Non-linear conductivity in Coulomb glasses

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We have studied the nonlinear conductivity of two-dimensional Coulomb glasses. We have used a Monte Carlo algorithm to simulate the dynamic of the system under an applied electric field $E$. We have compared results for two different models: a regular square lattice with only diagonal disorder and a random array of sites with diagonal and off-diagonal disorder. We have found that for moderate fields the logarithm of the conductivity is proportional to $\sqrt{E/T^2}$, reproducing experimental results. We have also found that in the nonlinear regime the site occupancy in the Coulomb gap follows a Fermi-Dirac distribution with an effective temperature $T_{\text{eff}}$ higher than the phonon bath temperature $T$.

1 Introduction

Electron transport in Coulomb glasses (CG) has been investigated for decades. These glasses are systems with electronic states localized by the disorder and long range Coulomb interactions between carriers. At low temperatures, conductivity in CG is by hopping, where the transition rates for electron jumps depend exponentially on an energy factor and on a spatial factor. In the limit of very low temperatures, an optimization of the total penalty paid through these two factors leads to the mechanism coined by Mott as variable range hopping (VRH). Mott obtained the precise law for the DC conductivity $\sigma$ of non–interacting systems in this regime [1] and Efros and Shklovskii (ES) [2] modified his argument to include the effects of Coulomb interactions by considering the specific form of the single–particle density of states in CG. The conductivity in this case is of the form

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

with the exponent 1/2 independent of the dimensionality of the system. $T_0 = \beta e^2/(\epsilon k_B a)$ is a characteristic temperature, $\epsilon$ the dielectric constant of the material, $a$ the localization radius of the electrons, and $\beta$ a numerical coefficient that depends on dimensionality. The conductivity of many different types of systems have been found to obey this law, Eq. (1).

Nonlinear effects in electron transport are specially important in CG. The universality of the CG ensures that in the linear regime the behaviour of the conductivity is fairly independent of the model used. For this reason, lattice models are often employed as they are computationally more efficient. In the nonlinear regime, the universality is not ensured and a comparison between different models is interesting. We simulate numerically a lattice model and a random site model of CG to study the conductivity as a function of the applied electric field and temperature in the nonlinear regime. We have first verified that in the linear regime both models reproduce the behavior of Eq. (1) at low temperatures. The slope obtained are quite
similar and also similar to results from a percolation simulation [3]. Here we concentrate in comparing the results of both models in the nonlinear regime.

2 Model
We consider two different Coulomb glass models: a square lattice with site disorder and an irregular array of random sites with both diagonal and off-diagonal disorder. Both models are described by the same Hamiltonian [4]

\[ H = \sum_i (\phi_i + x_i E) n_i + \sum_{i<j} (n_i - K)(n_j - K) \frac{1}{r_{ij}}, \]

where \( n_i = 0, 1 \) are occupation numbers, \( K \) is the compensation, equal to 1/2, and \( \phi_i \) are the random site energies chosen from a box distribution with interval \([-W/2, W/2]\). \( E \) is the value of the applied electric field. \( x_i \) is the coordinate along the direction of the applied field of site \( i \) and \( r_{ij} \) is the distance between sites \( i \) and \( j \). The unit of distance is the lattice spacing for the square lattice and \( L/\sqrt{N} \) for random sites, \( L \) being the lateral size of the sample and \( N \) the number of sites. The inverse of the unit of distance is our unit of energy and temperature. We implement periodic boundary conditions, but on the direction of the applied field we increment the energy by \( \pm EL \) every time an electron crosses a fix virtual surface, where the sign depends on the crossing direction. This arrangement induces a permanent current in the direction of the field when we set up our dynamical procedure.

The MC method employed is similar to the one introduced in [5]. It first chooses a pair of sites with a probability proportional to \( \exp(-2r_{ij}/\xi) \), where \( \xi \) is the localization length, which we have chosen equal 2/3 in the lattice model and 1 in the random site model. Then if one of the sites chosen is occupied and the other empty it performs the transition with an energy dependent probability given by

\[
f(\Delta E) = \begin{cases} 
1 - \frac{e^{\Delta E/T}}{1 + 1} & \text{for } \Delta E > 0 \\
1 - \frac{e^{-\Delta E/T}}{1 + 1} & \text{for } \Delta E < 0 
\end{cases}
\]

for the lattice model. \( \Delta E \) is the total transition energy, including the energy due to the applied field. For the random site model, this probability is

\[
f(\Delta E) = \min\{1, \exp(-\Delta E/T)\}
\]

for the lattice model. We concentrate in temperatures for which a stationary state is achieved relatively fast and so only single-electron transitions must be considered. The time step of our MC procedure is then equal to \( \tau_0/\sum_{ij} \exp(-2r_{ij}/\xi) \), where \( \tau_0 \) is the inverse phonon frequency, of the order of \( 10^{-13} \) s [6,7]. We believe that the differences between the two models in \( \xi \) and in \( f(\Delta E) \) do not change qualitatively the results.

We start from a random configuration and follow the dynamics at a given temperature, monitoring all relevant magnitudes. Once we are in a stationary situation, we obtain the conductivity of each sample through the displacement of the center of mass of the electrons for a given time interval. Then we average the logarithm of the conductivity.

3 Results and discussion
We have calculated the conductivity (defined as \( \sigma = j/E \)) for different values of the applied field and the temperature in the variable range hopping regime. In Fig. 1 we represent the conductivity \( \sigma(T, E) \) as a function of \( E \) for several values of \( T \) for both models, the random site model (a) and the lattice model (b). At any fixed \( T \), we observe a small linear regime for small values of the field and then a systematic
Conductivity as a function of $E$ for several temperatures. Fig. 1a is for the random site model and Fig. 1b for the lattice model.

As can be seen in Fig. 1, both models behave qualitatively similar. Probably the main difference between both models is at high field values where in the random model we approach the temperature independent regime faster than in the lattice model. For a field $E = 2$ we already get a roughly temperature independent conductivity, while for the lattice model much larger fields are required. We think that a factor contributing to this different behaviour is that the critical percolation jump is larger in the random site model than in the lattice model, and so the effect of the field is also larger. While the $T$ independent region is near the conductivity maxima in the random site model, it is far from these maxima in the lattice model.

To model in a compact way the field and temperature dependence of the nonlinear conductivity we have followed the same procedure as Aronzon et al. [8], who measured the nonlinear conductance in a p-Si layer and were able to collapse all the data by plotting $\sigma(T,E)/\sigma(T,0)$ as a function of $\sqrt{E/T}$. They studied the activated regime, while our results correspond to variable range hopping. A relatively good collapse of the data is obtained by plotting $\sigma(T,E)/\sigma(T,0)$, on a logarithmic scale, versus $\sqrt{E/T}$, as done in Fig. 2. The left part (a) corresponds to the random site model, while the right part (b) is for the lattice model. This collapse is only good at low and moderate values of the field and low temperatures. For $T = 0.5$ the gap is filled and there is no overlap with the data for lower temperatures. We have also observed that, for a fixed $T$, the CG fills as we increase $E$. The deviation from the collapse at high fields can also be related to the filling of the gap. So, for a good collapse of the data as a function of $\sqrt{E/T}$ it seems necessary to have a well developed CG. At intermediate field values, when the linear response is not a good approximation any more, the linear dependence of $\ln \sigma(T,E)$ with $E^{1/2}$, observed experimentally, is reproduced by both models.

Once we have reached a stationary situation we calculate the site occupation probability $f(\epsilon)$ and we have found that it follows pretty well a Fermi-Dirac distribution with an effective temperature $T_{\text{eff}}$, which depends on both $T$ and the applied field $E$, and is higher than the bath temperature. The results are similar for both models considered.
4 Conclusions

Both the lattice and the random site model produce qualitatively similar results in the nonlinear regime, except for the saturation region at high fields. At intermediate field values, the linear dependence of \( \ln \sigma(T, E) \) with \( E^{1/2} \), observed experimentally, is reproduced by both models. When the system maintains a Coulomb gap (for both \( T \) and \( E \) not too large) we obtain a good collapse of the data with respect to \( \sqrt{E/T} \). We plan to extend the study of the non linear regime in order to explain experimental results on hot electrons \([9]\).

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