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Monte Carlo simulation of hopping conduction in two-dimensional Coulomb glasses

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Abstract. We have carried out a Monte Carlo simulation of the conductivity of a two-dimensional strongly localized interacting system. A plot of $d\log\sigma/d\log T$ versus T, on a double logarithmic scale, clearly shows two distinct regimes, one activated at high T and a non-activated one at low T. The conductivity exponent in this later regime is close to $\frac{1}{2}$, in agreement with Efros and Shklovskii's predictions, although the characteristic temperature T_0' is about a factor of two smaller than predicted.

1. Introduction

Thermally assisted hopping between localized states is thought to be the dominant transport mechanism in strongly disordered systems. At relatively high temperatures the spatial (tunnelling) factor is most important in determining transition rates. Conduction then proceeds mainly by short one-electron jumps; as the temperature is decreased the electrons prefer to jump longer and longer distances in order to find states closer in energy. Such behaviour, called variable-range hopping (VRH), results in a temperature dependent activation energy. At even lower temperatures, the conductivity should be dominated by many-electron jumps that avoid the Coulomb gap and have very low excitation energies (Pollak and Ortuño 1985).

It is commonly believed that in the presence of interactions the conductivity in the VRH regime obeys Efros and Shklovskii's law:

$$\sigma \propto \exp\{-(T_0'/T)^{1/2}\} \tag{1}$$

with the exponent $\frac{1}{2}$ independent of the dimensionality of the system (Shklovskii and Efros 1984). This type of behaviour has been observed in many experimental works, some of them on two-dimensional systems (Bishop *et al* 1980, Liu *et al* 1992, Lee *et al* 1992). As the temperature becomes of the order of the Coulomb gap energy, this gap should be washed out and the conductivity should follow Mott's VRH law (Mott 1968):

$$\sigma \propto \exp\{-(T_0/T)^{1/(1+d)}\} \tag{2}$$

where d is the dimensionality of the system.

Recent experiments have shown a re-entrance to activated behaviour at very low temperatures, which sometimes is suppressed by a magnetic field (Terry *et al* 1992, Dai *et al* 1992), and sometimes is not (Kim and Lee 1993). This has been interpreted as due to the existence of a hard gap, of both magnetic and non-magnetic origin, in the single-particle density of states close to the Fermi level.

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We have performed a Monte Carlo computer simulation of the conductivity of a two-dimensional interacting and strongly localized system. The only previous simulation of this problem was done by Levin *et al* (1987) within the R model approximation, that we can now avoid due to the drastic increase in computer power. Our results show an activated regime at high temperatures and only one non-activated regime at low temperatures with an exponent close to $\frac{1}{2}$, as predicted by Shklovskii and Efros (1984).

In section 2 we present the model and the numerical algorithm employed to simulate conductivity. In section 3 we show the numerical results. We finally discuss the results and extract some conclusions.

2. Model and simulation algorithm

The model is based on a classical Hamiltonian which includes a diagonal disorder energy and an electron–electron $1/r$ Coulomb interaction. The sites are arranged in a two-dimensional square lattice, with the number of electrons equal to half the number of sites. The Hubbard energy is assumed to be much larger than the other relevant energies, so no more than one electron can occupy a site. The disorder energy is a random variable uniformly distributed in the interval $(-W, W)$. We first throw the electrons at random and obtain a pseudo-ground state by stabilizing the system against all possible one-electron transitions (Baranovskii *et al* 1979). Afterwards, we thermalize the system to a given temperature by means of the Metropolis algorithm, as described by Davies *et al* (1984).

To simulate electric conduction, we have extended the previous algorithm for thermalization. Specifically, we reduce the jumping probability by the factor $\exp\{-2r_{ij}/a\}$ to simulate correctly the transition rates, and we incorporate the electric field F by adding the energy $eF\tilde{x}_{ij}$ to the site energy. In the above, e is the electronic charge and a the localization radius. The electric field is applied along the x direction; $\tilde{x}_{ij}$ is equal to $x_j - x_i$ if the electron does not cross the initial edge of the square perpendicular to the x axis, and otherwise (Levin *et al* 1987)

$$\tilde{x}_{ij} = \begin{cases} x_j - x_i + L & \text{if } x_j < x_i \\ x_j - x_i - L & \text{if } x_i < x_j. \end{cases} \tag{3}$$

The conductivity is proportional to the difference between the number of electrons which cross the original edge of the sample in and against the direction of the field ($x_j < x_i$ and $x_i < x_j$, respectively).

We used 10 different samples of size 60×60. For each temperature and each sample, we attempted a total number of jumps ranging between 5×10^7 and 1.3×10^9. We use several localization radii and a disorder energy $W = 2$, in units of the Coulomb energy $e^2/\langle r \rangle$, $\langle r \rangle$ being the lattice constant. The electric field was chosen as $F\langle r \rangle = kT/10$, small enough to be within the linear regime (k is the Boltzmann constant). The difference between the numbers of jumps with and against F is about 10% of the sum of the two. We also tested that the electric current had reached a stationary state.

3. Numerical results

We calculated the temperature dependence of the conductivity in the range $0.04 \leqslant T \leqslant 0.6$, as a function of the localization radius. We assumed a functional dependence of the conductivity of the form

$$\sigma(T) \propto T^m \exp\{-(T_0/T)^x\} \tag{4}$$

and plotted $w(T) = \mathrm{d}\log\sigma/\mathrm{d}\log T$ versus T to determine the exponent x. For m small compared to $x(T_0/T)^x$, the previous form of σ implies that $\log w(T)$ against $\log T$ is a straight line, whose slope is equal to the exponent x.

To analyse the importance of sample to sample fluctuations, we have obtained the average of the conductance, of the resistance and of the logarithm of the conductance for each temperature. We have checked that the average conductance always differs by less than 1% from the inverse of the average resistance. Thus, we conclude that fluctuations are not relevant in the two-dimensional hopping regime considered.

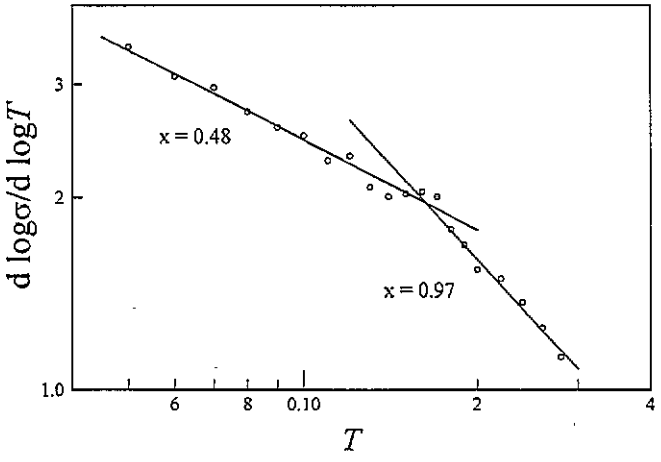

Figure 1. $\mathrm{d}\log\sigma/\mathrm{d}\log T$ as a function of T, on a double logarithmic scale, for a disorder energy $W = 2$ and a localization radius $a = 3$.

In figure 1 we represent $w(T)$ as a function of T, on a double logarithmic scale, for a localization radius $a = 3$. Two straight lines are visible, with slopes equal to 0.48 ± 0.05 and 0.97 ± 0.08, approximately corresponding to Efros and Shklovskii's law and to activated behaviour, respectively. The transition temperature between both regimes is $T_C = 0.18$. We have to note that any procedure to determine the conductivity exponent is necessarily very sensitive and generates big error bars in the exponent x.

Figure 2 shows $\log\sigma$ as a function of $T^{-1/2}$ for a localization radius $a = 3$. The low-T data are fitted quite well by a straight line which extends for almost two orders of magnitude of the conductivity. The slope of the straight line corresponds to a characteristic temperature $kT_0' = 2.37$. The inset in figure 2 represents $\log\sigma$ as a function of T^{-1} in the high-temperature regime. The conductivity follows an Arrhenius behaviour in this regime, with an activation energy equal to 0.31.

We have done an analysis, similar to the one shown for $a = 3$, for $a = 2$, 2.5 and 4. The main features are similar to the case $a = 3$, and the characteristic parameters are given in table 1. We can notice that in the non-activated regime, we always get an exponent close to $\frac{1}{2}$. The activated regime has already been studied in a previous publication (Pollak *et al* 1994). We obtained that the activation energy is proportional to the Coulomb gap and does not depend on the localization radius.

We have not found any sign of a re-entrance to activated behaviour at very low temperatures. The temperatures considered are probably a little bit too high for this new

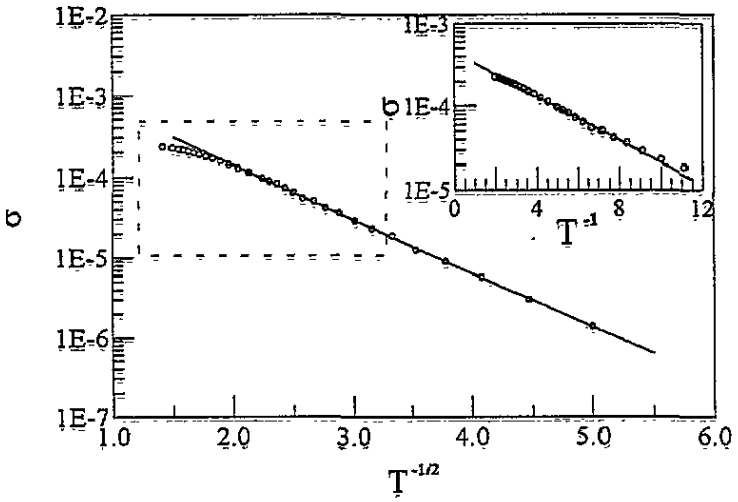

Figure 2. $\log\sigma$ as a function of $T^{-1/2}$ for $W = 2$ and $a \equiv 3$. The inset represents $\log\sigma$ against T^{-1} for the high-temperature regime of the main curve.

Table 1. Characteristic parameters for the VRH regime. a is the localization radius, x the conductivity exponent entering equation (4), T_0' the characteristic temperature obtained fitting the simulations of the conductivity to equation (1), T_{ES} the theoretical prediction of the Efros and Shklovskii temperature, equation (5), and T_C the crossover temperature between the activated and VRH regimes.

a	x	T_0'	T_{ES}	T_C
2	0.58	2.35	3.25	0.18
2.5	0.52	2.46	2.60	0.16
3	0.48	2.37	2.17	0.18
4	0.53	2.62	1.63	0.18

regime to be observed. But we also believe that we could never obtain this regime with only one-electron jumps, since this behaviour should be due to many-electron jumps and not to a hard gap in the density of states.

4. Discussion

The theoretical prediction T_{ES} for the characteristic temperature T_0' appearing in Efros and Shklovskii's law is given by (Shklovskii and Efros 1984)

$$kT_{ES} = \frac{\beta e^2}{\kappa a} \tag{5}$$

where β is a numerical factor of the order of six, and κ is the effective dielectric constant. In real experiments, κ (as well as the density of states in the Coulomb gap) depends on the localization radius, but for the interpretation of our simulations we have to consider $\kappa = 1$. In table 1, we show the values of T_{ES} obtained with equation (5) and $\beta = 6.5$ (Nguyen 1984).

We can notice that both the numerical fittings T_0' and the theoretical predictions T_{ES} for the characteristic temperature are of the same order of magnitude, but the theoretical predictions are inversely proportional to the localization radius a, while the numerical fittings are independent of a. This is so because our simulations do not correspond to the classical Coulomb gap regime characterized by a localization radius smaller than the intersite separation and where expression (5) is valid. If we extrapolate our results to $a = 1$, where the classical regime starts, we would obtain the estimate $\beta = 2.4$, less than half of Efros and Shklovskii's predictions. In the Arrhenius regime, the activation energy is also independent of the localization radius and proportional to the Coulomb gap (Pollak *et al* 1994).

Our Monte Carlo procedure is not very suitable to analyse the assumption underlying Efros and Shklovskii's model for VRH. For example, we cannot obtain direct evidence for the importance of successive correlations (the only ones involved in our simulations since we do not consider many-electron jumps). We cannot conclude whether the exponent of $\frac{1}{2}$ is a result of the linear (in two dimensions) single-particle density of states or whether it is due to (sequential) correlation effects.

We believe that in order to see a second non-activated regime, corresponding to the so-called Mott VRH, we would have to consider less strongly localized systems, closer to the insulator–metal transition, as is the case in most experimental situations where one sees a crossover. Close to the transition the jumps are longer, the screening is bigger and it is much easier to overcome the Coulomb gap effects. The transition temperature to the activated regime is $T_C \approx 0.18$, while the expected crossover temperature to Mott VRH is equal, in two dimensions, to

$$T_C' \equiv \gamma \frac{T_{ES}^3}{T_M^2} \tag{6}$$

where T_M is Mott's characteristic temperature, and γ is equal to 729/4096 if we use the typical hopping distance as the relevant magnitude for the crossover. Then, the critical temperature ranges between 0.2 and 3, but the activated behaviour sets in at lower temperatures. Our system is too interacting for Mott VRH to be observed. We would have to include a high dielectric constant in the interaction energy to be able to observe Mott's behaviour, but then it would be difficult to obtain Efros and Shklovskii's law for the same sample.

We can observe in table 1 that the transition temperature between the activated and VRH regimes is roughly independent of a and approximately equal to 0.18. We can explain this result by considering that the VRH regime only holds when the typical hopping distance is larger than the localization radius. This condition is satisfied for $T < T_0'/16 \approx 0.15$, in good agreement with our numerical simulations.

5. Conclusions

We have found a conductivity exponent in VRH in interacting systems close to $\frac{1}{2}$, in agreement with Efros and Shklovskii's predictions. The values of the characteristic temperature T_0' are independent of the localization radius, in disagreement with these predictions, which only apply to the classical Coulomb gap regime. Extrapolating our results to this regime would produce a constant β of the order of 2.5, about half the value predicted by Efros and Shklovskii. The value of T_0' is of importance in the interpretation

of conductivity experiments and in the variable-range hopping regime in the quantum Hall effect.

We are now extending our calculations to lower temperatures, which has to be done with a completely different approach based on percolation between many-electron configurations. This approach will also allow us to analyse the importance of correlations, since we will be able to identify the critical jumps in each percolation path. Nevertheless, the percolation approach only works at very low temperatures and for the temperature range considered here the Monte Carlo technique is more appropriate.

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