Elementary excitations and avalanches in the Coulomb glass

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Abstract. We study numerically the statistics of elementary excitations and charge avalanches in the classical Coulomb glass model of localized charges with unscreened Coulomb interaction and disorder. We compute the single-particle density of states with an energy minimization algorithm for systems of up to $100^3$ sites. The shape of the Coulomb gap is consistent with a power-law with exponent $\delta \simeq 2.4$ and marginally consistent with exponential behavior. The results are also compared with a recently proposed self-consistent approach. We then analyze the size distribution of the charge avalanches produced by a small perturbation of the system. We show that the distribution decays as a power law in the limit of large system size, and explain this behavior in terms of the elementary excitations. Similarities and differences with the scale-free avalanches observed in mean-field spin glasses are discussed.

1. Introduction
In this contribution, we study two related aspects of the physics of disordered systems of localized charges with long-range interaction. In Sec. 2, we reconsider the long-standing puzzle of the exponential suppression of the one-particle density of states in three dimensions, predicted long ago [1, 2] but never observed in numerical studies. In Sec. 3, we investigate the size distribution of the charge rearrangements, or avalanches, induced by a small displacement of a charge.

We consider the Coulomb glass model [1], in which $KN$ charges occupy $N = L^d$ sites arranged in a regular $d$-dimensional lattice of linear size $L$. The Hamiltonian in dimensionless units is

$$\mathcal{H} = \sum_{i<j}^{N} (n_i - K) \frac{1}{r_{ij}} (n_j - K) + \sum_{i=1}^{N} n_i \phi_i,$$

where $n_i \in \{0, 1\}$ is the occupation number for site $i$, and $\sum_{i=1}^{N} n_i = KN$. The $\phi_i$'s are independent, identically distributed Gaussian random variables with zero mean and standard deviation $W$.

2. Elementary excitations
As first pointed out by Pollak [3] and Srinivasan [4], the one-particle density of states (1-DOS), $g(\varepsilon) = N^{-1} \sum_{i=1}^{N} \delta(\varepsilon - \varepsilon_i)$, where $\varepsilon_i = \sum_{j \neq i}^{N} (n_j - 1/2)/r_{ij} + \phi_i$, is depleted near the Fermi level $\varepsilon_F$ due to the long-range interaction. Efros and Shklovskii [5] famously showed that the stability
of the ground state against one-particle hops requires \( g(\varepsilon) \) to vanish at \( \varepsilon_F \) (creating a so-called Coulomb gap) and to satisfy the bound

\[
g(\varepsilon) \leq c_d|\varepsilon - \varepsilon_F|^{d-1}
\]

near \( \varepsilon_F \), where the constant \( c_d \) depends on \( d \). Efros [1] and Baranovskii et al. [2] considered a self-consistent equation (SCE), that for \( K = 1/2 \) (which sets \( \varepsilon_F = 0 \)) and \( d = 3 \) reads

\[
g(\varepsilon) = g_0(\varepsilon) \exp \left[ -\frac{2\pi}{3} \int_0^\infty \frac{g(\varepsilon')d\varepsilon'}{(\varepsilon' + |\varepsilon|)^{\frac{3}{2}}} \right],
\]

where \( g_0(\varepsilon) \) is the bare 1-DOS. For asymptotically small \( \varepsilon \), the solution to Eq.(3) is \( g(\varepsilon) = (3/\pi)^{\frac{1}{2}} |\varepsilon| \), i.e. the bound in Eq.(2) is saturated. For \( d = 2 \), an analogous SCE gives asymptotically \( g(\varepsilon) = (2/\pi)|\varepsilon| \). The behavior \( g(\varepsilon) = c_d|\varepsilon - \varepsilon_F|^{d-1} \) is universal in the sense that it does not depend on the bare 1-DOS.

Due to the Coulomb gap, the low energy elementary excitations can be roughly divided [2] in charged excitations (adding or removing a charge from a site with \( |\varepsilon_i| < \Delta \), where \( \Delta \) is the gap width) and dipole excitations, i.e. electron-hole pairs at nearby sites \( i, j \) with \( (\varepsilon_j - \varepsilon_i) > \Delta \) and excitation energy \( \omega = \varepsilon_j - \varepsilon_i - 1/r_{ij} \ll (\varepsilon_j - \varepsilon_i) \).

If the dc conductivity is dominated by long one-particle hops, and the bound in Eq.(2) is saturated, the variable-range hopping \( T^{1/2} \) law follows [5, 1]. The dipole density of states (2-DOS) \( \phi(\omega) \) vanishes only logarithmically as \( \omega \to 0 \) in \( d = 3 \) [2, 6], thus low energy dipoles dominate ac conductivity and the specific heat.

Equation (2) does not consider the stability of the ground state against multi-particle hops, so an important question is whether these produce a harder gap in \( g(\varepsilon) \). In Refs.[1, 2] it was argued that, for \( d = 3 \), the stability against a charge excitation of energy \( \varepsilon \) and simultaneous excitation of dipoles at distance \( r < \varepsilon^{-1/2} \) from it requires \( g(\varepsilon) \) to vanish exponentially as \( g(\varepsilon) \propto P(\varepsilon) \) for \( \varepsilon \ll \Delta \), where \( P(\varepsilon) \) is given by Eq.(4) with \( f(x) = 1 \) and \( \gamma = 1.5 \). For \( d = 2 \), this criterion does not produce a hardening of the linear gap. Contrary to these results, recent mean-field studies [7] predict a quadratic \( g(\varepsilon) \) for \( d = 3 \), by connecting the shape of the gap to a putative glass transition. Subsequent numerical studies [8, 9, 10], however, provided evidence against the existence of such a transition.

Numerical computations of the 1-DOS in \( d = 3 \) have failed so far to observe an exponential gap, and generally favor a power law \( g(\varepsilon) = c_d|\varepsilon|^{\delta} \) with \( \delta \geq 2 \) [8, 11, 12, 13, 14]. Recently, Efros, Skinner, and Shklovskii (henceforth referred to as ESS) [15] proposed a modified SCE in which \( g_0(\varepsilon) \) in Eq.(3) is replaced by \( g_0(\varepsilon)P(\varepsilon) \), where

\[
P(\varepsilon) = \exp[-\gamma f(\Delta/\varepsilon)(\Delta/\varepsilon)\ln^{-7/4}(\Delta/\varepsilon)]
\]

and the crossover function \( f(x) = (1 - x)^\eta \theta(1 - x) \), with \( \eta > 7/4 \), is introduced to interpolate between the \( \varepsilon \ll \Delta \) regime and \( \varepsilon \simeq \Delta \) where \( P(\varepsilon) \simeq 1 \). The solution to this modified SCE gives asymptotically \( g(\varepsilon) \propto g_0(\varepsilon)P(\varepsilon) \) for \( \varepsilon \ll \Delta \) (a non-universal behavior since \( \Delta \) enters explicitly), and a softer behavior for \( \varepsilon \to \Delta \). ESS argue that this “delayed” onset of the exponential hardening is the reason why it has not been observed in numerical simulations.

2.1. Numerical results

We consider the Hamiltonian in Eq.(1) for \( d = 3 \) and \( K = 1/2 \) with periodic geometry, namely we surround the \( L^3 \) simulation cell with an infinite number of identical images, and sum over the interactions between site \( i \) of the central cell and site \( j \) of all the images using the Ewald method [10]. This gives an effective interaction \( r_{ij}^{-1} + v(r_{ij}) \), where \( v(r_{ij}) \) is a correction of order \( L^{-1} \) [16]. For each disorder realization (sample) \( \{\varphi_i\} \), we start from a random configuration and perform energy-decreasing one-particle hops chosen uniformly at random among all unstable
electron-hole pairs, until we reach a configuration stable against all one-particle hops, or pseudo ground state [17]. To this end, we use a modified version of the algorithm of Ref. [18] adapted to the periodic geometry [16].

We report here our results for $L = 100$. We simulate 32 (96) samples for $W = 2$ ($W = 4$). To reduce the sample-to-sample fluctuations of $\varepsilon_F$, which tend to fill the Coulomb gap, before averaging over samples we shift $g(\varepsilon)$ by $(\varepsilon_a + \varepsilon_b)/2$ for each sample, where $\varepsilon_a$ and $\varepsilon_b$ are such that $\int_{-\infty}^{\infty} d\varepsilon \, g(\varepsilon) = \int_{-\infty}^{\infty} d\varepsilon \, g(\varepsilon) = p$. In Fig.1 we plot $g(\varepsilon)W$ as a function of $\varepsilon W^{1/2}$, excluding energies affected by finite-size effects ($\varepsilon \lesssim 0.015$, as we determined from a finite-size scaling analysis [16]). For $0.1 < \varepsilon W^{1/2} < 0.4$ (or $0.07 < \varepsilon/\Delta < 0.26$, where we define $\Delta = (g_0(0)/\pi/3)^{1/2} = (18/\pi)^{1/4}/W^{1/2}$) the data are close to $g(\varepsilon) = (3/\pi)^2$, but a deviation is visible for small $\varepsilon$. We solved the modified SCE with the same numerical method and parameters ($\eta = 4, \gamma = 1.5$) as ESS for $g_0(\varepsilon) = (2\pi W^2)^{-1/2} \exp[-\varepsilon^2/(2W^2)]$. (For the box distribution, our solution agrees with theirs. Incidentally, we also solved numerically Eq. (3), finding oscillations in $\varepsilon$ around the asymptotic solution $3\varepsilon^2/\pi$ [19]). As shown in Fig.1, the solution for $W = 2$ is fairly close to the data at intermediate energies, but for small $\varepsilon$ it gives a steeper behavior. Taking $\eta = 3$ improves only slightly the agreement. For small $\varepsilon$ the data for $W = 2, 4$ are superimposed, consistent with the asymptotic scaling $g(\varepsilon) \sim g_0(\varepsilon)P(\varepsilon)$, but are actually far from the function $g_0(\varepsilon)P(\varepsilon)$, showing that much smaller energies are needed to see the exponential hardening.

The deviation from both the quadratic behavior and the modified SCE becomes very clear by plotting $g(\varepsilon)/\varepsilon^2$, see Fig.2. The data are also consistent with $g(\varepsilon) = c_d|\varepsilon|^\delta$ with $\delta \simeq 2.4$ for $\varepsilon W^{1/2} < 0.2$, displayed with the sloped line in Fig.2. In fact, the data for different $W$ are well described by $g(\varepsilon) = a_d|\varepsilon|^\delta W^{1-\delta/2}$ with $\delta \simeq 2.4, a_d \simeq 2$.

To estimate the systematic error due to pseudo ground states not being true ground states, we ran the algorithm 20 times per sample for a subset of 196 samples with $L = 60, W = 2$. The sample-averaged $g(\varepsilon)$ computed with the pseudo ground states $a$ and $b$ with lowest and highest energy for each sample agree within the error bars. In average, $a$ and $b$ differ in only $\simeq 1\%$ of the sites, and their relative energy difference is very small ($\simeq 2.5 \cdot 10^{-5}$, a factor $10^2$ smaller than the
sample-to-sample energy fluctuation). Hence, it seems unlikely that this systematic error affects our conclusion. We report elsewhere [16] these tests and a detailed finite-size scaling analysis.

In an earlier work [8] we found evidence for a quadratic gap from a scaling analysis of the temperature and energy dependence of the 1-DOS obtained with equilibrium Monte Carlo. While those results are unaffected by the above systematic error (equilibration was carefully checked), they are limited to $L \leq 10$, so because of the finite-size effects below $\varepsilon \sim L^{-1}$ we could only explore the energy range in which the data in Figs.1,2 are approximately quadratic. In this energy range the present data and those of Ref.[8] agree quantitatively, despite being obtained with completely different algorithms.

In conclusion, the data from pseudo ground states show a clear deviation from a quadratic gap and are consistent, in the energy range reached, with a power-law gap with exponent $\geq 2.4$, in agreement with Refs.[11, 12]. The data also agree qualitatively but not quantitatively with the scenario of ESS. Much larger systems will be needed to discriminate between an exponential and a power-law gap.

3. Charge avalanches

Let us now consider the following numerical experiment. Starting from a pseudo ground state found as in Sec.2, we perturb it by inserting an extra charge or by exciting a dipole. This will in general destabilize some electron-hole pairs. We then relax one of the unstable pairs, which in turn creates new unstable pairs, and continue in this way until we stop upon reaching a new pseudo ground state, after a number $S$ of hops. Avalanche processes of this kind have been studied in disparate systems such as earthquakes, sandpiles, and Barkhausen noise in magnets [20]. A well studied theoretical example is the random field Ising model (RFIM). The RFIM Hamiltonian is identical to Eq.(1) when we take $K = 1/2$ and truncate the interaction to nearest neighbors. In Ref.[21] avalanches were triggered by a small uniform external field that destabilizes only one spin, and evolved via zero-temperature single spin-flip dynamics. At a critical value of the disorder $W = W_c$, the probability distribution of the avalanche size was found to decay as

$$p(S) \sim S^{-\tau}\exp(-S/S_c)$$

(5)

for large $S$, where $\tau = 1.60 \pm 0.06$ and $S_c$ is a cutoff that diverges with the system size. Hence, $p(S)$ is scale-free in the thermodynamic limit, $L \rightarrow \infty$. For $W > W_c$, the cutoff tends to a finite value $S_c \rightarrow S^*$ for large $L$, with $S^* \rightarrow \infty$ as $W \rightarrow W_c$. For $W < W_c$ there are system-size avalanches with finite probability [21].

Pazmandi et al. [22] simulated the same dynamics in the infinite-range Sherrington-Kirkpatrick (SK) spin glass model and found a power-law behavior with a cutoff proportional to the system size, and estimated $\tau \approx 1$. Unlike in the RFIM, however, this did not require fine-tuning of parameters (the criticality is “self-organized” [22]). Recently, the authors of Ref.[23] related the equilibrium avalanches in the SK model to the marginal criticality of its equilibrium glass phase, and obtained the analytical result $p(S) \sim S^{-\tau}$ with $\tau = 1$. It was suggested that a scenario similar to that of the SK model might be at play in the Coulomb glass [24, 23]. Although a glass phase was ruled out numerical studies down to very low temperatures [8, 9, 10], the possibility remains that the system is critical at zero temperature. It is thus interesting to ask whether the avalanches are scale-free. Avalanches in the Coulomb glass provide a mechanism for nonlinear screening [25, 26], which is relevant for capacitance and conductance experiments on disordered insulators and granular metals [27, 28].

Figure 3 shows $p(S)$ from the numerical experiment described above for $d = 3$, $W = 2$, and $K = 1/2$. The avalanches are triggered by exciting the lowest energy dipole that produces an instability and are evolved by random hops as in Sec.2. The most important feature of Fig.3 is the exponential cutoff that increases linearly with $L$. As shown in Fig.4, the data can be rescaled according to Eq.(5) with $\tau \approx 1.5$ and $S_c = aL$, $a \approx 0.48$. A form $p(S) \sim S^{-\tau}\exp[-(S/\alpha T)^2]$ also
fits reasonably well $\tau \simeq 1.7$ and $S_c \propto L$. This scale-free behavior (extrapolating to $L \to \infty$) is robust and does not require fine tuning. In fact, we observe a divergent cutoff for other values of $K$ near $1/2$, when hops are performed in order of increasing hopping length instead of uniformly at random, and even for huge disorder ($W = 32$).

**Figure 3.** Avalanche size distribution for dipole-triggered avalanches. The data are averaged over 20000, 48000, 29000, 2135 samples for $L = 8, 16, 30, 60$ respectively.

**Figure 4.** Scaling plot of the avalanche size distribution assuming Eq.(5) with $\tau = 3/2$ and $S_c = aL$. $A(a,L)$ is a normalization factor slowly varying with $L$, computed analytically from the branching process model.

Although these results may suggest an analogy with the self-organized critical avalanches of the SK model, we argue that they can be understood more simply in terms of the elementary charged and dipole excitations, without invoking a critical glass phase. We repeated our numerical experiment forbidding hops longer than a certain fixed length $R_{\text{max}}$ independent of $L$, and found that in this case $p(S)$ has an exponential cutoff that does not increase with $L$ [16]. If we choose $R_{\text{max}}$ proportional to $L$, we find again $S_c \propto L$, which demonstrates that scale-free avalanches require arbitrarily large hops. In a glass phase the critical avalanches arise due to an infinite correlation length [7, 23], thus in our understanding the scale-free behavior should be present also for finite $R_{\text{max}}$, contrary to our results.

We can understand qualitatively how scale-free avalanches arise by considering the response to dipole and charge excitations, neglecting correlations among successive hops. When a dipole is excited, a number $O(\phi(0) \log L)$ of dipoles become unstable due to the $1/r^3$ dipole-dipole interaction (we neglect here the logarithmic gap of the 2-DOS $\phi(\omega)$). These are mostly near the excited dipole (the probability to find an unstable dipole at distance $r$ decays as $1/r$), thus the avalanche cannot propagate far if only short hops are allowed. In addition to the dipoles, a certain number of arbitrarily long pairs also become unstable. A long hop can create a charged excitation in a region still untouched by the avalanche. The charged excitation destabilizes a number $O(\phi(0)L)$ of dipoles. When one of these dipoles flips it creates, as we just argued, a local finite avalanche and, with finite probability, new long unstable pairs. This process can be thought of as a branching process with branching ratio unity, which gives critical avalanches with $\tau = 3/2$. The above argument also explains why $S_c$ is linear in $L$. In fact, the cutoff is determined by long hops that reach the boundary of the system. Since a long hop creates a
number \( O(L) \) of subsequent hops, \( S_c \propto L \) follows. By the same argument, for \( d = 2 \) the cutoff scales as \( S_c \propto \log L \), which indeed we observe numerically [16].

An avalanche exponent \( \tau = 3/2 \) is typical of mean-field models [29]. In this spirit, the branching process model considers the avalanche as a collection of independent events. Let us just mention that in this model, \( p(S) \) for avalanches triggered by a charge injection (instead of a dipole excitation) is given by a convolution of \( M \) Galton-Watson processes, corresponding to subavalanches initiated by dipoles made unstable by the charge injection, where \( M \) is a Poisson variable with \( O(L) \) mean, and fits well our numerical results [19].

We conclude by noting that in a physical dynamics with distance-dependent hopping probability, time introduces a cutoff on the maximal hopping length, and thus on the power-law tail of \( p(S) \). We expect that a nonzero temperature produces a similar effect. Avalanches at finite temperature could be studied with a “damage spreading” algorithm [30].

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