Variable-range-hopping in two-dimensional system.

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Computer modeling of the VRH conductivity in the two-dimensional system has been done by kinetic Monte Carlo method, which includes some new elements. Study of the temperature dependence of the conductivity, testing of the different scaling relations, and study of the size effect show that the Efros-Shklovskii mechanism of the VRH is valid in the slightest details. It has been also shown that simultaneous transitions of many electrons are not important. The reasons of disagreement with previous works are thoroughly analyzed.

The concept of the variable range hopping (VRH) of localized electrons belongs to Sir Mott [1]. He has considered the phonon assisted tunneling of localized electrons between different sites. Mott has found that the typical hopping length for a two-dimensional (2D) case \( R_M \approx (a/3)(T_M/T)^{1/3} \) increases with the decreasing temperature. This is the origin of the term “VRH”. Here \( T_M = \beta_M (g_0 a^2)^{-1} \), \( a \) is the localization length of an electron, \( g_0 \) is the density of states at the Fermi level, \( \beta_M \) is a numerical coefficient. The conductivity obeys the Mott’s law [1,2]

\[
\sigma_M \sim (\gamma e^2/T) \exp\left(- (T_M/T)^{1/3}\right),
\]

where \( \gamma \) is a typical phonon frequency of the order of \( 10^{12} \text{sec}^{-1} \).

Electron-electron interaction has added a new chapter to the theory of VRH. The study of the interaction in localized regime has been initiated by Pollak [6] and Srinivasan [7]. Later on Efros and Shklovskii [8] have shown that the single particle density of states (DS) in 2D case linearly tends to zero as energy tends to the Fermi energy. This phenomenon, which is called the Coulomb gap (CG), is due to the long range part of the Coulomb interaction which, in a sense, remains non-screened. At large disorder the DS \( G(\epsilon) = 2|\epsilon|/\pi e^4 \) has a universal form. The DS is given by the only combination of the energy and electron charge which has a proper dimensionality. In fact, the CG results from the Coulomb law and from the discrete nature of electron charge.

Simple arguments based upon single-electron excitations show that the VRH with the Coulomb interaction (CI) obeys Efros-Shklovskii (ES) law [8]

\[
\sigma_c \sim (\gamma e^2/T) \exp\left(- (T_0/T)^{1/2}\right),
\]

where \( T_0 = \beta_0 e^2/a \). The percolation approach (See references in [8]) gives \( \beta_M = 13.8, \beta_0 = 6.5 \). The hopping length \( R_C \approx (a/4)(T_0/T)^{1/2} \).

Many experimental works on the 2D structures report the ES law, but very often the data are ambiguous because one should have a really large interval of \( \sigma \) to distinguish between the two laws. We think that the most important results have been obtained recently by groups of Jiang and Dahm and Adkins [9]. Using an artificial screening provided by metallic electrode, parallel to a plane with the 2D electrons, they have proved that the VRH transport reflects the crucial feature of the CG, the sensitivity to the long range interaction.

The theoretical understanding of the VRH is controversial. Efros and Shklovskii argue that in 2D case only the single electron transition with the typical hopping length are important [10] and the VRH has the same universal nature as the CG. Pollak and his followers [11,13] claim that both sequential and simultaneous transitions of different groups of electrons are very important for the VRH, so that the physics of the CG which is valid for the long hops only is not relevant. These claims are based upon the theoretical idea that simultaneous transition of many electrons may provide a gain in the activation [10]. Computer simulations of the VRH and the similar phenomena made by this group also show importance of the many-electron transport both in 3D and 2D cases but no new T-dependence of the conductivity has been proposed. The simulation of our group [8] reveals scaling typical for the CG, but in this work a simplified model has been used which does not take into account any simultaneous transitions and underestimates sequential transitions with the short length.

We present here the results of computations which takes into account all the sequential transitions and the most important simultaneous transitions of two electrons. We show that the VRH both in the CI case and without interaction (M-case), closely obeys the laws Eqs. (2,3) and different scaling laws which reflect the physics of the both cases. We also confirm earlier prediction that simultaneous transitions of many electrons are not important for the VRH in 2D case at low temperatures and analyze the discrepancy with the simulations by Pollak group.

We consider the standard lattice model with the Hamiltonian

\[
H = \sum_i \phi_i n_i + \frac{1}{2} \sum_{i\neq j} \frac{1}{\nu_i} (n_i - \nu) (n_j - \nu),
\]

where \( n_i = 0,1 \) are the occupation numbers. The quenched random site energies \( \phi_i \) are distributed uniformly within the interval \([-1,1]\). \( \nu \) is the average occupation number which is taken to be 1/2 everywhere below. The magnitude of the quenched disorder is enough
to provide the universal CG at all energies important in our temperature range \[\begin{equation}
\end{equation}\]. Here and below the lattice constant is a length unit and the nearest Coulomb energy which is equal to the amplitude of the disorder is both energy and temperature unit. In the M-case the interaction term in Eq. (3) is neglected.

To simulate the VRH by the kinetic Monte Carlo (MC) method we add an electric field \( E \) and consider the periodic boundary conditions (See details in Ref \[\end{equation}\]). To get conductivity we calculate the dipole moment due to electron transitions in the \( E \)-direction and divide it by the number of MC steps and by \( E \). This assumes that our time unit is \( 1/\gamma \). We check that the result is \( E \)-independent. In fact we take \( E \) from the condition \( E R_{C,M} = 0.1T \). The array size is taken \( 100 \times 100 \) for the temperatures above 0.05 and \( 200 \times 200 \) for the temperatures below 0.05. In the first approximation we neglect simultaneous transitions of many electrons. The new element of our algorithm is that we do not include tunneling probability into MC process \[\begin{equation}
\end{equation}\]. Instead we choose a pair of sites \( i \) and \( j \) with the probability \( \exp(-2\epsilon ij / a) / Z_1 \), where \( Z_1 \) is the normalization factor. Then the transition is rejected if both sites are occupied or empty, and finally it is performed with the probability \( 1/(1 + \exp(-\epsilon ij / T)) \), where \( \epsilon ij \) is the energy difference between the two configurations. This new scheme dramatically decreases the runtime of the simulation and leads to \( L^2 \), rather than \( L^4 \), algorithm in number of MC steps. Note that for the CI-case each MC step consists of \( L^2 \) operation itself due to recalculation of site energies after each transition.

To test the origin of the VRH we check the scaling laws which reflect an intimate physics of both CI- and M-cases: \( T_0 \) and \( T_M \) respectively are the only characteristic temperatures (energies) in the problem. These laws can be written in the universal form

\[
\sigma_M = (\gamma e^2 / T_M) f_M(T_M / T),
\]

\[
\sigma_{CI} = (\gamma e^2 / T_0) f_{CI}(T_0 / T),
\]

where \( f_M(x) \) and \( f_{CI}(x) \) are some functions. It follows from the scaling laws Eq. (4) and the above definitions of \( T_M \) and \( T_0 \) that \( \sigma_M / a^2 \) and \( \sigma_{CI} / a \) are functions of \( Ta^2 \) and \( Ta \), respectively. Thus, if one changes both \( T \) and \( a \) in the M-case in such a way that \( Ta^2 \) is constant then \( \sigma_M / a^2 \) will be also constant. For CI-case one should change \( T \) and \( a \) keeping \( Ta \) constant to get \( \sigma_{CI} / a \) constant. This test has been successfully performed and the convincing results are shown in the inset of Fig.1. Note that the small deviation of \( \sigma / a^2 \) from the constant value for the M-case is due to the lattice effect. Since \( R_M < R_C \), the lattice effect in the M-case appears at larger \( a \) than in the CI-case.

In Fig.2 we present the results for the size effect in the CI-case. We have calculated the average value of the conductivity \( \langle \sigma \rangle = \sigma_L / \sigma_\infty \), where \( \sigma_L \) is the logarithmic average of the conductivity over arrays with different disorder at given \( L \) and \( T \), \( \sigma_\infty \) is the conductivity at the maximum \( L \) at a given \( T \). We have also calculated dispersion \( \text{dis} = \delta \sigma / \sigma \), where \( \delta \sigma \) is the dispersion of the conductivity and \( \sigma \) is the arithmetic average of the conductivity at given \( L \) and \( T \).

We did these computations not only to get an idea how large the size of an array should be to obtain the macroscopic value of the average conductivity and what value of the dispersion one should expect at a given \( L \) and \( T \). Another reason is that the \( L \)- and \( T \)-dependences of the average and the dispersion give us a new insight into the physics of the VRH. One can see from Fig. 2 that the dispersion is a function of only one argument \( TL \), as it follows from the ES theory. Indeed, the correlation length \( L_c \) of the percolation network is \( L_c = R_C(T_0 / T)^{\nu / 2} \). Since the exponent of the correlation length \( \nu = 1.33 \), one gets that \( L_c \) is very close to \( 1/T \). Thus, \( L / L_c \approx LT \).
which explains the $L$- and $T$-dependence of the dispersion.

The behavior of the average is completely different. It does not change until very low values of $TL$. At even smaller $TL$ it decreases dramatically and it is not any more a function of $TL$. We believe that it is a function of $L/R_{C1} \sim L\sqrt{T}$, and the decrease of the average conductivity appears due to the hard gap in the DS. It is known \[17\] that the hard gap between occupied and empty states results from the size effect and its value is of the order of $1/L$. At $L < R_C$ the energy stripe of the VRH is completely within this gap. We suggest that this is the reason of the decrease of the average conductivity. Fig. 2 confirms qualitatively this suggestion. Unfortunately, we are unable to check it quantitatively.

![FIG. 2. The size dependence of the dispersion (left axis, open symbols) and of the logarithmic average of the conductivity (right axis, solid symbols) at $T = 0.1$ ($\triangle, \filledtriangle$) and $T = 0.05$ ($\square, \bullet$) for the CI-case. Inset: the conductivity at the presence of the simultaneous transitions of two electrons for the CI-case. The contribution to the conductivity due to single hops (●) and due to double hops (○) at $a = 0.5$ should be compared. The conductivity with single hops only at $a = 1$ ($\square$) is also shown.](image)

Now we come to the simultaneous transitions of many electrons in the interacting system. We consider only two-electron transitions, which are the most important.

Suppose that in the initial state electrons occupy sites 1 and 3 and in the final state they are in the sites 2 and 4. The activation energy of this process $\epsilon_{1234}$ is the energy difference between the final and the initial states. Due to Pollak it may be smaller than the sum of the energies of the single-electron transitions. Moreover, the increase in the activation exponent may beat an extra tunneling exponent, which appears because of the tunneling of two electrons. That is why Pollak and his followers insist on many-electron processes.

First we calculate the probability of the process. Let us consider the case when $r_{12}, r_{34} \ll R$, where $R$ is the distance between pairs (1,2) and (3,4). Following Ref. \[14\] we concentrate on the single phonon transitions. It is obvious that these transitions only cannot provide anything but independent hops of electrons. The result is different if one considers the CI as well. We think that the amplitude of the most important process is described by the second order perturbation theory. It consists of a product of two matrix elements. The first one gives the electron transition in one of the close pairs, say (1,2), due to the phonon absorption without energy conservation. This element has a factor $\exp(-r_{12}/a)$. The system comes to the intermediate state, where sites 2 and 3 are occupied. The second element describes the transition of the second electron from 3 to 4 in the external electrostatic potential created by the dipole (1,2). This element has a factor $\exp(-r_{34}/a)$. The $R$-dependence is due to the dipole-dipole interaction. Use of the Golden rule gives the correct energy conservation law and a factor $\sim \exp(-2(r_{12} + r_{34})/a)/R^4$. The result is the same as for the Förster diffusion of molecular excitons \[13\], very similar but not identical problem. The transition rate used in Ref. \[11,13\] and many others is taken to be $R$-independent at large $R$. We cannot understand this result because to get the common energy conservation law one should assume that the remote pairs can “talk” to each other, which means there should be an interaction between them with some $R$-dependence. We argue below that the contradiction between our results originates from the $R$-dependence.

To accommodate this fast decay with $R$ we assume that the simultaneous transitions occurs only if the initial or final position of the second electron is within the spheres with the radii $R_C$ from the initial or final position of the first electron. Note that this assumption overestimates the role of the double electron transitions in the most important case when one electron makes a long hop $R_C$ and the other one makes a short hop. The interaction between such pairs decreases (as $1/R^2$) at distances smaller than $R_C$.

To simulate the double hop transport we use the same idea as for single hop case. This time, however, we choose a pair of sites $i$ and $j$ for single hop transition with the probability $p_1 = \exp(-2r_{ij}/a)/Z_2$, and sites $i$, $j$, $k$ and $l$ for double hop with the probability $p_2 = \exp(-2(r_{i2} + r_{k3})/a)/Z_2$, where $Z_2$ is found from the normalization condition for the sum of two probabilities.

If the double hop is chosen, we check the occupation for both pairs of sites $(i,j)$ and $(k,l)$ and then use the same Boltzman factor as before with $\epsilon_{ijkl}$ instead of $\epsilon_{ij}$. The algorithm is also $L^2$ in the number of MC steps. However, since the number of possible transitions of two electrons is much larger than the number of single transitions, one can show that there are $\approx 4R_C^2\exp(-2/a)$ attempts of double transition per one attempt of a single one, which makes simulation much more time consuming.
The contribution of single and double hops to the total conductivity can be separated by collecting their dipole moments in the different cells. We have checked that the single hop contribution does not change in the presence of double hops. The results of the simulation are shown on the inset of Fig.2. We are able to calculate double hop contribution for the case $a = 0.5$, because at larger $a$ the value of $R_C$ is too large. The single hop contributions are shown for both $a = 1, 0.5$. Note that a small deviation from the universal behavior at high temperatures is a result of the lattice effect for $a = 0.5$. One can see that the double hop contribution is from one to two orders of magnitude smaller than the single hop contribution at VRH region of temperatures. Moreover, the relative fraction of double hops in the total conductivity decreases with decreasing temperature. This result does not support Pollak's prediction $[10]$ of the gain in the activation energy for simultaneous transition of two electrons as compared with the single electron transition.

The computational data, obtained in the papers $[11, 13]$ and many other works of this group show the importance of the many-electron hops which contradicts to our result. In our opinion the $R$-independent probability of the simultaneous hops assumed by this group is responsible for the contradiction.

Indeed, if in a large array each pair has an equal probability to make a transition with any other $L^2$ soft pairs in the system the number of transitions for the pair per time is proportional to $L^2$. This is a giant overestimate of the role of many-electron transitions. The abnormal size effect should be a manifestation of this mistake. Unfortunately, we have found only one work $[12]$, where authors take care about the size effect and this work deals with the 3D case. However, we think that the infinite range interaction between pairs should provide the same effect in the 3D-case. Looking at Fig. 3 of Ref. $[12]$ one can see an exponential size effect without any signs of a saturation. The resistivity increases with the size because the algorithm include the selection of states with the highest transition rate among them. The selected states must consist of soft pairs which are far from each other and do not contribute to the dc conductivity.

Another reason for contradictions is that the method used in all these papers is applicable to the mesoscopic systems only. It consists of selecting a number of low-energy states of the total system to study transitions between them. It looks nice because it takes into account all many electron transitions, while we could afford the simultaneous transitions of two electrons only. The problem is in the necessary number of states, which provides reasonable thermodynamic and kinetic description. This number increases exponentially with the number of sites in the array. Due to the sensitivity of the CG to the long range interaction the size of the array $L$, which provides macroscopic regime, increases with decreasing $T$. One can estimate from Fig. 2 that $L \approx 3/T$ gives a reasonable dispersion. For example, $T=1/400$ is the middle of the temperature interval in Ref. $[1]$. It follows that $L$ should be at least 1000. Instead, authors compute few samples with different disorder at $L \approx 22$. These samples have very different values of conductivities and different patterns of the $T$-dependences (See Fig.1 of Ref. $[1]$. This is a typical mesoscopic result.

Finally, our computer simulation confirms the ES theory of the VRH transport in 2D systems and shows that the attempts of its revision have no ground.

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[1] N. F. Mott J. Non-Crystal. Solids 1,1 (1968).
[2] The derivation of preexponential factor can be found in Ref. $[3]$.
[3] E. I. Levin et al., Sov. Phys. JETP 85, 842 (1987).
[4] M. Pollak, Disc. Faraday Soc. 50, 13 (1970);
[5] G. Srinivasan, Phys. Rev. B, 4, 2581 (1971);
[6] A. L. Efros and B. I. Shklovskii, J. Phys. C, 8, L49 (1975).
[7] F. W. Van Keuls et al. Phys. Rev. B56, 13263 (1997); A. I. Yakimov et al. Phys. Rev. B61, 10868 (2000).
[8] Note that in 3D case the situation is much more difficult, but the law Eq. (2) should be still valid. See recent review A. L. Efros in Phase Transitions and Self-Organization in Electronic and Molecular Networks Ed. by J.C. Phillips and M.F. Thorpe (Kluwer Academic/Plenum Publishers, New York, 2001), p. 247.
[9] A. L. Efros and B. I. Shklovskii in Electron-Electron Interaction in Disordered Systems, Ed. by A.L. Efros and M. Pollak, (North-Holland, Amsterdam 1985) p.409.
[10] M. Pollak and M. Oruto, ibid p.287. The references to the original works can be found in this review.
[11] A. Perez-Garrido et al., Phys. Rev. B 55, 8630 (1997).
[12] A. Diaz-Sanchez et al., Phys. Rev. B 59, 910 (1999).
[13] K. Tenelsen, M. Schreiber, Phys. Rev. B 52,13287 (1995).
[14] F. G. Pikus, A. L. Efros, Phys. Rev. Lett. 73, 3014 (1994).
[15] This idea has been proposed by O. Biham (private communication).
[16] B. I. Shklovskii, A. L. Efros Electronic Properties of Doped Semiconductors (Springer-Verlag, Berlin 1984) p. 219
[17] S. D. Baranovskii et al. J. Phys. C 12, 1023 (1979).
[18] Förster Th. In: Modern Quantum chemistry, N.Y.,1965, pt3, p.93