Numerical studies of relaxation in Electron Glasses

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Abstract. We study numerically strongly localized systems with long-range Coulomb interactions. We obtain a set of low-energy many-electron configurations. We calculate transition rates between states involving up to six electron jumps. We obtain the density of configurations and the density of metastable states. We also analyze the stability of these metastable states. We use the master equation to simulate the dynamic of the system, both without and with an applied electric field. We obtain in this way the energy relaxation from excited states and the behaviour of the conductivity as the system relaxes. We observe a drastic change in this behaviour for relaxation times close to the Maxwell time.

1. Introduction
Coulomb glasses are systems with localized electronic states and Coulomb interactions between carriers. Very slow relaxation rates are commonly observed in these systems due to the exponential dependence of the transition rates with hopping length and energy and due to the many-valley structure of the phase space.

Experimental studies on indium oxides by the group of Ovadyahu [1], have shown typical glassy phenomena such as logarithmic relaxation and aging. Similar effects have been found on granular metals [2], on ultrathin metal films [3] and on ferromagnetic granular nickel (Frydman).

Slow relaxation in Coulomb glasses has been studied theoretically (Pollak, Yu, Weizmann, Müller) and by Monte Carlo (MC) simulations (Grempel, Efros, Murcia).

2. Model and numerical procedure
We consider two–dimensional Coulomb glasses in the strongly localized regime, described by the standard tight–binding Coulomb gap (CG) Hamiltonian [4, 5]

\[ H = \sum_i \epsilon_i n_i + \sum_{i<j} n_i n_j \frac{1}{r_{ij}}, \tag{1} \]

where \( n_i = 0, 1 \) are occupation numbers and \( \epsilon_i \) are the random site energies chosen from a box distribution with interval \([-W/2, W/2]\). \( r_{ij} \) is the distance between sites \( i \) and \( j \). We consider square samples of lateral size \( L \) and sites placed at random. \( l_0 = L/\sqrt{N} \) is our unit of distance and \( 1/l_0 \) is our unit of energy and temperature. We study systems ranging from 500 to 2000 sites, and establish a minimum separation between sites equal to 0.2. The range of the disorder is \( W = 2 \) and the localization length \( a \) is equal to unity. We choose the number of electrons to be half the number of sites, and use cyclic boundary conditions.

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We used a numerical algorithm to obtain the ground state and $2.5 \times 10^5$ lowest energy many-particle configurations of the system. The algorithm [1, 2] consists of the following two stages. In the first stage, we repeatedly start from states chosen at random and relax each sample by means of a local search procedure. In an iterative process, we look for neighbors of lower energies and always accept the first such state found. The procedure stops when no lower energy neighboring states exist, which insures stability with respect to all one-electron jumps and compact two-electron jumps. We then consider a set of metastable states found by the process just described and look for the sites which present the same occupation in all of them. These sites are assumed to be frozen, i.e. they are not allowed to change occupation, and the relaxation algorithm is now applied to the unfrozen sites. The whole procedure is repeated until no new frozen sites are found with the set of metastable states considered.

In the second stage, we complete the set of low-energy configurations by generating all the states that differ by one- or two-electron transitions from any configuration stored. In order to speed up this process, which is very CPU time consuming, we again assume frozen and unfrozen sites and in first place look for neighboring configurations by changing the occupation of unfrozen sites only. We later relax this restriction in the final stage.

We are also interested in storing metastable states and we have developed a variant of the previous algorithm to this aim. In this case, we only relax by one-electron hops of length smaller than a critical value that we take equal to 6. This allows us to obtain metastable states with respect to jumps shorter than the critical one and also with respect to one-electron transitions. In this version of the algorithm we do not employed the second stage of the original method and we consider a huge number of initial random configurations.

To check the degree of completeness of the set of metastable states obtained, we have plotted in figure the evolution of the energy of the highest energy configuration stored as a function of the number of relaxation processes attempted on a logarithmic scale. Each relaxation process consists in choosing an initial random configuration and let it relax by one-electron hops until a metastable state is reached. Each of the four curves in figure corresponds to a different disorder realization, i.e. position of the sites and random site energies. The curves start when 250,000 different metastable states have been stored. We note that the convergence is fairly good when the number of attempts is larger than $\approx 10^8$. There are important fluctuations from sample to sample in the starting point of each curve and in the final energy, reflecting the variations in the complexity of the different energy landscapes.

**Figure 1.** Energy of the highest configuration stored as a function of the number of relaxation attempts.

**Figure 2.** Number of times that a configuration is reached from different initial configurations as a function of the energy of the configuration.
In figure 2 we have plotted the number of times that a configuration is reached from any initial random state versus the energy of the final configuration. We notice that for energies in the first half of the figure each configuration is visited at least almost ten times and often more than a thousand times. It is unlikely that there are configurations in this energy range that have not been visited at all. For energies above 0.4 (for the disorder realization of figure 2 there are many states that have been reached once, and we expect to be also many other states that still have not been visited at all.

3. Master equation

We have studied the time evolution of our system through the master equation in configuration space. The system is described by the time dependent probability vector, \( \mathbf{p}(t) \), whose components are the occupation probabilities of the different many-electron configurations. The evolution depends on the transition rates between configurations. In this work, we assume that the system evolves through single–electron hops. The transition rate for a jump from site \( i \) to site \( j \) when the system is in configuration \( \alpha \) is

\[
\Gamma_{ij}^{(\alpha)} = \tau_0^{-1} \exp \left( \frac{-2r_{ij}}{a} \right) \min \left[ 1, \exp \left( \frac{-E_{ij}^{(\alpha)}}{kT} \right) \right]
\]

(2)

where \( \tau_0 \) is the inverse phonon frequency, of the order of \( 10^{-13} \) s.

The master equation setting the evolution of our system is

\[
\frac{d\mathbf{p}(t)}{dt} = \mathbf{A} \mathbf{p}(t)
\]

(3)

The dynamical matrix \( \mathbf{A} \) gives us the rate of change from one configuration \( \alpha \) to another \( \beta \). Its non–diagonal matrix elements are \( \Gamma_{ij}^{(\alpha)} \), if configurations \( \alpha \) and \( \beta \) differ by a single jump from \( i \) to \( j \), and zero otherwise. Its diagonal elements are \( -\sum_{i,j} \Gamma_{ij}^{(\alpha)} \), so that the total probability is conserved.

We choose for the initial state the mixture of all configurations with weights equal to the Boltzmann factor for a temperature 40 times larger than the phonon bath temperature, which in this study we take as \( T = 0.002 \). We checked that the results do not depend on the initial state considered, provided it is widely distributed between configurations.

When we want to study how it relaxes the conductivity of the system, we simulate the application of an electric field \( F \) with an extra energy contribution equal to \( -FS\sum_{i}x_{ni} \), where \( x_i \) is the coordinate along the direction of the field of site \( i \). The inclusion of this term modifies the transition rates, equation (2), depending on whether the transition is in favour of or against the electric field.

In order to characterize the degree of stability of the metastable states, we have considered an extension of equation (2) for the transition rates of many-electron jumps. We have assumed that in this case equation (2) is still valid provided that \( r_{ij} \) is substituted by the total hopping distance of all electrons involved and \( E_{ij} \) by the energy difference between the final and the initial configurations. The total hopping distance is minimized with respect to all possible transitions between the initial and final occupations.

4. Density of metastable states

We have first calculated the density of configurations as a function of energy. In figure 3 we represent the integrated density of many-electron configurations as a function of energy (black, upper curve). We have also obtained the densities of metastable states according to their degree of stability and their accumulated values are also plotted in figure 3. The red curve corresponds
to configurations that are stable with respect to all one-electron transitions, i.e. that cannot lower its energy via a single electron jump, but there is a two electron transition that do lower its energy. The green and blue curves correspond to accumulated densities of states stables with respect to two and three electron transitions, respectively. Finally the magenta dashed curve represents the accumulated density of configurations that can lower their energy by a single electron jump longer than the critical hopping distance considered, 6 in our case.

All curves in figure 3 can be fitted relatively well by expressions of the form

$$\log N(E) = A \exp\{BE^{1/2}\}$$

with $A$ and $B$ constants. It is surprising that there is no sign of saturation of the density of metastable states up to the relatively high energies considered. Also, except for a small crossover at low energies between the curves for metastable states with respect to one- and two-electron jumps, there is no predominance of highly stable states at low energies, as could be reasonably expected.

![Figure 3](image-url)

**Figure 3.** Integrated density of configurations as a function of energy for different degrees of stability. The black curve corresponds to all configurations, the red, green and blue curves to configurations stable with respect to one, two and three electron jumps, respectively. The magenta dashed curve corresponds to states stables with respect to one electron jumps shorter than the critical hopping distance.

### 5. Stability of metastable states

For each of the metastable configurations found, we calculate all transitions downward in energy to other metastable states. We consider $T = 0$ and so we concentrate only in the total hopping distance. It is clear that the direct transition between two metastable states, i.e. the bottom of two valleys, is not in general the most effective transition between the valleys, but we assume that represents a rough estimate of the stability of the valleys. For each metastable state we store the fastest of all previously calculated transitions downward in energy. In figure 4 we have plotted the hopping distances of the fastest relaxation transition from any metastable state arranged in decreasing order. These distances are proportional to the logarithm of the transition
Figure 4. Hopping distance of the optimal transition from metastable states arranged in decreasing order.

Figure 5. Energy relaxed in the optimal transition from metastable states versus the initial energy.

rates and so to the logarithm of the relaxation times. A constant distribution of these logarithms should corresponds to a straight line in our figure.

In figure 5 we have represented the energy decrease of the fastest relaxation transitions as a function of the energy of the relaxing configuration. When a transition ends up in a configuration with a larger transition rate (shorter relaxation time) than the original one we add to the energy difference of the transition the energy decrease of the subsequent transition. The red line in figure 5 is a smoothing of the data. We see that on average the energy difference of the transitions grows linearly with the initial energy, although the constant term is fairly important.

6. Evolution towards equilibrium

We have integrated numerically the master equation with an adaptative Runge-Kutta algorithm starting from configurations at thermal equilibrium at \( 40T \), where \( T = 0.002 \) is the phonon bath temperature, determining the evolution of the system. The system size is \( N = 1000 \). The occupation probability of the low energy configurations after a relaxation time \( t = 10^5 \) is represented in figure 6. The straight line is proportional to \( \exp\{−E/kT\} \) and at equilibrium all configurations should lie in a line parallel to this one. We can appreciate that many configurations have arranged in lines with the slope of equilibrium. They correspond to configurations belonging to the same valley. We have reached equilibrium within valleys, but not between different valleys.

7. Conductivity

To study the conductivity of the system as it relaxes, we have integrated the master equation in the presence of an applied electric field. In this case we have considered eight different systems of size \( N = 500 \), at \( T = 0.04 \) and an electric field \( F = T/20 \). The conductivity as a function of time is plotted in figure 7 (red curve, left axis). We also plot the energy (blue curve, right axis) and note that their behaviours are quite different. The solid circle corresponds to the conductivity in equilibrium at the Maxwell time, i.e. the inverse of the conductivity in units of \( e^2/h \). The conductivity decreases quickly at times shorter than the Maxwell time, when it reaches a value close to the equilibrium value and then relaxes slowly.

In figure 8 we represent the same conductivity data as in figure 7 on a logarithmic scale (red curve). The straight line has slope one and it represents a conductivity inversely proportional to the relaxation time. We have also plotted \( −E^{-1/4} \) (blue curve, right axis), which should
Figure 6. Occupation probability of low-energy configurations after the system has relaxed for a time $t = 10^5$. The straight line is proportional to $\exp\{-E/kT\}$.

Figure 7. Conductivity as a function of time for eight different samples (dashed curves) and their average value (continuous curve) for $T = 0.04$. The solid circle corresponds to the conductivity in equilibrium at the Maxwell time.

Figure 8. Conductivity as a function of time for eight different samples (dashed curves) and their average value (continuous curve) for $T = 0.04$. The solid circle corresponds to the conductivity in equilibrium at the Maxwell time.

be roughly proportional to $-T_{\text{eff}}^{-1/2}$, where $T_{\text{eff}}$ is the effective temperature. If both curves in figure 8 would coincide, the conductivity would follow Efros and Shklovskii’s law in terms of the effective temperature. We see that the curves are not very different, but the important feature of the change of behaviour at the Maxwell time is not captured by the energy relaxation.

8. Conclusions

The approach based on the master equation is very promising to study relaxation in electron glasses. To address the most interesting problems (shape of the dip, logarithmic relaxation, aging) we have to develop a renormalization technique adequate to the calculation of the
conductivity. This is a problem much harder to solve than the previously developed renormalization approaches for the study of the energy.

Acknowledgments

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