Study of three-dimensional Coulomb Glass model using mean field approximations

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Recently a mean-field theory about a local minimum was used by [Amir et al., Phys. Rev. B 77, 165207 (2008)] to discuss the relaxation of the Coulomb glass system. In this paper, we present the analysis of the dynamics of the Coulomb Glass lattice model in three dimensions near a local equilibrium state by using mean-field approximations. We specifically focused on understanding the role of localization length and the temperature on small fluctuation about the equilibrium state. We used the eigenvalue distribution of the dynamical matrix to characterize relaxation laws as a function of localization length at low temperatures. The variation of the minimum eigenvalue of the dynamical matrix with temperature and localization length is discussed numerically and analytically. We show that our results for the slow relaxation can be well understood by understanding the role played by the density of states in relaxation dynamics.

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I. INTRODUCTION

The term Coulomb Glass (CG) refers to that category of disordered insulators that have a sufficiently high disorder, which leads to localized electronic states coupled with the Coulomb interactions. The presence of a glass phase in this model has been predicted theoretically by several authors [2–6]. In dimensionless units, the Hamiltonian for CG lattice model is defined [7] as

\[
\mathcal{H}\{n_i\} = \sum_{i=1}^{N} \epsilon_i n_i + \frac{1}{2} \sum_{i \neq j} \frac{e^2}{\kappa |r_i - r_j|} (n_i - 1/2)(n_j - 1/2)
\]

(1)

Where, \(\epsilon_i\)'s are the on-site random field energy and the occupation number \(n_i \in \{0, 1\}\). The electrons at site \(i\) and \(j\) interact via unscreened Coulomb interaction \(\frac{e^2}{\kappa r_{ij}}\) where \(\kappa\) is the dielectric constant.

Much work has been done to find the ground state of the CG model at high disorder. Using mean fields approach [3], Monte Carlo simulation [8–10] and other optimization [11, 12] approaches it has been found that there exist many metastable states (pseudo ground states) at low temperatures. This metastability is responsible for glassy behaviour. The density of states (DOS) found in all these approaches shows a soft gap \(g(E) \sim E^\delta\) around the Fermi level \(E_F\). The value of \(\delta\) is very near to the theoretical prediction of \(d-1\) (\(d\) is the dimensionality of the system) given by Efros and Shklovskii [7]. Recently Müller and Ioffe have established a connection between the presence of a glassy phase and the appearance of a soft gap in three dimensional CG model using locator approximation [20]. The formation of a gap in DOS effects the conductivity (\(\sigma\)) quiet significantly. One can see that the conductivity changes from the Mott’s law [21, 22] of \(\ln \sigma \sim (T_M/T)^{1/4}\) to the Efros-Shklovskii’s \((T_{ES}/T)^{1/2}\) law [7] at low temperatures.

The existence of glass transition in three dimensional CG is still controversial and a matter of active research [23–26]. Some mean-field analysis of this system also suggests the existence of stable a glassy phase [21, 27–29]. Experiments on CG systems have exhibited non ergodic behaviour [30–37]. Non-equilibrium dynamics of Structural and spin glasses has been studied using scaling properties of non-stationary correlation and response functions [38–43]. Various numerical simulations claim that the CG model exhibits glassy behaviour i.e. slow relaxation [44–49], aging [38, 47] and memory effects [36, 57]. The numerical and theoretical work mostly uses transitions between different minimas (pseudo ground states) to explain the non equilibrium experimental results. However few authors have approached this problem differently, by considering the system in the vicinity of a single valley [1, 47, 48, 50]. Amir et al [1] showed that the small fluctuations about an equilibrium relax as \(\ln(t)\). They show that the slow relaxation is primarily due to isolated localized states that have a long lifetime. In their work on the CG model (a disorder in site energies as well as the position of sites) with small localization lengths, slow dynamics occur without interactions. The soft gap in the DOS exists, but it is not relevant to
dynamics. In this paper, we are also concentrating relaxation of fluctuations about a minimum (single valley picture) for the lattice CG model. In the lattice model, the disorder comes only from site energies, so the question of having isolated states does not exist. Instead, we find that the states near the Fermi level are very stable and any fluctuations in them relax very slowly. The existence of a gap in DOS means that these states are in a certain sense isolated energetically, which for long times leads to a power-law ($t^{-\alpha}$) like decay, where $\alpha$ depends upon the localization length.

The goal of this paper is to develop a formalism that accounts for the correlations between the dynamics of a system with the occurrence of the Coulomb gap. The paper is organized as follows. In Sec. II we have provided an overview of our derivation of the linear dynamical matrix. In Sec. III we present a detailed discussion of our mean-field results obtained numerically and analytically. And finally in Sec. IV we provide the conclusions of our work.

II. DYNAMICS

The most general non-conserved dynamics on the total probability distribution of the spins was developed by Glauber [51]. This was extended to conserved dynamics by Kawasaki who incorporated the constraint of fixed magnetization. The Kawasaki formulation [52, 53] applies to CG as the electron number is conserved - which is equivalent to fixed magnetization. Here we deal with the probability distribution of $P(n_1 \ldots n_N; t)$, which involves the occupation of all the sites in the system. The Kawasaki dynamics holds for the interacting system as well as multi-particle dynamics. Since this approach is general, it can be taken beyond the mean-field theory. However, since several approximations are involved, one has to choose them such that results of the single-particle master equation are recovered.

Now, the time evolution of a system can be described using a generalized master equation [54]

$$\frac{d}{dt} P(n_1 \ldots n_N; t) = - \sum_{i \neq j} W_{i \rightarrow j} P(n_i, t) \times P(n_1 \ldots n_N; t) + \sum_{j \neq i} W_{j \rightarrow i} P(n_j, t) \times P(n_1 \ldots n_N; t)$$

(2)

where $W_{i \rightarrow j}$ denotes the transition rates from state $i$ to $j$ and $P(n_i, t)$ is the probability of finding the system in state $i$ at time $t$. The transition rates can be single or multi-electron transfer. Since we are interested in Kawasaki dynamics, only transitions that conserve the particle (electron) number will be considered. Using single-particle transitions, the Kawasaki dynamics equation can be rewritten as

$$\frac{d}{dt} P(n_1 \ldots n_N; t) = - \sum_{i \neq j} \omega_{i \rightarrow j} n_i (1 - n_j) \times P(n_1 \ldots n_N; t) + \sum_{i \neq j} \omega_{j \rightarrow i} \tilde{n}_j (1 - \tilde{n}_i) \times P(n_1 \ldots n_N; t)$$

(3)

where $\omega_{i \rightarrow j}$ is the transition probability from site $i$ to $j$ and $\tilde{n}_i = 1 - n_i$. Now we impose the condition of "detailed balance", so that the evolution is towards thermal equilibrium. In thermal equilibrium,

$$\omega_{i \rightarrow j} n_i (1 - n_j) = \omega_{j \rightarrow i} \tilde{n}_j (1 - \tilde{n}_i)$$

(4)

$$\omega_{i \rightarrow j} = \frac{\exp(-\beta E_i)}{\exp(-\beta E_j)}$$

(5)

The energy required to transfer an electron from $i$ to $j$ is

$$\Delta E_{ij} = E_i(1, \ldots, \tilde{n}_i, \ldots, \tilde{n}_j, \ldots) - E_i(1, \ldots, n_i, \ldots, n_j, \ldots),$$

$$= \epsilon_j - \epsilon_i + \sum_{m \neq i} K_{jm} n_m - \sum_{m \neq j} K_{im} n_m,$$

$$= \tilde{E}_j - \tilde{E}_i.$$

(6)

where

$$\tilde{E}_j = \epsilon_j + \sum_{m \neq i} K_{jm} n_m,$$

$$\tilde{E}_j = E_j - K_{ij} n_i,$$

(7)

and $E_j$ is the Hartree energy: $E_j = \epsilon_j + \sum_m K_{jm} n_m$. We can then rewrite eq. (6) as

$$\Delta E_{ij} = E_j - E_i - K_{ij}(n_i - n_j),$$

$$= E_j - E_i - K_{ij}.$$  

(8)

hence we get $\omega_{i \rightarrow j} = e^{-\beta \Delta E_{ij}}$. So we choose our transition probability as

$$\omega_{i \rightarrow j} = \frac{\gamma_{ij}}{2\tau} \frac{1}{\exp(-\beta \Delta E_{ij}) + 1}$$

(9)

where $\tau$ is a hopping time scale. With this choice, master equation takes the form

$$\frac{d}{dt} P(n_i; t) = - \sum_{i \neq j} \frac{\gamma_{ij}}{2\tau} n_i (1 - n_j) \times$$

$$f(\Delta E_{ij}) P(\ldots, n_i, \ldots, n_j, \ldots; t) -$$

$$f(\Delta E_{ij}) P(\ldots, \tilde{n}_i, \ldots, \tilde{n}_j, \ldots; t)$$

(10)

Here $f(E) = \frac{1}{\exp(\beta E) + 1}$ is the Fermi-Dirac distribution, $\gamma_{ij} = \gamma(\epsilon_{ij})$ is a factor independent of temperature, but
depends on the distance between sites \( i \) and \( j \). For hopping electrons \( \gamma_{ij} = \gamma_0 e^{-r_{ij}/\xi} \), where \( \gamma_0 \) is a constant.

From this one, can derive an equation for time-dependent averages or moments. To connect to the one-particle master equation, we consider

\[
N_i(t) = \sum_{\{n_i\}} n_i P(n_1 \ldots n_N; t)
\]

who time derivative gives

\[
\frac{d}{dt} N_i(t) = -\frac{1}{2\tau} \sum_{j \neq k} \gamma(r_{jk}) \sum_{\{n_i\}} n_i n_j (1 - n_k)
\]

\[
[f(\Delta E_{kj}) P(n_1 \ldots n_v; t) - f(\Delta E_{jk}) P(n_1 \ldots \tilde{n}_j \ldots \tilde{n}_k \ldots ; t)]
\]

Again if \( i \neq j \) or \( i \neq k \), a change of summation variables \( j = k \) makes the two terms cancelled. The only surviving terms comes from \( i = j \),

\[
\frac{d}{dt} N_i(t) = -\frac{1}{2\tau} \sum_{k \neq i} \gamma(r_{ik}) \sum_{\{n_i\}} n_i (1 - n_k)
\]

\[
[f(\Delta E_{ki}) P(\ldots n_i \ldots n_k \ldots ; t) - f(\Delta E_{ik}) P(\ldots \tilde{n}_i \ldots \tilde{n}_k \ldots ; t)]
\]

\[
= -\frac{1}{2\tau} \sum_{k \neq i} \gamma(r_{ik}) [(n_i (1 - n_k) f(\Delta E_{ki}))_t - \langle (1 - n_i) n_k f(\Delta E_{ik}) \rangle_t] 
\]

Here \( \langle \ldots \rangle_t \) denotes average at time \( t \). Though this is an exact equation, the rhs contains higher-order correlations in occupation numbers. To get a closed set of equations, one needs to apply mean-field approximation to eq. (13).

**Mean-Field Approximation**

The mean-field approximation consists of making the assumption

\[
\langle f(n_1 \ldots n_N; t) \rangle = f(N_1(t) \ldots N_N(t))
\]

With this assumption we get

\[
\frac{d}{dt} N_i(t) = -\frac{1}{2\tau} \sum_{k \neq i} \gamma(r_{ik}) \left[ N_i (1 - N_k) f_{FD}(E_k - E_i) - N_k (1 - N_i) f_{FD}(E_i - E_k) \right]
\]

where \( E_i \) and \( E_k \) are the Hartree energies at site \( i \) and \( k \) respectively. Now let us linearise this equation about an equilibrium solution.

\[
N_i(t) = f_i + \delta N_i
\]

\[
E_i^e = \epsilon_i + \sum_l K_{il} f_i
\]

where \( f_i = \frac{1}{\exp(\beta E_i^e) + 1} \). Putting eq. (16) and eq. (17) into eq. (15) one gets,

\[
\frac{d}{dt} \delta N_i = -\frac{1}{2\tau} \sum_{k \neq i} \gamma_{ik} \left[ (f_i + \delta N_i)(1 - f_k - \delta N_k) f_{FD}(E_k^e - E_i^e + \sum_l (K_{kl} - K_{il}) \delta N_l) - (f_k + \delta N_k)(1 - f_i - \delta N_i) f_{FD}(E_i^e - E_k^e + \sum_l (K_{il} - K_{kl}) \delta N_l) \right]
\]
where we define

\[ \Gamma_{ik} = \frac{1}{2\pi} \gamma(r_{ik}) \ f_i(1 - f_k) \ f_{FD}(E_k^* - E_i^*) \] (20a)

\[ \Gamma_{ki} = \frac{1}{2\pi} \gamma(r_{ki}) \ f_k(1 - f_i) \ f_{FD}(E_i^* - E_k^*) \] (20b)

\[ A_{ii} = -\sum_{k \neq i} \frac{\Gamma_{ik}}{f_i(1 - f_i)} \] (20c)

\[ A_{il} = \frac{\Gamma_{li}}{f_i(1 - f_l)} + \frac{1}{T} \sum_{k \neq i} \frac{\Gamma_{ik}}{f_k(1 - f_k)} (K_{ki} - K_{li}) \] (20d)

And the final linear equation using the detailed balance is,

\[ \frac{d}{dt} \delta N_i = \sum_{k \neq i} \left[ \frac{\delta N_i}{f_i(1 - f_i)} \Gamma_{ik} - \frac{\delta N_k}{f_k(1 - f_k)} \Gamma_{ki} + \frac{1}{T} \sum_{k \neq i} \Gamma_{ik} (K_{ki} - K_{li}) \delta N_l \right] \]

\[ = \sum_i A_{il} \delta N_l \] (19)

where we define

\[ \Gamma_{ik} = \frac{1}{2\pi} \gamma(r_{ik}) \ f_i(1 - f_k) \ f_{FD}(E_k^* - E_i^*) \] (20a)

\[ \Gamma_{ki} = \frac{1}{2\pi} \gamma(r_{ki}) \ f_k(1 - f_i) \ f_{FD}(E_i^* - E_k^*) \] (20b)

\[ A_{ii} = -\sum_{k \neq i} \frac{\Gamma_{ik}}{f_i(1 - f_i)} \] (20c)

\[ A_{il} = \frac{\Gamma_{li}}{f_i(1 - f_l)} + \frac{1}{T} \sum_{k \neq i} \frac{\Gamma_{ik}}{f_k(1 - f_k)} (K_{ki} - K_{li}) \] (20d)

It is easy to verify that \( \Gamma_{ik} = \Gamma_{ki} \). Thus the final linear equation has the form which is the same as used by Amir et al. Here \( A \) is the linear dynamical matrix governing the dynamics of the system near equilibrium and \( \Gamma_{ik} \) are the equilibrium transition rates.

\[ \text{FIG. 2: (Colour online) (a)-(c) Distribution of the eigenvalues obtained by solving Eq.20 at different temperatures (} T = 0.33 \text{ in blue, } T = 0.20 \text{ in red and } T = 0.10 \text{ in black). } \xi \text{ is the localization length here. The graph is averaged over 100 instances. System size is } N = 16^3. \text{ (d)-(f) Low eigenvalue distribution at each correlation length is fitted into a power-law function for } T = 0.1. \]

\[ \text{FIG. 3: (Colour online) Comparison of the eigenvalue distribution of the full A-matrix (in black) with the ones obtained after neglecting the second term in Eq.20(b) (in red) at different } \xi \text{ for } T = 0.10 \text{ is done here.} \]

\[ \text{III. RESULTS AND DISCUSSIONS} \]

\textbf{A. Coulomb Gap}

The method: To calculate the Hartree energy \( (E_i) \) given in Eq. 17, we have first calculated the magnetization, which, approximated within the mean-field theory is defined as

\[ m_i = \tanh \beta \left( \epsilon_i + \sum_k \frac{m_k}{f_k} \right) \] (21)

The above equation was solved self-consistently and the final \( m_i \)'s were then used to calculate \( E_i \)'s using \( f_i = (m_i + 1)/2 \). We have annealed our data from \( T = 1 \) to \( T = 0.1 \), and the on-site energy \( \epsilon_i \) was chosen randomly from a box-distribution of width \( \pm W/2 \) where \( W = 1 \) and \( \beta = 1/T \).

It is well established now that in the CG model, a soft gap, also called the Coulomb gap, is observed in single-particle DOS at low temperatures. The gap gets filled as the temperature increases. In this paper, the temperatures where the soft gap is well established are referred to as low temperatures (i.e. \( T = 0.2 - 0.1 \)). Efros and Shklovskii have further argued that at zero temperature, DOS follows the relation \( g(E) \approx E^{d-1} \) in d-dimensional CG model. In Fig. 4(a), one can see formation of a soft gap in DOS after \( T = 0.33 \). We further found that at \( T = 0.1 \), the DOS can be well fitted by the relation \( g(E) \propto E^2 \) (see Fig. 4(b)) as suggested by Efros and Shklovskii.

\[ \text{B. Linear Dynamical Matrix} \]

In Fig. 5(a-c), we show the distribution of the eigenvalues of a linear dynamical matrix \( (A - \text{matrix}) \) at different temperatures and localization lengths. The eigenvalues (\( \lambda \)) here determine the rate of decay in the system.
With the decrease in temperature, the shifting of $\lambda$ towards zero indicates a slowing down of relaxation with decreasing temperature. The important question here is what relaxation law does the system obey at low temperatures where one expects slow relaxations. At $T = 0.1$, we found that the low eigenvalue distribution follows a power-law relation $P(\lambda) \sim \lambda^\alpha$ (see Fig.2(d-f)). This implies that the correlation function $C(t) = \langle \delta n(t)\delta n(0) \rangle$ obeys $C(t) \sim 1/t^{(\alpha+1)}$ at long times. Fig.2(d-f) also shows that the value of $\alpha$ is increasing as the localization length decreases.

It is well known that for $t \gg \lambda_{\text{min}}$, the correlation function behaves as $e^{-\lambda_{\text{min}}t}$. We now want to look at the behaviour of $\lambda_{\text{min}}$ as a function of temperature and correlation length. Note that the interaction part in the $A$-matrix (second term in Eq.(20(d))) does not contribute much to the eigenvalue distribution at low temperatures as shown in Fig. 3(a-c) for all localization lengths considered. In fact for $\xi = 1$, the eigenvalue distributions (at low $T$) are mostly determined by the diagonal part of the $A$-matrix. This means that the lowest eigenvalue ($\lambda_{\text{min}}$) is the smallest value of $A_{ii}$ (which is defined as $A_{\text{min}}$). In Fig.3(a), we found that $A_{\text{min}} \propto T^3$ for $\xi = 1$, the proof of which is as follows:

**Proof:** $A_{\text{min}} \propto T^3$.

Using Eq.(20(c)), we calculated the $A_{ii}$’s and found that they are smallest for sites around the Fermi level ($E \approx \mu$ and so $f_i \approx 0.5$), which makes Eq.(20(c)) as

$$A_{\text{min}} = -4 \sum_{k \neq i} \Gamma_{ik}$$

$$= -4 \sum_r \sum_{E_{\text{electron}}} e^{-r/\xi} e^{-|E|} F(r,E)$$

(22)

here $F(r,E)$ is the probability of finding an electron or hole having the Hartree energy $E$ at a distance $r$ from a site $i$. Since $\xi$ is large, the electrons will hop to a site so as to minimize the factor $(r/\xi + |E|)$. Neglecting the correlation between $r$ and $E$, then the above Eq.(22) can be rewritten as

$$A_{\text{min}} \approx -4 \sum_r e^{-r/\xi} \int_0^{E_{\text{max}}} g(E) e^{-|E|} dE$$

(23)

$g(E)$ is the density of states (DOS) of single-particle Hartree energies ($E$). As discussed earlier, our results (see Fig.3(b)) shows that $g(E) \propto E^{2.0}$. Substituting that in Eq.(23) we get

$$A_{\text{min}} \propto T^3$$

(24)

We now look at the behaviour of low temperature $\lambda_{\text{min}}$ values at small correlation length ($\xi = 0.2$). In this case, firstly the $A_{ii}$ distribution is different from the eigenvalue distribution, but the minimum value remains almost the same. More importantly, one should note that the above arguments for $A_{\text{min}}$ for the temperature range considered ($T = 0.2 - 0.1$) does not work well when the correlation length is very small. For instance, when $\xi = 0.2$, the major contribution to $A_{\text{min}}$ comes from the nearest neighbour sites only (i.e. $r = 1$). This means that the correlation between $r$ and $E$ cannot be neglected. So one has to find $F(r = 1, E)$ which is the two particle nearest neighbour DOS and insert it in Eq.(20(c)). We show $F(r = 1, E)$ at different temperatures in Fig. 0 for $0 < E_i \leq -0.1$. Unlike Fig.1(a), there is a hard gap in $F(r = 1, E)$ for small energy electrons at low temperatures. This is not surprising, since if one was working with true ground state, then there is a hard gap $O(1)$ in $F(r = 1, E)$. The reason behind it is that the ground state is stable against any single electron-hole transition which implies $E_h - E_e - 1/\tau_{eh} > 0$. This means that $|E_h| + |E_e| > 1$ for any nearest neighbour electron-hole pair. This implies that Eq.(20(c)) now reduces to

$$A_{\text{min}} \approx -e^{-1/\xi} \sum_j e^{-\Delta E_{ij}/T}$$

(25)

where $\Delta E_{ij}$ is the energy difference between site $i$ and its nearest neighbours $j$. In Fig.2 we have shown that $A_{\text{min}}(T)$ indeed follows the above relation at $\xi = 0.2$. So our analysis of $A_{ii}$ matrix shows that $\lambda_{\text{min}}$ obeys different scaling laws as one reduces the correlation length at low temperatures.

**IV. SUMMARY**

We have studied the relaxation properties of three dimensional Coulomb glass lattice model using mean-field approximations. The eigenvalues of a linear dynamical matrix were used to find out the rate of decay in the system. Analysis has been done at low temperatures where the gap in the single-particle density of states is almost quadratic as expected from the Efros-Shklovskii’s law. We found that at small temperatures, the system will show a power-law decay at long times for all localiza-
\[ \ln (A_{ii}) = -3.9218 - \left(\frac{0.5596}{T}\right) \]

FIG. 5: (Colour online) Lowest value of the diagonal part of $A$ – matrix at $\xi = 0.2$ calculated using Eq. (20(c)), which is averaged over 100 configurations are plotted against temperature. The solid line shows that the data fits well with $\ln(|A_{ii}|) = -3.9218 - \left(\frac{0.5596}{T}\right)$ relation.

FIG. 6: (Colour online) (a)-(d) Distribution of the Hartree energy on site $k$, $E_k$ (where $k$ are the 6 nearest neighbour sites of $i$) at different temperatures, when the Hartree energy on site $i$, $E_i$ are chosen from the interval $[-0.1, 0.0]$. The relaxation becomes slower as the localization length decreases. Finally, we have found that although the full eigenvalue distribution is not much affected by the Coulomb interaction term in the linear dynamical matrix but one can gain a better understanding of the behaviour of low temperature dynamics if you look at the role of gap in the density of states in the decay process. The gap in density of states exists due to long range nature of Coulomb interactions and so the interactions play an important role in the relaxation process.

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