Excitation probability and effective temperature in the stationary regime of conductivity for Coulomb Glasses

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1 Introduction

Coulomb glasses are complex systems with strongly localized states and Coulomb interactions among carriers. They are characterized by quite slow relaxation rates due to the exponential dependence of the transition rates with hopping length [1, 2]. For instance, if we apply a strong electric field to place the system into a stationary state of conductivity or follow its relaxation starting from a quenched state, it holds that Coulomb glasses exhibit phenomena such as loss of ergodicity, slow relaxation and aging, among others [3–7]. Even a temperature is not well-defined, strictly speaking [8].

Concerning the study of conductivity, the standard two-dimensional tight-binding Coulomb gap Hamiltonian that describes the system is [1, 2]

\[ H = \sum_i \phi_i n_i + \sum_{i<j} (n_i - K)(n_j - K) + \sum_i \varepsilon x_i, \]

where \( n_i = 0, 1 \) are occupation numbers and \( \phi_i \) are the random site energies lying in the interval \([-W/2, W/2]\), where \( W \) denotes the range of disorder. Also, \( K \) is the compensation, equal to \( 1/2 \), \( r_{ij} \) is the distance between sites \( i \) and \( j \), \( \varepsilon \) is an external electric field (applied in the \( x \)-direction) and \( x_i \) is the cartesian coordinate of the \( i \)-th site.

The transition rate from configuration \( \alpha \) to \( \beta \) is given by

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

(c.f. [1]), where \( \tau_0 \) is the inverse phonon frequency, \( k_B \) is the Boltzmann constant, \( a \) is the localization length, and \( \Delta E_{a,\beta} \) is the change of energy between configurations, also known as excitation. In numerical simulations, it is usually considered that the system evolves through single-electron hops, so \( \Gamma_{\beta,\alpha} \) is not zero only if configurations \( \alpha \) and \( \beta \) are connected by a single jump from site \( i \) to site \( j \).

Numerical approaches have shed light on the thermodynamics of Coulomb glasses when they are placed out of equilibrium. It has been found that for both relaxation and nonlinear conductivity, the probability of occupation of sites follows a Fermi-Dirac distribution (FDD in the sequel), as it also occurs in equilibrium, but at a higher temperature than that of the phonon bath [9]. It is the so-called effective temperature, \( T_{\text{eff}} \), which may be a common feature of strongly localized systems out of equilibrium including spin glasses [10, 11]. Such a temperature tends to...
the real during the relaxation processes and remains constant at stationary states produced by the application of a strong electric field [12]. Traditionally, the probability of occupation has been employed to calculate $T_{\text{eff}}$ via the numerical integration of the FDD. However, it critically depends on the choice of the chemical potential [13].

In this paper, we show an alternative to the occupation probability to numerically calculate $T_{\text{eff}}$ in systems placed into stationary states by applying a strong electric field, namely, the excitation probability, which also follows a FDD in relaxation simulations [9]. In general, such a function constitutes a better alternative, since it does not depend on the choice of the chemical potential, which may be critical for small sample sizes. Thus, its statistics are much better than those presented by occupation probabilities, so we propose this as a standard procedure to determine the effective temperature in stationary states for Coulomb glasses.

In all our simulations we follow the dynamics of two-dimensional systems via single-electron hops by employing the hybrid Monte Carlo algorithm provided by Tsiganov and Efros [14]. Regarding the simulation of equilibrium, we have followed the same approach at high temperatures, along with the statistics of the lowest energy levels, obtained via optimization algorithms [15, 16]. We have considered square samples of lateral size $L$ and $n$ sites randomly placed. To set the system into a stationary state of conductivity, we set $\varepsilon = T$ (c.f. [17]). Notice that $l_0 = L\sqrt{n}$ 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. The range of disorder is $W = 2$ and the localization length, $a$, is equal to 1. We choose the number of electrons to be the half of the number of sites and shall use cyclic boundary conditions. The site energies are defined as $\varepsilon_i = \phi_i + \sum_j (n_j - K)/r_{ij}$.

Regarding the finite size effects, we refer the reader to the Appendix.

## 2 Excitation probability in equilibrium

Let $N(\Delta E)$ be the number of electron-hole excitations of energy $\Delta E$. The excitation probability, $F(\Delta E)$, is defined as follows:

$$F(\Delta E) = \frac{N(\Delta E)}{N(\Delta E) + N(-\Delta E)}.$$  \hspace{1cm} (3)

In equilibrium, if $\Delta E$ is the change of energy between the initial and the final configurations of the system, the inverse excitation, once redefined the site energies, has energy $-\Delta E$. From Eq. (2), we have

$$\frac{\Gamma(\Delta E)}{\Gamma(-\Delta E)} = \exp(-\beta\Delta E).$$  \hspace{1cm} (4)

The probability per unit of time for an excitation of energy $\Delta E$ is proportional to the number of excitations at that particular energy. Thus,

$$\frac{\Gamma(\Delta E)}{\Gamma(-\Delta E)} = \frac{N(\Delta E)}{N(-\Delta E)}.$$  \hspace{1cm} (5)

From Eq. (3), we obtain that $F(\Delta E)$ follows a FDD at temperature $T$, i.e.,

$$F(\Delta E) = \frac{\Gamma(\Delta E)}{\Gamma(\Delta E) + \Gamma(-\Delta E)} = \frac{1}{1 + \exp(-\Delta E/k_{B}T)}.$$  \hspace{1cm} (6)

In equilibrium, it also holds that the probability of occupation follows a FDD at $T$ [13].

The natural variable for both $N(\Delta E)$ and $F(\Delta E)$ is the difference of energy between initial and final configurations in which occupations differ in generic sites $i$ and $j$, namely, $\Delta E_{ij} = \varepsilon_j - \varepsilon_i - 1/r_{ij}$ [2]. In Figure 1, it is shown the dependence of $N(\Delta E)$ on $\Delta E$ for $N = 2000$ and three equilibrium temperatures: 0.1 (black squares), 0.08 (red dots), and 0.06 (blue triangles). From this plot we can infer that excitations with $\Delta E \geq 0$ are dominant in equilibrium. From the ground state, all excitations must be positive. Figure 2 shows the dependence of $F(\Delta E)$ for $N = 2000$ and temperatures 0.1 (black squares) and 0.06 (red dots) in equilibrium. Solid curves represent the theoretical FDDs. Further, it has been verified that the fit to a FDD remains valid for smaller sizes, e.g., $n = 1000$ or $n = 500$.

![Figure 1: Single-particle number of excitations, $N(\Delta E)$, for temperatures 0.1 (black squares), 0.08 (red dots), and 0.06 (green triangles). Sample size is $N = 2000$. Positive excitations are dominant in equilibrium](image-url)
3 Excitation probability and effective temperature for stationary states

The occupation probability also follows a FDD at $T_{\text{eff}}$ in the simulations for relaxation, as pointed out. That result remains valid for excitations, once they have been divided into fast and slow ones. Some excitations of the system, mainly consisting of near sites, quickly reach equilibrium at $T$, so we shall label them as fast. By contrast, some other excitations are considered as slow, which are far from the ergodic limit and do not equilibrate at $T$. In this way, we find different time scales in the dynamics of Coulomb glasses [1, 8]. The standard procedure for choosing fast or slow excitations consists of a cut in distances. In our simulations, distances between sites $\leq 1$ are chosen as a limit for fast excitations, whereas excitation distances $> 10$ limit slow ones.

Traditionally, occupation probability has been employed to calculate $T_{\text{eff}}$ since it constitutes an unique FDD. However, its calculation depends on the selected chemical potential, which can be fixed at zero, half of the sum of the highest energy of an occupied site plus the lowest energy of an empty one for the ground state, or the same for each occupation state along time. When $n \rightarrow \infty$, the three criteria should lead to the same results, though numerical simulations in Coulomb glasses are still far from this limit. In Figure 3, it is shown the dependence of $T_{\text{eff}}$ on $1/L$ at equilibrium for the three criteria at $T = 0.01$, labeled as zero (black squares), ground (red dots) and levels (green triangles), respectively. Electric field is set as zero. When the system is in equilibrium, all the values of $T_{\text{eff}}$ should be equal to $T$, plotted as a horizontal line in the figure. In general, the best choice for the chemical potential regarding the occupation probability is the one that corresponds to the ground state. In fact, it presents a better behavior.

In general, the excitation probability, despite the cut in distances, does not depend on the chemical potential and shows better statistics than the occupation probability. Although it is employed in relaxation simulations ($\bar{\varepsilon} = 0$), the results obtained for stationary systems are even better, so we propose it as a standard method for calculating the effective temperature out of equilibrium in Coulomb glasses and other complex systems, including spin glasses. In Figure 4, there are shown the results of the simulations carried out under nonlinear conductivity for $n = 2000$ at $T = 0.1$ and $\bar{\varepsilon} = T$. The plot of $\Delta E$ vs. $F(\Delta E)$
The hopping length in Coulomb glasses is $l_H = \frac{1}{T} \sqrt{T_0}$ (c.f. [2]). According to [2], finite-size effects can be neglected when $l_H$ is much less than half the lateral dimension of the system, $L/2$. In our simulations, both the lowest temperature, $T = 0.06$, and the theoretical value $T_0 = 6.5$ (c.f. [2]) lead to $l_H \sim 2.6$. The lateral dimension of the samples is $L/2 \approx 22.4 \gg l_H$. Thus, the dynamics of our simulations do not present finite-size effects.

References