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Low-temperature saturation of variable-range hopping and delocalization of electron states by entanglement with phonons in two dimensions

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We investigate low-temperature transport properties in a two-dimensional electronic system coupled with phonons. It is found that some of the localized states will be delocalized by the entanglement with phonons even when the temperature approaches the absolute zero. The distribution of phonons near the zero temperature is departed from the Boson distribution because the entangled states are preferred from the energy point of view. This leads to the low-temperature saturation of the variable-range hopping of electrons and the existence of a metal-like behavior in two dimensions.

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The metal-insulator transition in two-dimensional (2D) systems has been of great interest in the past two decades. Within the standard scaling theory, all carriers are localized in the absence of an external magnetic field.[1] Seven years ago, metallic behavior was observed in metal-oxide-semiconductor field-effect transitor.[2] Although the origin of this phenomenon is still in controversy, one school of thought believes that it is related to a crossover from the quantum to classical transport.[3–8] Thus, the understanding of this phenomenon will shed light on the bridge connecting classical and quantum physics and may introduce new concept on the transport in low dimensions. One mechanism leading to the transition from quantum to classical behavior is the inelastic scattering of electrons by phonons or other bosonic excitations, which eliminates the quantum coherence of electron wave functions. In early years the phonon-assisted transport of electrons has been studied by many authors. In his pioneering work, Mott has proposed variable-range hopping (VRH) model describing finite conductance of amorphous semiconductors at finite temperatures.[9] In this model the hoppings between quantum-mechanically localized states are assisted by phonons. Other authors have theoretically studied the delocalization effect of phonons in disordered systems.[10–13] This effect, however, has been shown to vanish at the zero temperature due to the usage of the Bose thermal distribution for free phonons in these studies. It is believed that at zero temperature the metal-insulator transition is still related to a quantum transition, and the 2D systems should have zero conductance in this sense. In VRH model, the classical-like processes connected with inelastic scattering vanish when approaching zero temperature, leading the the $T^{-1/3}$ divergence of the logarithmic resistance in two dimensions. Recently, the vanishing of classical-like behavior at zero temperature is questioned experimentally by the observations of the low-temperature saturation of the dephasing.[14] A theoretical calculation on quantum dot has shown that the inelastic scattering for the electron cannot vanish at zero temperature, leading to the saturation of the dephasing. This implies that the combined electron-phonon states, rather than the separated ones, are in equilibrium with the thermal bath.[15] In this paper, a 2D electronic system coupled with phonons is studied. We focus on the delocalization effect of phonons at the zero temperature. According to the Heisenberg uncertainty principle, the entanglement of electron and phonon states lowers the energy of the combined system. From this the VRH theory is extended to the case of temperature approaching the absolute zero by replacing the Bose distribution for free phonons with the thermal statistics of the coupled electron-phonon system. We argue that such kind of phonon-assisted mechanism can also saturate at very low temperatures, leading to the metal-like behavior.

At the beginning, let us consider a model Hamiltonian that describes the coupling between electrons and phonons in a 2D disordered system,

$$H=\sum_i \epsilon_i c_i^\dagger c_i+\sum_{\langle i,j\rangle}(c_i^\dagger c_j+\text{H.c.})+\sum_{i,q} g_{i,q} c_i^\dagger c_i(a_q^\dagger+a_q)+\sum_q \hbar\omega_q\left(a_q^\dagger a_q+\frac{1}{2}\right), \quad (1)$$

where c_i and $c_i^\dagger$ are electronic annihilated and creation operators for electrons at site i, ϵ_i is the random site energy uniformly distributed between $-w/2$ and $w/2$, $a_q^\dagger$ and a_q are annihilated and creation operators for phonons of mode q, $\hbar\omega_q$ is energy of a phonon in mode q, and $g_{i,q}$ is the coupling strength between electron at site i and phonon of mode q which is randomly distributed between 0 and q. Here the second term describes the nearest-neighbor hopping of the

electrons and the hopping integral is set to be in the energy units. We assume that only a fraction of the phonon modes has enough coupling strength with electrons, and the number of these modes M is proportional to the area of the system, $M=\alpha N^2$, with α being a constant and N the linear size of the system.

In this paper we restrict ourselves to the study of the electron-phonon coupling and the correlation between electrons is ignored, thus, we only consider the motion of one electron on a lattice. A full quantum-mechanical description of a state in Hamiltonian (1) is a linear combination of basis wave functions consisting of an electron state and a number of phonons:

$$|\Psi\rangle=\sum_{i,\mathcal{D}} C_{i,\mathcal{D}}|\phi_i\rangle\otimes\prod_{q\in\mathcal{D}} a_q^{\dagger}|0\rangle, \tag{2}$$

where $|\phi_i\rangle$ is the electron orbital on site i, $\mathcal{D}$ is a set of phonon numbers with m_q being the number in the qth mode for q ranging from 1 to M, $|0\rangle$ is the state with zero phonon, and $C_{i,\mathcal{D}}$ is the corresponding coefficient. It is interesting to note that by this description the Hilbert space for the motion of a single electron is extended from $N\times N$ dimensions in the case without the electron-phonon interaction to $N\times N\times(m+1)^{\alpha N\times N}$ dimensions, if we only include at most m phonons for each mode ($m_q\leqslant m$ for all sets $\mathcal{D}$). This is a tremendous increase of the effective dimensions of the system even though $g_{i,q}$, α, and m are small, and may lead to the violation of the conclusion of the scaling theory in Ref. 1. The Hilbert space consists of a large number of planes, each of which corresponds to a specific set of the phonon states. Among them the basic plane is the one with zero phonon, in which the site energies are the original values given by ϵ_i in Hamiltonian (1). For the other planes the site energies are increased by an amount of the energies of the corresponding phonons. This increase of site energies may weaken the effect of tunneling paths provided by these planes. However, this effect still cannot be neglected if there is a small fraction of phonon modes which has low energies and is strongly coupled with electrons.

To illustrate this effect, we use the standard transfer matrix method (TMM) to study the delocalization of the electronic states on a 2D disordered system via the coupling with phonons. To simplify the calculation, we only include at most one phonon for each mode, and the phonon induced hoppings between different sites are ignored. We calculate the rescaled localization length λ_N/N where λ_N is the localization length of a strip with width N and length L, much larger than N. The number of phonon modes involved in this calculation is αN^2, corresponding to the number of modes in an $N\times N$ square. Thus, the obtained rescaled localization length corresponds to the conductance of the square system. In the TMM calculation we project the input and output amplitudes of the wave function to the basic plane with zero phonon, although there are many planes with nonzero phonons in the intermediate states. This procedure guarantees that the incoming and outgoing electrons are from and to the zero-temperature reservoirs. In Fig. 1, we plot the size dependence of the rescaled localization length for different

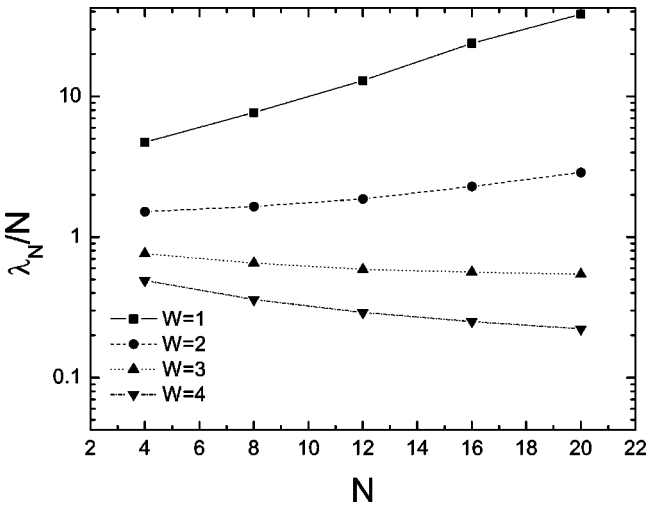

FIG. 1. Rescaled localization length as a function of the system size. The parameters are the following: $g=0.2$, the energy of electron is 0.1, the density of relevant phonon modes is described by $\alpha=1/16$, and the phonon energy is $\hbar\omega=0.2$.

strengths of disorder W. It is obvious that there appear states for which the rescaled localization length is increased with the system size. This behavior could be regarded as metallic-like. However, with this calculation we could not determine a sharp point of the transition, as there is not a value of W_c, for which the rescaled localization length is size independent (fixed point). This implies the failure of the use of the standard TMM, since the increase of the effective dimensions with the size N is rather nonregular, and the processes involved are in fact not quantum mechanical. Nevertheless, the trend of the delocalization is evidently shown from this calculation. This trend occurs at the zero temperature. The tunneling paths in planes corresponding to nonzero phonons can be considered as ''virtual processes,'' which have effect even at the zero temperature. Especially, if $\hbar\omega\ll W$, the paths with nonzero phonons can always provide tunneling probability for the originally localized states.

A more suitable description for these processes is some type of the classical treatments, such as the VRH model or the percolation theory. However, as mentioned above, in the previous VRH model the effect of phonons vanishes at the zero temperature. This is because the number of phonons is zero if the phonon system is regarded as in equilibrium with the thermal bath. This is true only if the energy of the total system of electron and phonons is exactly equal to the sum of the electron energy and the phonon energy. In this case the statistical distribution function is the product of those of the subsystems.[16] The situation will be changed when the coupling between the subsystems alters the energy of the total system from the sum of the subsystems. In this case the energies of the subsystems are no longer meaningful quantities which can be used in the ensemble averaging. The only quantity which can be used is the total energy. In a simplest situation let us consider an electron at a single energy level coupled with a phonon mode of energy $\hbar\omega$ and the coupling strength is g. If the energy change is considered as far as to the second order of g, the phonon number at temperature T is

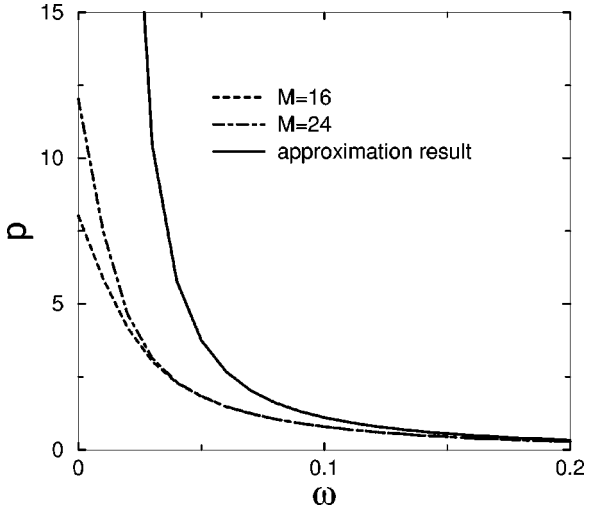

FIG. 2. The distribution of phonons p as a function of ω. The parameters are $w=0$, $g=0.1$, and $kT=0.1$.

$$p(\omega,T)=\frac{\dfrac{\exp(-\beta\hbar\omega)}{[1-\exp(-\beta\hbar\omega)]^2}+\dfrac{g^2}{\hbar^2\omega^2}\exp(\beta g^2/\hbar\omega)}{\exp(\beta g^2/\hbar\omega)-1+\dfrac{1}{1-\exp(-\beta\hbar\omega)}}. \tag{3}$$

Here, $\beta=1/kT$ with k being the Boltzmann constant. It can be seen that the phonon number saturates to $g^2/\hbar^2\omega^2$ at low temperature which is different from the usual Bose distribution. On the other hand, for $kT\gg g^2/\hbar\omega$, the thermal fluctuations smear out the energy difference caused by the coupling, the phonon number becomes the same as that of the phonon subsystem. Of course, in a real world there are many phonon modes coupled to many electron states, and the combined states become more entangled and complicated.

In Fig. 2, we compare the above equation with numerical results by diagonalizing the Hamiltonian. The electron subsystem is a 10×10 square lattice with on-site disorder and nearest-neighboring hopping. The maximum number of phonons in the state $\hbar\omega$ is considered up to M, $M=16,32$. This will limit the statistically averaged phonon number p, leading to a finite value of p in the numerical results even at the limit of $\omega=0$ which corresponds to a complete softening of the lattice. During the calculations, it is found that the strength of the on-site disorder in the electron plane has little effect on the average phonon number. So we take $w=0$ as default in all calculations. It seems that the result from the approximation in Eq. (3) tends to overestimate the phonon number compared to numerical results when ω is small. However, it does indicate the basic fact that the coupling with the electron system will excite more phonons than that from the ordinary Bose statistics for an isolated phonon system in equilibrium with the bath and, especially, the average phonon number saturates to a finite value in approaching the zero temperature. So, for simplicity we will use this approximate result in the next stage.

In the VRH model the electron can be transferred from one localized state to another localized state with the assistance of phonons. This can produce a finite conductance even though all the states of electrons are localized. According to Mott, the VRH process takes place in a lattice with the following Hamiltonian:

$$H_{\mathrm{VRH}}=\sum_m \xi_m n_m, \tag{4}$$

where index m denotes a localized state, ξ_m is the corresponding energy, and $n_m=0,1$ is the occupation of electrons in this state. The probability of transferring an electron from a localized state m to another localized state m', $P_{mm'}$, is obviously proportional to the number of the available phonons, but exponentially decays with the distance between the localization centers of states m and m' denoted as $r_{mm'}$. This consideration leads to the following expression:[9]

$$P_{mm'}\propto\exp\left(-\frac{2r_{mm'}}{\lambda}\right)p(E_{mm'},T), \tag{5}$$

where λ is the average localization length of the electron states and $E_{mm'}$ is the energy difference between states m and m', assumed to be the same as the energy of the mediated phonon. In the Mott theory $P_{mm'}$ vanishes at zero temperature, since from the ordinary Bose distribution the number of phonons is zero. However, this probability should be finite at zero temperature if we calculate it from the pure quantum mechanics of the electron system, since the electron-phonon coupling produces nondiagonal elements for states $\{m\}$. A straightforward perturbation estimation from the coupling in Hamiltonian (1) gives $P_{mm'}\propto[g^2/(\hbar^2\omega+E_{mm'})^2]\exp(-2r_{mm'}/\lambda)$. This coincides with Eq. (5) at $T\rightarrow0$ if $p(E_{mm'},T)$ is replaced with Eq. (3). Thus, it is reasonable to replace the Bose distribution with the phonon number in the composite electron-phonon states so that the VRH theory can be generalized to the low-temperature and strong electron-phonon coupling limit.

The resistivity of the system is proportional to the inverse of the maximum probability with respect to the variation of $r_{mm'}$, and the energy difference $E_{mm'}$ is approximated by

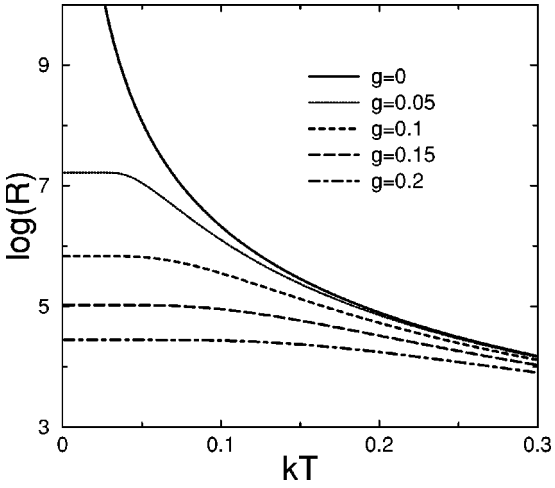

FIG. 3. Resistivity as a function of the temperature. The parameters are $\lambda=1$ and $\rho=0.6$.

$$E_{mm'} = \frac{1}{\rho r_{mm'}^2}, \tag{6}$$

where ρ is a quantity proportional to the density of states of electrons. In Fig. 3, we plot the temperature dependence of the resistivity obtained from the above consideration. It can be seen that there exist states with finite resistivity at zero temperature. For these states the resistivity is almost saturated at low temperatures. If the scattering effects of the thermal excitations are included, the metalliclike behavior of the temperature dependence could be expected in this regime. On the other hand, the transition probabilities between localized states are randomly distributed. Among them the states with transition probabilities larger than a certain threshold can be connected to form clusters that are similar to those in classical percolation models. In this sense the percolation models may also be suitable for the description of the metal-insulator transition in such systems.

In summary, we have investigated the effect of the electron-phonon coupling on the transport of electrons in 2D disordered systems at very low temperatures. The delocalization effect of phonons, which has been studied in the case of finite temperatures in earlier works,[9–13] is investigated in the case of temperature approaching the absolute zero. Due to the redistribution of the phonon number in the composite states of electron and phonons, the VRH theory is modified at the low-temperature limit, and the saturation of the VRH probabilities can produce a finite value of the resistivity at the zero temperature and the metalliclike behavior of the system, which cannot be accounted for by the theory of the quantum metal-insulator transition.

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