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Title of the Thesis: “Numerical and Theoretical Study of Coulomb Glasses”

ABSTRACT

This thesis is concerned with the study of phase transition in the Coulomb glass system. The Coulomb glass refers to a disordered system in which electrons localized at lattice sites interact with each other via unscreened Coulomb interaction. In addition, like Anderson insulator model there is on-site random energy associated with each site. The term “glass” is due to many features which this system shares with other glasses, including the slow dynamics, aging and memory effects. Few examples of such systems are compensated doped semiconductors, granular metals and ultra thin films.

The Coulomb Glass (CG) system is characterized by the Hamiltonian

$$H = \sum_i \phi_i n_i + \frac{1}{2} \sum_{i \neq j} \left(n_i - \frac{1}{2} \right) \left(n_j - \frac{1}{2} \right) \frac{e^2}{\kappa R_{ij}} \quad (1)$$

where n_i are the occupation numbers which can take values 0 and 1. ϕ_i is the on-site energy. For half filling case, this model has an important property that the chemical potential $\mu = 0$. Efros and Shklovskii used stability considerations for the ground state and showed that there is a soft gap in the density of states. They showed that the long range nature of the Coulomb interaction is responsible for the occurrence of gap in density of states (DOS). The gap is defined by the equation

$$g(\varepsilon) \propto \varepsilon^{D-1} \quad (2)$$

where ε_i are the single particle Hartree energies defined as,

$$\varepsilon_i = \phi_i + \sum_j \frac{e^2}{\kappa R_{ij}} \left(n_j - 1/2 \right) \quad (3)$$

An important question addressed in this thesis is the study of Density of states with disorder. Another important question in the study of any disordered system is how does its phase diagram look as a function of temperature and strength of disorder.

We investigated the CG model as a function of disorder and temperature. At $T = 0$, we have shown that the system exhibits a first order transition from charge-ordered phase to disordered phase at $W_c = 0.2253$. The transition was characterized by the exponents $\nu = 1.0$, $\beta = 0$ both corresponding to first order transition. The distribution of staggered magnetization at W_c possessed three peaks indicating phase coexistence. In addition to this we also found that the domain picture is appreciably different from the Imry and Ma assumptions at all disorders. From our work at finite temperature and disorder we have shown that the phase transition from paramagnetic phase to charge-ordered phase was of second order type. We found no evidence of spin glass phase between the charge-ordered phase and paramagnetic phase. An important observation here was that the critical exponents at $W = 0$ are different from $W \neq 0$ which suggests that for the finite temperature phase transition disorder is relevant. We have also given a theoretical argument that the Imry-Ma argument for short range RFIM can be extended to CG system at half filling. The last problem that we studied was the possible dynamical phase transition at high disorder using mean-field approximation. We did not find any phase transition in this case. We found that the gap exponent of DOS is close to $\delta \approx d - 1$ as predicted earlier. Analysis of eigenvalue distribution of Linear Dynamical matrix shows that the dynamics of the system gets slower as the temperature is lowered. Analysis of eigenvalue distribution of inverse susceptibility matrix did not show any phase transition. The calculation of Inverse Participation Ratio shows that the states are localized at low T which is the reason for slow dynamics in the system.