Chapter 3

Simulations in Coulomb Glass

Introduction

The numerical work in Coulomb glass problem has been a key to test the various theoretical ideas and to understand experimental results. The key physical results are concerned with the density of states (DOS) of site Hartree energies and DOS of the electron-hole excitations. As mentioned in the section 1.8.2, Efros and Shklovskii (ES)[16, 17] have argued that the DOS $g(\epsilon)$ for the Hartree energies is proportional to $g(\epsilon) \propto \epsilon^{d-1}$, where ϵ is measured from the Fermi energy. They further pointed out that this result has profound influence on the conductivity in the VRH regime. Due to the depletion of the DOS around the Fermi level, the conductivity will obey Efros-Shklovskii law, $\sigma = \sigma_0 \exp[-(T_{ES}/T)^{1/2}]$, rather than the Mott's $T^{1/4}$-law.

There is lot of controversy regarding the exact nature of DOS in the numerical literature. The first set of numerical studies were done by Baranovskii *et al* [42]. They found that numerical results for DOS for Hartree energies to be in good agreement with the ES theory. But the later studies by Mochena and Pollak [47, 48] found DOS to be a more rapidly increasing function of energy than predicted by theory. They claim that they have found many more of the low lying energy states of the system than is possible by the method of Baranovskii *et al* [42]. The next set of studies have come from Mobius *et al* [71] and Sarvestani *et al* [72]. They find the opposite result that the

DOS is smaller than the theoretical predictions especially for energies close to the Fermi level. They report the exponent of energy to be greater than $d-1$ in both two and three dimensions. Mobius *et al* have obtained the ground states by stabilizing the system with respect to two electron hops, in contrast to the earlier work [42] (Baranovskii *et al*), in which the ground states were stabilized for one-electron hops only. The idea was to look for constraints imposed by low-energy dipole excitations which as Efros argued lead to an exponential form for the density of states given in equation (1.49). No evidence of the exponential behavior resulting from such excitations was found. This indicates that the density of dipole configuration as envisaged by Efros [37] and Baranovskii *et al* [73] is not very significant. Davies *et al* [40, 41] also found that for a two and three dimensional system $g(\epsilon)$ to be smaller than the theoretical predictions for energies close to chemical potential. For a two dimensional system they find that the DOS obeys a power law with exponent 3/2. For a three dimensional system their DOS fitted the exponential form very well. The parameters were though in poor agreement with the predictions of Efros. To calculate the exponential form Efros had assumed that density of states of dipole excitations is a constant. The density of dipole excitations is the number of electron-hole pairs with excitation energy $\epsilon_h - \epsilon_e - 1/r_{eh}$ per unit volume. Davies *et al* found a gap in the density of states of dipole excitations for a three dimensional system. Since the lowering of DOS near the chemical potential seem to happening for both two and three dimensions one can just conclude that a mechanism different from Efros (constraints imposed by low energy dipole excitations) is responsible for lowering the DOS.

The calculation of conductivity involves density of states of electron-hole excitations. At low temperatures, it is believed that the multi-electron excitations will have a greater role in determining the dc conductivity of the system rather than the single electron excitations. Knotek and Pollak [38, 39], and Efros [16] have stressed that many electron excitation like polarons will be important at low temperatures. Little evidence of pola-

ronic type multi-electron excitation has been found in the numerical studies by Mochena and Pollak [47, 48]. They find that most of the excitations at low temperatures to be cascade or successive correlations type. Pollak and Knotek [38, 39] have argued that these excitations play a key role in determining the conductivity at low temperatures. Perez *et al* [74] have also used percolation method to calculate the conductivity between the low lying energy configurations of the interacting system. They found that conductivity obeys the ES-law, but the value of T_{ES} was found to be much smaller than that predicted by the theory. They attributed this decrease to the effect of successive and collective correlations on conductivity. They found both hop distance and hop energy to be proportional to the critical conductance of the network. They concluded that VRH mechanism aided by sequential or successive correlation is the correct hopping picture at low temperatures. The cascade type excitations do not seem to be important.

We have undertaken numerical calculations for two-dimensional Coulomb glass to resolve some of the above issues. As described earlier, the Hamiltonian for the Coulomb glass system can be written as,

$$H = \sum_i \phi_i s_i + \frac{1}{2} \sum_{ij} V_{ij} s_i s_j \tag{3.1}$$

where $s_i = \pm 1/2$, ϕ_i is the random energy on site i, $V_{ij} = e^2/\kappa r_{ij}$ is the Coulomb interaction between sites i and j separated by the distance r_{ij}. For a lattice of spacing l_0, $e^2/\kappa l_0$ is the scale of electrostatic energy, and we take this to be the unit of energy. The random energies ϕ_i's are distributed according to the distribution given in the equation (1.4). The single particle Hartree energies are defined as,

$$\epsilon_i = \phi_i + \sum_j V_{ij} s_j \tag{3.2}$$

If an electron is moved from an occupied site i to an empty one j, the change in energy of the system due to this one electron hop (or particle-hole excitation) is

$$\Omega_{ji} = \epsilon_j - \epsilon_i - \frac{1}{r_{ij}}. \tag{3.3}$$

where r_{ij} is measured in units of l_0. For the ground state all the single electron and hole excitation energies must be positive. This implies a minimum separation between pairs of sites whose single-particle energies lie on either side of the chemical potential, and if the states are assumed to be homogeneously distributed through space it leads to a bound on the single-particle DOS $g(\epsilon)$ of the form

$$g(\epsilon) \propto |\epsilon - \mu|^s \tag{3.4}$$

with $s = d - 1$ in d dimensions.

In this chapter we are interested in checking the various hypothesis made by different authors in the derivation of Coulomb gap. The stability condition, $\Omega_{ij} > 0$, will lead to correlations between electrons and holes in the psuedo-ground states. Since the particle number is conserved, the stability condition will also lead to correlation between holes (electrons). This can be checked by calculating the electron-hole and hole-hole correlation functions. The electron-hole correlation function can yield important information about the screening of interaction. The hole-hole correlation function helps us to check the homogeneity of the system. Homogeneity of the system and the unscreened nature of the Coulomb interaction are the two important hypothesis on which the ES theory is based. In the mean field approximation of Srinivasan, the occupation numbers of the sites in the ground state and the non-interacting state are same. This is a byproduct of his derivation. Comparing the minimum energy states with the initial state we can find out whether Srinivasan's derivation takes into account all the correlations present in the ground state accurately. The psuedo-ground states are the minimum energy Hartree states which are stable against single electron-hole transitions, for a given configuration of $\{\phi\}$. They are reached from a variety of initial conditions following the algorithm to be described in the next section. For high disorder, the present program finds the psuedo-ground states very accurately. For a single $\{\phi\}$ configuration the number of psuedo-ground states is small and they occur quite frequently as the initial conditions are varied. We want to look at how these psuedo-ground states differ from the ground

state in energy and difference in occupation numbers. This should give us some useful information about the nature of multi-electron excitations.

This chapter is organized as follows. In section 1, we give the algorithm used. In section 2, we calculate the density of states $g(\epsilon)$ for different disorder strengths. In section 3, we calculate the electron-electron and hole-hole correlation functions. In section 4, the correlation between initial non-interacting state and the resultant minimum energy state is checked. In section 5, we look at the nature of the minimum energy states for $A = 3$.

3.1 Algorithm

The computer program to generate ground states is similar to the one used by Davies *et al* [41] which is a modified version of the algorithm used by Baranovskii *et al* [42]. A set of random energies is generated and assigned to sites on a lattice. Then the electrons are put on half of the sites randomly with no correlation between ϕ_i's and the initial occupation numbers. The system was allowed to relax by successive electron hops, each of which lowered the total energy. In the first stage, called "$\mu-$sub" by Baranovskii *et al*, the single-particle energies were checked to see whether all occupied sites had lower energies than empty ones. If they did not, an electron was moved from the filled site with the highest energy to the empty one with the lowest energy. The single particle Hartree energies were recalculated, and the process was repeated until the ordering was correct. Most of the excess energy was released in this stage.

The next stage of our program, like that of Baranovskii *et al*, checks that the excitation energy equation (3.3) for an electron-hole excitation is non-negative for every pair of sites. We checked all the pairs first and then made the most favorable hop, as we found this to give final states of lower energy. The search for this most favorable hop is speeded greatly by the elimination of unnecessary tests. If a hop was made, the program returned to "$\mu-$sub"; if not, the model state is now stable against all single

electron-hole transitions. The final state will not in general be the true ground state of the system. Starting with the same set of random energies but with different initial occupations, a distribution of different minimum energy states which are stable against an electron-hole transition resulted. These minimum energy states are called "psuedo-ground states". These psuedo-ground states are separated by high energy barriers and are thus inaccessible to each other. This is consistent with the picture of glassy landscape. If the state of lowest energy occurred frequently in this distribution, we believe (following Baranovskii *et al*) that this is the true ground state. It is possible that the true ground state has peculiar properties which make it difficult to reach by the Monte Carlo procedure outlined above, and that our identification of it is therefore wrong. However, this may mean that the true ground state is difficult to reach for a real system, and that the "selected ground state" which we have calculated may well be the one of physical interest. The program is time consuming because after each electron-hole transition, all the Hartree energies have to be recalculated. One can calculate the new Hartree energies from the old Hartree energies by taking in the account the electron-hole transition. This is not as efficient as the "Ewald" [75] summation algorithm but has served our purpose.

To test the efficiency of the program we try to find the ground state of a pure system. For a 10×10 two dimensional system we found 10% ground states in 1000 attempts. If one does not use periodic boundary conditions one finds 1% ground states in 1000 attemps. So the use of periodic boundary condition does increase the efficiency of the program. The chemical potential μ is found by finding the mean of the final Hartree energies.

3.2 Single particle density of states

The single particle DOS for a $d = 2$, 40×40 systems for $A = 1, 2, 3$ was found. The averaging over disorder was done over 300 $\{\phi\}$ configurations. The resultant DOS is shown in fig. 3.1 for $A = 1, 2, 3$. The DOS is found to be linear in Hartree energies

in accord with the theoretical result. It can be seen that the qualitative nature of DOS is independent of the value of A. The width of Coulomb gap decreases with increasing disorder strength A. The ES theory is valid in the regime where there is no long range order in the system. We have seen in the last chapter that phase transition from paramagnetic to antiferromagnetic phase takes place at $V = (2/\pi)^{1/2}A$. So the results are consistent with the ES theory.

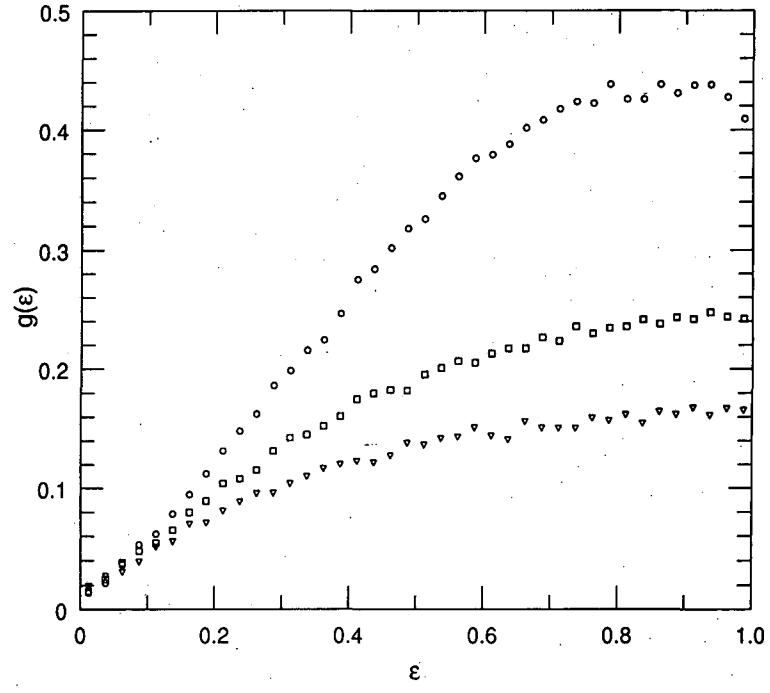

Figure 3.1: Plots of $g(\epsilon)$ with ϵ for ($\circ$) $A = 1$, ($\square$) $A = 2$ and ($\triangledown$) $A = 3$.

3.3 Correlation Functions

We will now calculate the electron-hole correlation function for the minimum energy configurations. The correlation function $cr(\epsilon_h, \epsilon_e, r_{eh})$ is defined as the probability of finding a hole with energy in the interval ϵ_h and $\epsilon_h + d\epsilon_h$ within the radius r_{eh} and $r_{eh} + dr$ from an electron in the energy interval ϵ_e and $\epsilon_e + d\epsilon_e$. Our idea is to determine whether the correlation function obeys the constraint imposed by the stability requirements. Efros has further argued that this function is just $\Theta(\epsilon_h - \epsilon_e - 1/r_{eh})$ implying a total

lack of correlations outside the range prescribed by the constraint. If the correlations die out faster with distance, this implies that the interaction is screened.

To calculate the correlation function $cr(\epsilon_h, \epsilon_e, r_{eh})$, we first considered one ϕ configuration. The total number of electrons in the energy interval ϵ_e and $\epsilon_e + d\epsilon_e$ were found. Then number of holes within the radii r_{eh} and $r_{eh} + dr$, in the energy interval ϵ_h and $\epsilon_h + d\epsilon_h$ for each of the electrons in the above energy interval was found. The resultant number was divided by the total number of electrons and holes in the energy intervals considered. Finally for each r_{eh} we divided by the corresponding coordination number of the lattice and got the correlation function for a single random energy configuration. The correlation function was disordered averaged over 80 $\{\phi\}$ configurations. The results for different electron energies ϵ_e, are shown in figures 3.2, 3.3 and 3.4. We see that correlation function can be well approximated by $\Theta(\epsilon_h - \epsilon_e - 1/r_{eh})$. This clearly implies that electrons and holes have long range correlations, which in turn implies that the electron-electron interaction is unscreened.

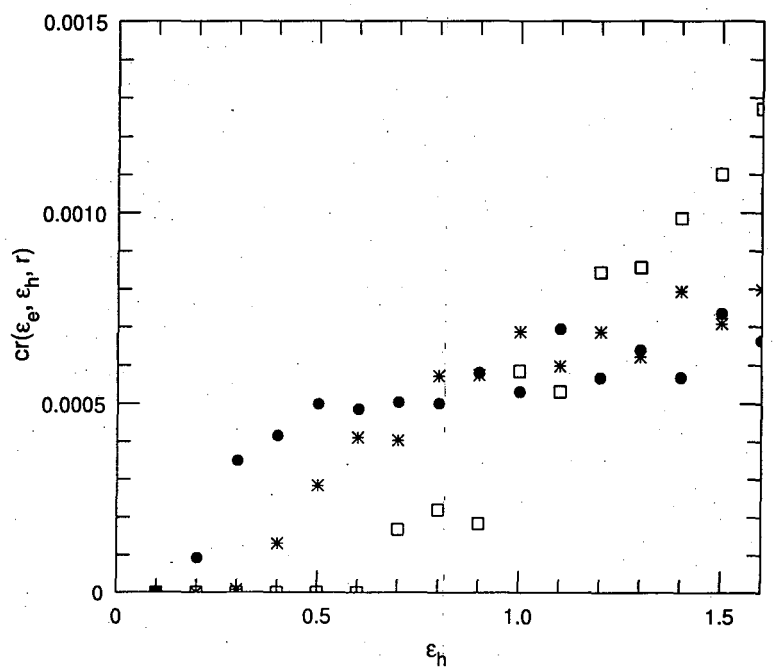

Figure 3.2: Plots of $cr(\epsilon_h, \epsilon_e, r_{eh})$ with ϵ_h at $\epsilon_e = -0.1$ for ($\Box$) $r_{eh} = 2$, ($\star$) $r_{eh} = 3$ and ($\circ$) $r_{eh} = 5$.

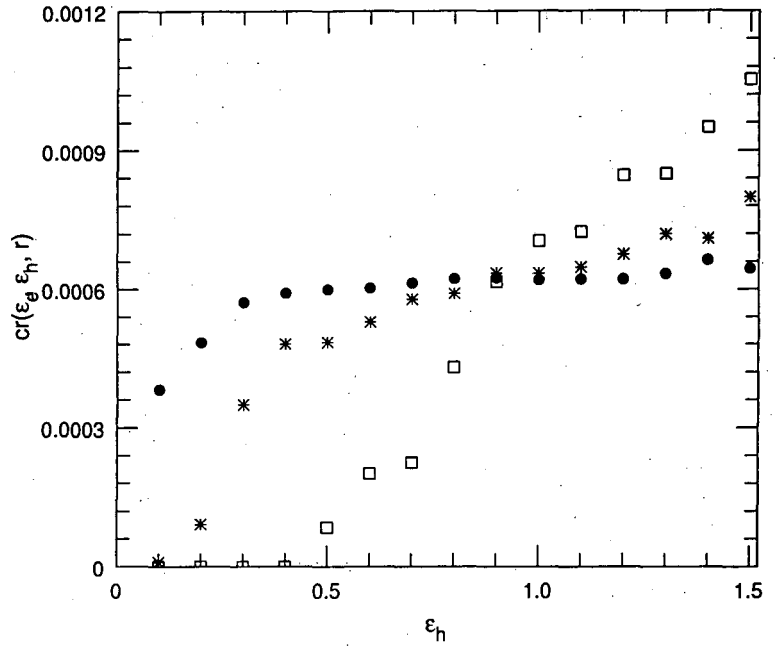

Figure 3.3: Plots of $cr(\epsilon_h, \epsilon_e, r_{eh})$ with ϵ_h at $\epsilon_e = -0.3$ for ($\Box$) $r_{eh} = 2$, ($\star$) $r_{eh} = 3$ and ($\circ$) $r_{eh} = 5$.

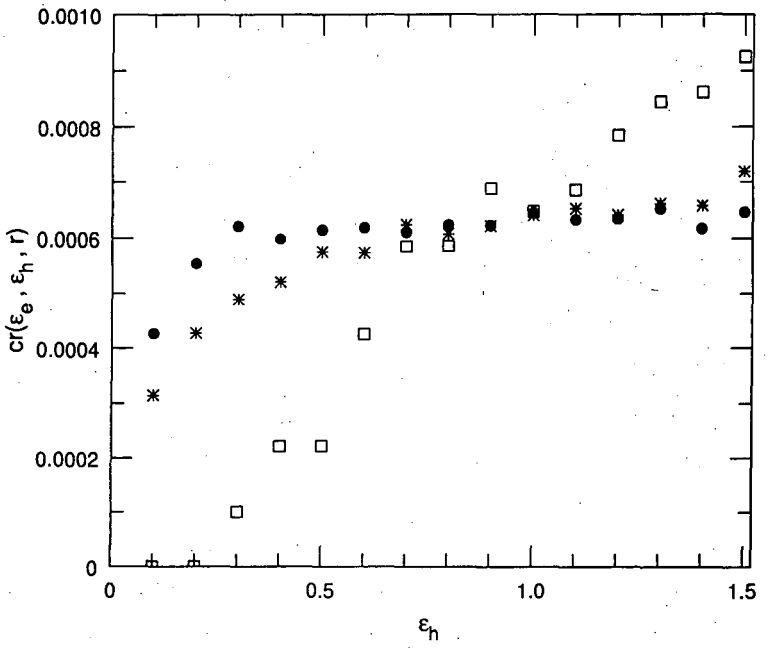

Figure 3.4: Plots of $cr(\epsilon_h, \epsilon_e, r_{eh})$ with ϵ_h at $\epsilon_e = -0.5$ for ($\Box$) $r_{eh} = 2$, ($\star$) $r_{eh} = 3$ and ($\circ$) $r_{eh} = 5$.

Davies *et al* [40, 41] have shown that at $A = 1/2$, one has clustering of hole states (electron states) if one looks at hole states (electron states) around the Fermi level. This is consistent with the fact that no hole state with low energies can be around an electron with low energy. Davies *et al* claimed that this hole-hole correlation will decrease with increasing disorder. To check this, we have computed the hole-hole correlation function $ch(\epsilon_h, \epsilon_h, r)$ for $A = 1, 2$. This correlation function is the probability of finding a hole in the energy range μ and $\mu + \epsilon_h$ within the radius r and $r + dr$ for a hole in the same energy range. The correlation function $ch(\epsilon_h, \epsilon_h, r)$ for $A = 1, 2$ is shown in fig. 3.5 and fig. 3.6 respectively. The hole-hole correlation is present for all energies considered and decays with increasing r for both $A = 1, 2$. We now try and see how is the correlation function $ch(\epsilon_h, \epsilon_h, r)$ changes with disorder. We compare $ch(\epsilon_h, \epsilon_h, r)$ for $\epsilon_h = 0.5$ for $A = 1$ and $\epsilon_h = 0.4$ for $A = 2$. The different values of ϵ_h are chosen for different disorder strengths to keep track of decreasing width of Coulomb gap with increasing disorder. The result is shown in fig. 3.7 and we find that the correlation functions to be in good agreement. We have taken the energy inhomogeneity (DOS is a function of ϵ) into account by dividing by the total number of holes in the energy interval considered. This means that though the total number of low energy holes around a hole may decrease with increasing disorder, the probability does not. This establishes that the hole-hole correlation function has a scaling property $ch(\epsilon_h, \epsilon_h, r, A) = f(\epsilon_h/\Delta, \epsilon_h/\Delta, r)$. This is contrary to the results of Davies *et al* [40, 41].

3.4 Correlation in Occupation Numbers

In Srinivasan's mean field derivation of Coulomb gap, we saw that the sites below the Fermi level in the initial state $\{\phi\}$ lowered their energy by creating a hole around themselves. Likewise the sites above the Fermi level (holes) in the initial state $\{\phi\}$ increased their Hartree energy by attracting electrons. So the occupation numbers of sites in the initial state and the ground state were the same. We will test this result by looking at

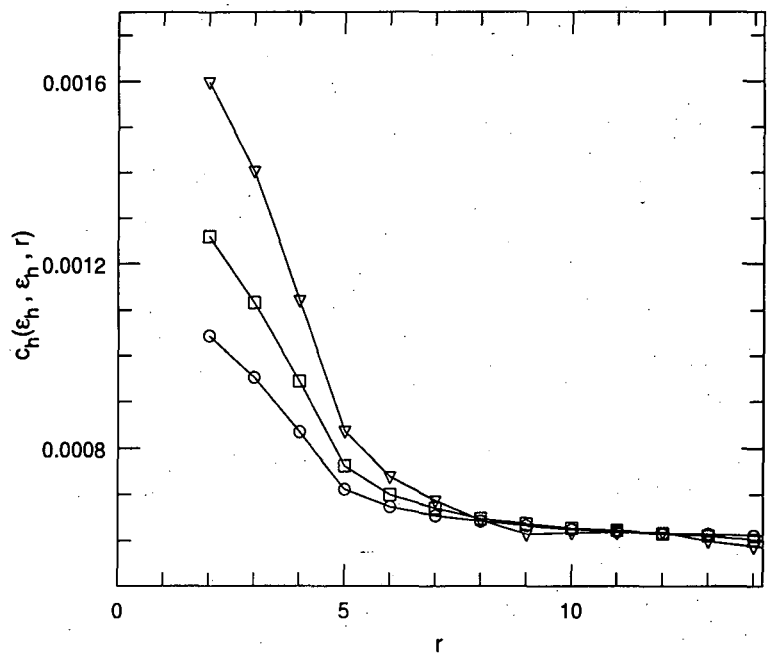

Figure 3.5: Plots of $ch(\epsilon_h, \epsilon_h, r)$ with r at $A = 1$ for ($\circ$) $\epsilon_h = 0.5$, ($\square$) $\epsilon_h = 0.4$, ($\bigtriangledown$) $\epsilon_h = 0.3$.

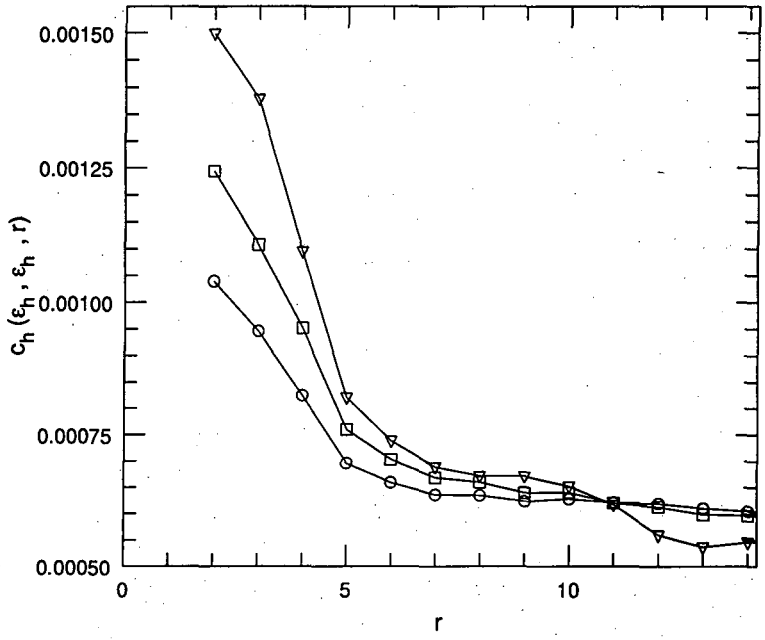

Figure 3.6: Plots of $ch(\epsilon_h, \epsilon_h, r)$ with r at $A = 2$ for ($\circ$) $\epsilon_h = 0.4$, ($\square$) $\epsilon_h = 0.3$, ($\bigtriangledown$) $\epsilon_h = 0.2$.

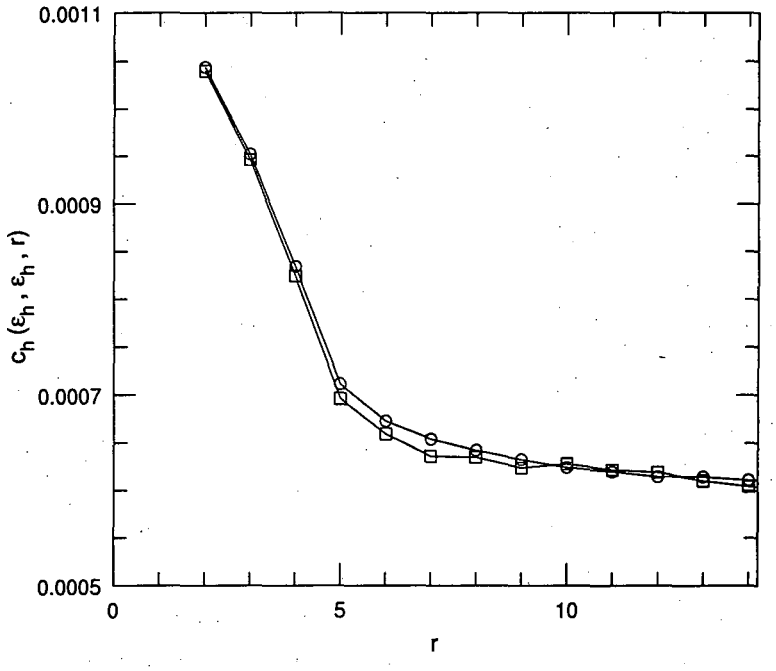

Figure 3.7: Plots of $ch(\epsilon_h, \epsilon_h, r)$ with r at $A = 1$ for ($\circ$) $\epsilon_h = 0.5$ and at $A = 2$ for ($\square$) $\epsilon_h = 0.4$.

the function $\delta n(\phi)$,

$$\delta n(\phi) = \left\langle \sum_i \frac{n(\phi_i) - n(\epsilon_i)}{2n(\phi_i)} \right\rangle_{av}. \tag{3.5}$$

We look at $\delta n(\phi)$ for $A = 1$ and two dimensional 40×40 system. We have disorder averaged over 100 $\{\phi\}$ configurations. The $\delta n(\phi)$ is shown in fig. 3.8. One can see that a lot of sites within the energy range $-.3 + \mu$ to $\mu + .3$, reverse their occupation numbers. So the minimum energy state is far more correlated than the mean field results of Srinivasan would imply. This is the key effect of the correlations in occupation numbers. Physically, only the states within an energy neighbourhood of the chemical potential would change their occupation. This energy range over which $\delta n(\phi) \neq 0$) can be regarded as the Coulomb gap.

3.5 Configuration Space

We look at the various psuedo-ground states for a two dimensional 40×40 system with $A = 3$. For every random energy set $\{\phi\}$ we find psuedo-ground states for 300 initial oc-

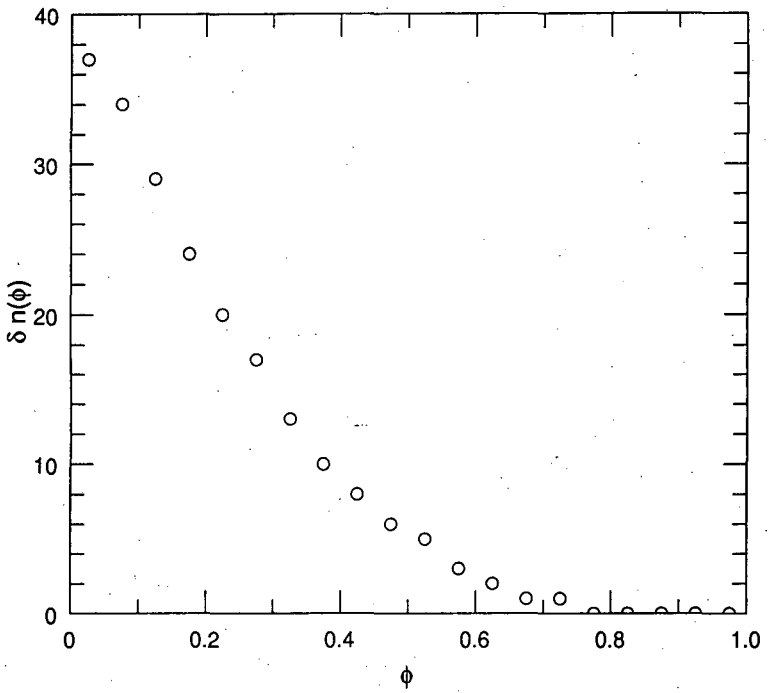

Figure 3.8: Plot of $\delta n(\phi)$ with ϕ

cupation number configurations. The state with lowest energy is taken to be the ground state. The psuedo-ground states are then characterized by their difference in energy with the ground state and their Hamming distance from the ground state configuration. Hamming distance is number of electrons and holes having different occupation numbers in the two configurations one is comparing. We look at the psuedo-ground states with energy difference less than 0.3. We found a large number of configurations with Hamming distance four and six. The energy (energy difference) of these configurations was very small. Most of these configurations had electrons and holes clustered together. For these low energy psuedo-ground states, the differences occur in the form of localized defects, such that the Hamming distance is confined to just these few defects. In psudeo ground states with higher Hamming distances, one again finds the occurrence of the above defects in addition to larger defect configurations. Most of these configurations were chain like with electrons and holes separated by small distances. We are not a position to give any quantitative estimates here since many more multi-particle excita-

tions can be created. Though for the low energy spectrum our analysis should give good qualitative estimates. In fig. 3.9 we show the density of states of the psuedo-ground states. We have disordered averaged over 200 random $\{\phi\}$ configurations. The density of states of the psuedo-ground states has no gap. This is due to large number of metastable configurations with small Hamming distances. More insight can be obtained if we plot DOS of these states at different Hamming distances separately. The density of states as a function of Hamming distance and energy is shown in fig. 3.10 and fig. 3.11. It is clear as the Hamming distance increases beyond 14 the DOS for the psuedo-ground states starts to show a gap. This has an interesting implication for conductivity which we can discuss only qualitatively at this point. A larger Hamming distance implies a longer chain and thus a longer distance over which electron can be transported. Thus possibly the configurations which can contribute to conductivity more significantly do have a gap. The relative importance of configurations with different Hamming distance for conductivity can only be checked by using the percolation method in configuration space as suggested by Perez *et al* [74].

Conclusions

The correlation functions largely validate the ideas of Efros and Shklovskii. The absence of correlations between initial and final occupation numbers point to the inadequacy of Srinivasan's theory. As explained in Chapter 1, the Srinivasan's analysis leads to screening of interaction. This seems to us to be a major problem as the electron-hole correlation function shows that the interaction is unscreened. The absence of gap in the density of states of psuedo-ground states was due to large number of low Hamming distance configurations. For conductivity the high Hamming distance configurations (long chains) might be more important. These configurations do have a gap in their density of states. The high number of configurations with Hamming distance four and six shows that stabilizing the ground state with respect to two and three electron transfer

will be quite important. Such stabilization would most likely relax a large number of configurations with low Hamming distance and they will then merge with the ground state. This will bring us closer to the glassy nature of the Coulomb glass system, which is different valleys separated by high energy barriers and high Hamming distances.

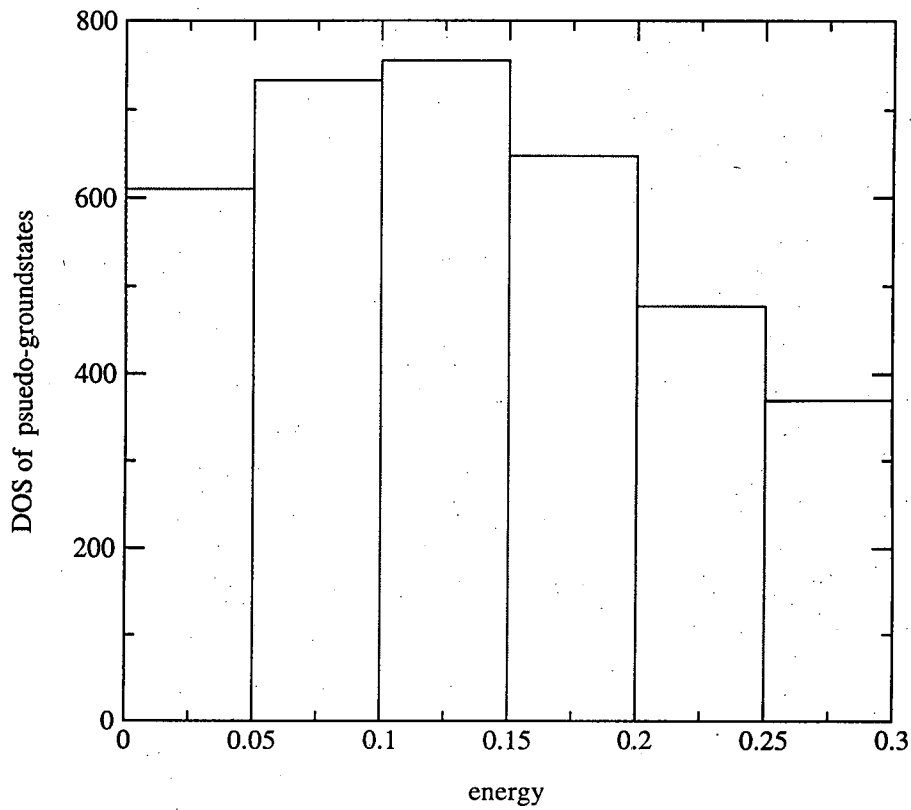

Figure 3.9: Plots of density of states of psuedo-ground states with energy of the psuedo-ground states.

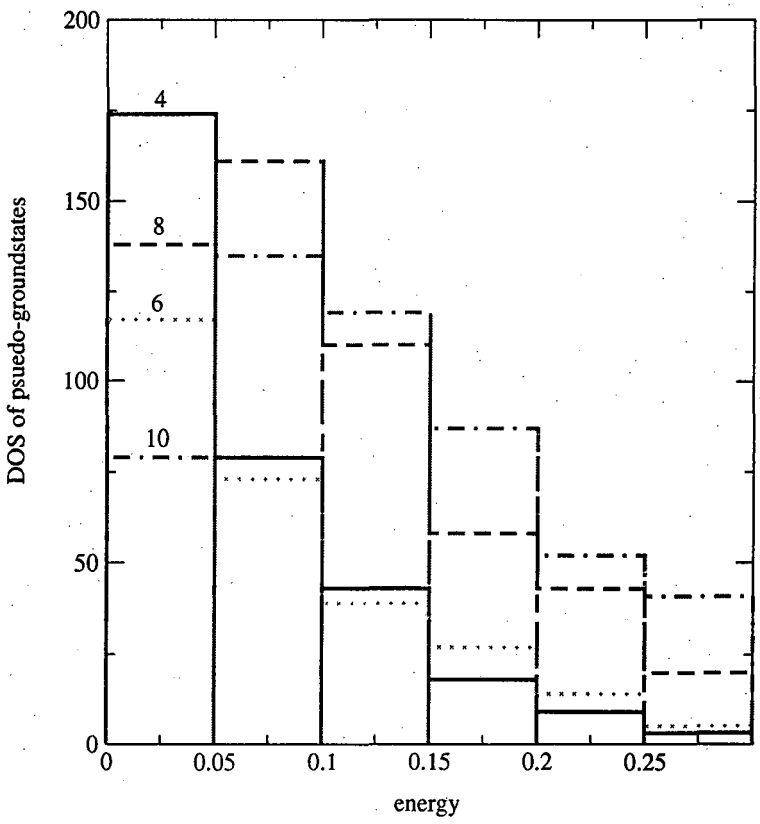

Figure 3.10: Plots of density of states of psuedo-ground states with energy of the psuedo-ground states for different Hamming distances 4, 6, 8, 10.

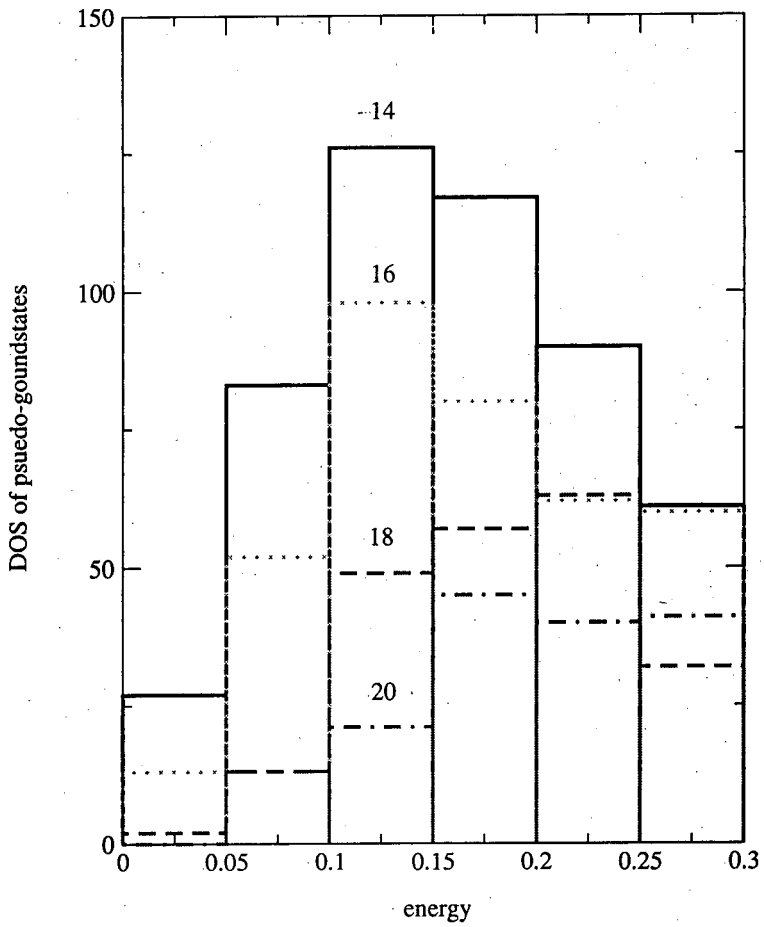

Figure 3.11: Plots of density of states of psuedo-ground states with energy of the psuedo-ground states for different Hamming distances 14, 16, 18, 20.