a=8$. This was to be expected, since the HCC should make to the index ξ_c of the exponential electrical-conductivity function a contribution $\Delta\xi_c$(HCC) that is proportional to ξ_c, and the value of ξ_c for $2r_c/a=15$ is significantly higher. On the basis of the data obtained by us, we can conclude that in the region of the Mott law $\Delta\xi_c(\text{HCC})\approx 0.03\xi_c$, i.e., three times greater than the rough estimate obtained in the analysis of isolated tetrads (Sec. 2).

In order to verify that we correctly understand the cause of the deviation of σ_{MA} from σ, we calculated σ and σ_{MA} for the case of slight compensation $K=0.05$. In this case, as the temperature is lowered, the Fermi level quite quickly becomes fixed near the energy 0.45Δ, and the electrical conductivity is realized in a gradually narrowing energy band. In contrast to the $K=0.5$ case, at not too low temperatures, this band is asymmetric about the Fermi level, and includes many more occupied states than empty ones. It follows from the analyses performed in Secs. 1 and 2 that the HCC can play a role only when many transitions occur between states lying on different sides of the Fermi level. In the case of strong band asymmetry such transitions are rare; therefore, the role of the HCC should be significantly smaller here than in the $K=0.5$ case. The computational results given in Figs. 2(b), 2(d), and 3 confirm these conclusions. The effects of the HCC for $K=0.05$ are two-four times weaker than the effects for $K=0.5$.

Thus far, we have been discussing the results obtained for one random set of coordinates and energies of 800 donors. It is natural to ask: What is the import of these results for a macroscopic sample? Can we consider them to be a stochastic property of the investigated set? It seems to us that we cannot. The point is that at the various temperatures and $2r_c/a$ values investigated by us the critical resistors and the tetrads containing them are entirely different, and we have, as it were, essentially independent sets to deal with. At the same time, at low temperatures $\Delta\xi_c$(HCC) has the order of magnitude $0.03\xi_c$ in all cases.

To verify directly the dependence on the random set, we investigated four other random sets for $K=0.5$, $2r_c/a=15$, $kT=\Delta/28$, and $eEN^{-1/3}/\Delta=\pm 0.005$. It turned out that the spread in the ratio σ_{MA}/σ for all the five sets does not exceed 20%. Thus, it can be assumed that the estimate ($\Delta\xi_c(\text{HCC})=0.03\xi_c$) obtained

by us for the effects of the HCC at low temperatures is valid for the majority of random donor-coordinate and energy sets and, consequently, for macroscopic samples.

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[1)]Strictly speaking, the lifetime of the system in the state in question is a random quantity, and, to stimulate the system correctly, we must use the expression $\delta t = -W^{-1}(t)\ln X$, where X is a random numerical variable whose values are uniformly distributed in the range from zero to unity. But we need the values of δt only for the computation of $t = \Sigma_i \delta t_i$. It is easy to show that the two methods of computing δt yield the same estimate for the physical time t, but the dispersion of the estimate obtained without $\ln X$ is smaller, and it is more economical in terms of machine time.

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