Distribution function of mesoscopic hopping conductance

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We study by computer simulation distribution functions (DF) of mesoscopic hopping conductance. The DFs obtained for one-dimensional systems were found to be quite close to the predictions of the theory by Raikh and Ruzin. For $D = 2$, the DFs both for narrow system and thin film look similar (and close to the $1D$ case).The distribution function for the conductance of the square sample is nearly Gaussian.

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Mesoscopic conductance fluctuations in the insulating regime of small, disordered transistors were first observed by Pepper [1] in GaAs MESFETs and then studied in detail in Si MOSFETs by Fowler, Webb and coworkers [2] in the early 1980s. Extremely strong random fluctuations, spanning several orders of magnitude, were observed at low temperatures in the conductances of narrow-channel devices as the gate voltage was varied. The explanation was provided by Lee [3] who proposed a model in which electrons move by variable-range hopping (VRH) along a one-dimensional (1D) chain. A number of elementary hopping resistances, each depending exponentially on the separation and energy difference between sites, are added in series to give the overall resistance of the chain. In this model it is assumed that, because of the extremely broad distribution of the elementary resistors, the total chain resistance can be well approximated by that of the single most resistive hop. The fluctuations then arise as a consequence of switching between the pairs of localized sites responsible for the critical hop as each elementary resistance reacts differently to a change in the chemical potential. These fluctuations are therefore of "geometrical" origin, arising from the random positioning of localized sites in energy and space, as distinct from the "quantum" nature of the tunneling mechanism which would be strongly affected for example by an applied magnetic field. Serota, Kalia and Lee [4] went on to simulate the ensemble distribution of the total chain resistance R and its dependence on the temperature T and the sample length L. In their ensemble, the random impurities are distributed uniformly in energy and position along the chain. In experiments a single device is generally used, so that the impurity configuration is fixed, and fluctuations are observed as a function of some variable external parameter such as the chemical potential. An ergodicity hypothesis is then invoked to the effect that the same ensemble is sampled in both cases, something that has been verified experimentally by Orlov *et al.* [5]. Using the natural logarithm of the resistance, the authors of Ref. [4] obtained for the mean and standard deviation:

$$\langle \ln \rho \rangle \sim \left(\frac{T_0}{T}\right)^{1/2} \left[\ln\left(\frac{2L}{\xi}\right)\right]^{1/2} \tag{1}$$

$$s \equiv \langle (\ln \rho - \langle \ln \rho \rangle)^2 \rangle \sim \left(\frac{T_0}{T}\right)^{1/2} \left[\ln\left(\frac{2L}{\xi}\right)\right]^{-1/2} \tag{2}$$

where ξ is the localization radius and T_0 is the characteristic temperature for Mott VRH: $T_0 = 1/k_B\rho\xi$ (ρ is the density of states at the Fermi energy). It can be seen that the size s of the fluctuations decreases extremely slowly with length, a result characteristic of 1D which was first pointed out by Kurkijarvi [6]. The explanation is simply that exceptionally large resistance elements, even though they may be statistically rare, dominate the overall resistance since they cannot be by-passed in this geometry. The averaging assumed in the derivation of Mott's hopping law for 1D does not occur and the total resistance takes on the activated form of the largest individual element.

A detailed analytical treatment of this model was undertaken by Raikh and Ruzin (RR) [7,8] who divided the problem into a number of length regimes. Their theory introduces the concept of the "optimal break", the type of gap between localized states (on an energy versus position plot) which is most likely to determine the overall resistance. The optimal shape of such a state-free region has maximal resistance for the smallest area and turns out to be a rhombus. A sufficiently long chain will have many such breaks in series to give a most probable resistance

$$R = R_0 \frac{L}{\xi} \left(\frac{T_0}{T}\right)^{1/2} \exp\left(\frac{T_0}{2T}\right)^{1/2} \tag{3}$$

where R_0 is the prefactor in the Mott VRH formula, and $\rho = R/R_0$. This formula is valid only for substantially

long samples. More exactly, it is valid when $\nu \gg 1$, where ν is a parameter defined implicitly by

$$\nu = \frac{2T}{T_0} \ln\left(\frac{L\nu^{1/2}}{\xi}\right). \tag{4}$$

When the expected number of optimal breaks in the chain becomes of order one ($\nu \leq 1$), which corresponds to the normal experimental situation, the resistance of the chain is determined by a few sub-optimal breaks of which the expected number occurring in a chain of length L is approximately one. In this case, the most probable value of the resistance (or its logarithm $Q = \ln \frac{R}{R_0} = \ln \rho$) is

$$Q = \frac{\nu^{1/2} T_0}{T} \approx \left\{ 2\frac{T_0}{T} \ln\left[\frac{L}{\xi}\left(\frac{T_0}{T}\right)^{1/2} \ln^{1/2}\left(\frac{L}{\xi}\right)\right]\right\} \tag{5}$$

The probability distribution function (DF) for the quantity $f(Q)$ is best written in terms of ν and a new parameter Δ

$$\Delta = Q - \frac{\nu^{1/2} T_0}{T}, \tag{6}$$

For $\nu < 1$ it is given by the following integral:

$$f(\Delta) = \frac{e^{\Delta}}{\pi} \int_0^{\infty} \exp\left(-x^{\nu^{1/2}} \cos\frac{\pi\nu^{1/2}}{2}\right) \cdot \cos\left(xe^{\Delta} - x^{\nu^{1/2}} \sin\frac{\pi\nu^{1/2}}{2}\right) dx, \tag{7}$$

where $f(\Delta)$ is a function with a peak close to $\Delta = 0$ and width determined by ν. There is a simple relationship between ν and the variance of Q:

$$\langle Q^2 \rangle - \langle Q \rangle^2 = \frac{\pi^2}{6}\left(\frac{1}{\nu} - 1\right) \tag{8}$$

This theory is equally applicable [9] to the case of the transverse conductance σ of a thin film or barrier. Instead of a sum of series resistances, the required quantity is the sum of parallel conductances representing conducting chains of hops traversing the film. Whereas in 1D the total resistance is determined by the blocking effect of the critical hop, here the total conductance is dominated by an optimal "puncture": an uncommonly high-conductance hopping chain through the barrier which effectively shorts out all other current paths. On a logarithmic scale, since $\ln \rho = \quad - \ln \sigma$, the DFs for the two geometries are simply reflections of each other. The variation of the width and peak position with ξ and ρ is different, however, in the two cases. In 1D the importance of blocking resistors adds weight to the contribution of extremely high resistances and produces a long tail out to low values of $\ln \sigma$. For a short 2D barrier the DF has the opposite asymmetry with a tail out to high conductances, reflecting the effect of punctures in shorting out less conductive paths. In fact the form of the DF is universal, the theory requiring only that the elementary quantities to be summed are independent and come from an exponentially wide distribution. The microscopic details of the conduction mechanism enter only into the dependence of ν and Δ on external parameters such as the temperature and magnetic field. The requirement of independence in the case of the barrier means that conductive chains must be sufficiently far apart, which should be satisfied for a barrier with a sufficiently large aspect ratio W/L. We use the description "short 2D" for this short-, wide-channel geometry to distinguish it from the square 2D geometry in which conduction is via an interconnected percolation network.

The aim of the present work is to do numerical simulation on the 1D and 2D mesoscopic systems in Mott hopping regime, and find the distribution functions of conductance in these systems. We start by replacing the transport problem with a random-resistor network in which the hopping between sites i and j is equivalent to having a resistor ρ_{ij} such that

$$\ln \rho_{ij} = 2\alpha d + (|E_i - \mu| + |E_j - \mu| + |E_i - E_j|)/2kT, \tag{9}$$

Here ρ_{ij} is the resistor between sites i and j, α is the inverse localization length, d is the distance of two localized sites, E_i and E_j are energies of site i, j, and μ is the chemical potential, T is the temperature. Thus the mesoscopic system is reduced to a random resistor network. To find the resistance of the network, the resistors joining electrodes are selected in ascending order until the first percolation path connects the reservoirs. The resistance of the percolation path is taken to be the resistance of the entire system.

In the simulation, first, a number of different impurity configuration is generated. Sites are randomly distributed along dimensions of the system and their energies are chosen randomly from a uniform distribution between $-0.5 \sim +0.5$. For each configuration we randomly chose the position of the chemical potential μ. Thus we can consider the chemical potential distributions (for a fixed impurity configuration) and the ensemble and chemical potential distributions. Typical results for a given configuration and given value of chemical potential are presented below. For a 1D system of $L = 1000$ When chemical potential $\mu = 0$ and temperature $T = 0.001$, by the method described above, the threshold is $\ln \rho_c = 11.9$. Among about 500,000 resistors, there are 53 resistors satisfying unequality $\ln \rho_{ij} \leq \ln \rho_c$, among which there are 12 resistors in the percolation path. The profile of their resistances is shown on Fig. 1a. We see that the single largest hop in fact determines the conductance of the system. With temperature increasing, the resistors in percolation path become closer in resistance, which can

been seen on Fig. 1b, which presents the results of similar calculations, but with $T = 0.01$.

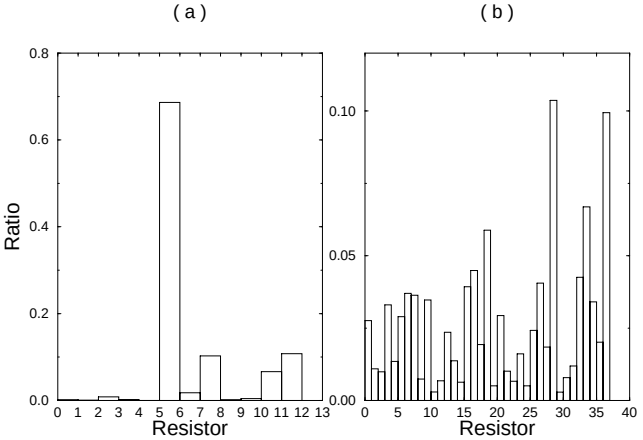


FIG. 1. The ratio of individual resistances in the percolation path to the path resistance: a)$T = 0.001$; b)$T = 0.01$.

We simulate the 1D system at first, and compare the numerical results with the RR theory. The 1D system has a length of 1000, and a localization length of 50. We consider three cases:

1. $T = 0.001$, which gives $\nu = 0.225$;

2. $T = 0.01$, which gives $\nu = 3.6$;

3. $T = 0.015$, which gives $\nu = 5.8$.

For each temperature we consider 1000 ensembles, and chemical potential range is $\mu = -0.1 \sim +0.1$. The results of the first case is shown below.

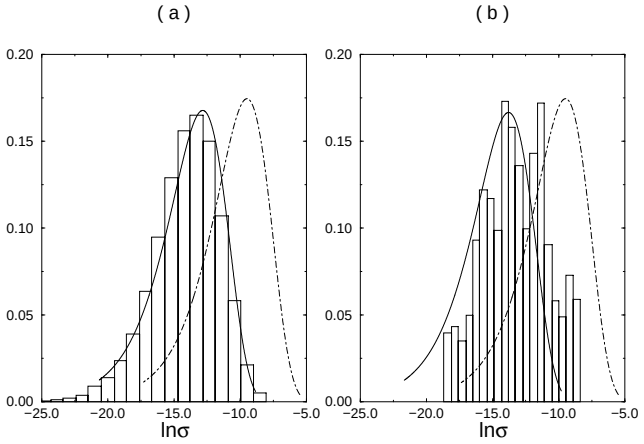


FIG. 2. The conductance of 1D system for $\nu = 0.225$: a) ensemble distribution function; b) chemical potential distribution function. The histograms in both figures are the numerical result, the solid lines correspond to the fitting curves, and the dash-dot lines are the prediction by the RR theory.

The numerical simulation results for $\nu = 3.6$, where according to the theory, the distribution function should be Gaussian, are presented below.

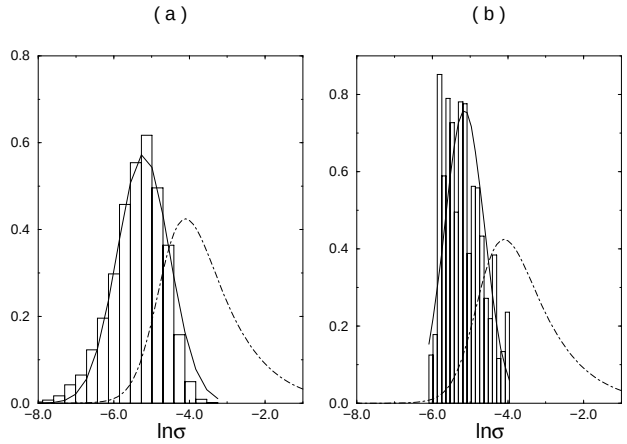
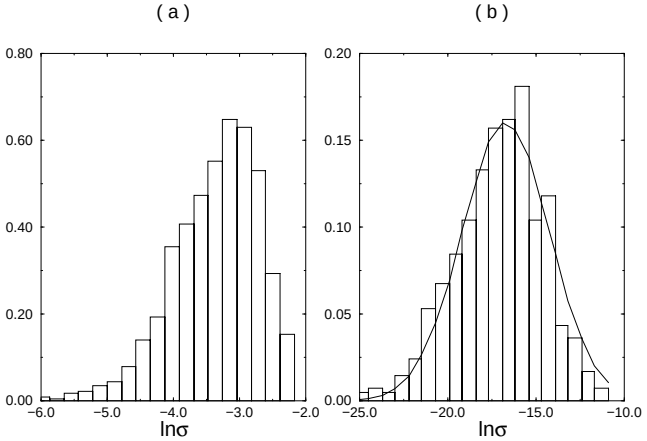


FIG. 3. The conductance of 1D system for $\nu = 3.6$: a) ensemble distribution function; b) chemical potential distribution function. The histograms in both figures are the numerical result, the solid lines correspond to the fitting curves, and the dash-dot lines are the prediction by the RR theory.

The result of $T = 0.015$ leads to the similar figures above except for thiner and higher DFs, which shifts a little towards the higher conductance.

For 2D system, we consider three particular cases: narrow 2D system, square sample and thin film. We expect that the DF of narrow 2D system should be close to that of 1D system and according to the RR theory, the thin film DF on a logarithmic scale should be a reflection of the 1D case distribution function. It is natural to expect that the DF of the square system would be close to a Gaussian. For a 2D system all parameters are chosen to be the same as in the 1D case, except $w = 100$ in the case of narrow sample; $w = 1000$ and $L = 100$ for thin film and $w = L = 1000$ for square 2D system. The number of impurity configurations = 50 in each case. The results are shown below.



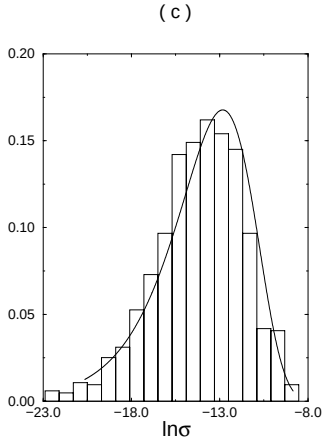


FIG. 4. The ensemble distribution function for the conductance of 2D system: a) thin film; b) square sample; c) long system. Histograms are numerical results. The solid curve in b) is the Gaussian fitting, in c) is the RR theoretical fitting for the 1D case.

We see that the situations of narrow 2D is close to the 1D case as expected, and the normal 2D is close to Gaussian. But, unexpectedly, the DF for thin film is similar to the 1D case distribution function and not a mirror reflection of it, as argued by RR.

In conclusion, the paper has studied the DF of the conductance in mesoscopic systems by numerical simulation. We have found that the distributions obtained by choosing randomly the chemical potentials (for a fixed impurity configuration), which corresponds to a typical experimental situation, coincide with those obtained when both impurity configuration and chemical potential is chosen randomly, in agreement with the ergodicity hypothesis. The DFs obtained for one-dimensional systems were found to be quite close to the predictions of the theory by Raikh and Ruzin. For $D = 2$, the DF both for narrow system and thin film looks similar (and close to the $1D$ case).The distribution function for the conductance of the square sample is close to Gaussian.

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