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Disorder dependence of phase transitions in a Coulomb glass

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We have performed a Monte Carlo study of a three dimensional system of classical electrons with Coulomb interactions at half filling. We systematically increase the positional disorder by starting from a completely ordered system and gradually transitioning to a Coulomb glass. The phase transition as a function of temperature is second order for all values of disorder. We use finite size scaling to determine the transition temperature T_C and the critical exponent ν. We find that T_C decreases and that ν increases with increasing disorder.

Electrons with long range Coulomb interactions in three dimensions display a rich and complex behavior. If there is translational invariance and a background of compensating positive charge, the system forms a Wigner crystal at low densities where the potential energy dominates the kinetic energy [1, 2]. In the presence of quenched disorder the competition between interactions and disorder produces a Coulomb glass. Comparing these two extremes reveals similarities and differences. For example both undergo a phase transition when the temperature is lowered. In one case an ordered arrangement of electrons is formed while in the case of the Coulomb glass a highly disordered arrangement is frozen into place. Yet both low temperature phases have a gap in their single particle density of states.

In this paper we study the effect of gradually introducing disorder into a three dimensional system of electrons with long range Coulomb interactions. The system is discrete in the sense that the electrons sit on half of the available sites. In the ordered case the sites form a cubic lattice. The disorder is introduced in the positions of the sites and their deviation from a cubic lattice. The Hamiltonian is

$$H = \sum_{i>j} \frac{(n_i - K)\,(n_j - K)}{r_{ij}} \tag{1}$$

where we set the charge $e = 1$, n_i is the number operator for site i, $r_{ij} = |\boldsymbol{r}_i - \boldsymbol{r}_j|$, and K is a compensating background charge making the whole system charge neutral. $n_i = 1$ (-1) for an occupied (unoccupied) site. We consider half–filling with $K = 1/2$.

We have simulated three dimensional systems of linear size $L = 4$, 6, and 8. We place $N = L^3$ sites in the system. We have only considered the case of half filling in order to take advantage of the particle-hole symmetry. For the ordered case the sites form a cubic lattice. In the ground state, every other site is occupied; the occupied sites form a face centered cubic (FCC) lattice. We can gradually introduce disorder by allowing the deviation of a site from its position in a cubic lattice to be chosen from a Gaussian distribution with a standard deviation of σ. This gives the radial distance from the cubic lattice site. The angular coordinates of the site are chosen randomly using a uniform distribution. The ordered case corresponds to $\sigma = 0$. $\sigma = 1$ corresponds to a very disordered case with a standard deviation equal to the cubic lattice constant a. For all values of the disorder, the system

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undergoes a second order phase transition as the temperature is lowered. (In the ordered case, constraining the electrons to sit on lattice sites rather than allowing them to have continuous translational degrees of freedom results in a second order phase transition. This is consistent with our observations of the lack of coexistence of the ordered and disordered phases at T_C and with the absence of hysteresis.) We study the effects on the thermodynamics of this phase transition as a function of the disorder.

We use infinite periodic boundary conditions in which the simulation box is infinitely replicated in all directions to form a lattice. We use an Ewald summation technique [3] so that an electron on a given site interacts with the other electrons and all their images via the Coulomb interaction.

We used a Monte Carlo heat bath algorithm. We keep a table of the potential energy at each site. Each electron is looked at sequentially and moved to one of the available $N/2+1$ sites (its own site or one of the available $N/2$ unoccupied sites), chosen with a Boltzmann probability. If the site chosen is the electron's originial location, the potential energies are unchanged; if the electron hops to a new site, we update all the potential energies. If the electron chooses its initial site, which it does with high probability at low temperatures, we do not have to recompute the potential energies. This speeds up the simulation considerably, partially compensating for the much longer equilibration times needed at low temperatures. Our longest run (for $L=4$ at $T=0.01$) had 3×10^6 Monte Carlo steps per electron. Depending on the system size and temperature, the sample averages involved between 5 and 190 disorder configurations.

Let $S_i = 2(n_i - K)$ be an effective spin associated with the occupation of site i so that $S_i = 1$ (-1) for an occupied (unoccupied) site. The Edwards–Anderson order parameter is defined as $q \equiv [\langle S_i\rangle^2]$; we will denote thermal averages by $\langle\ldots\rangle$ and disorder averages by $[\ldots]$. We use the moments of the overlap to define Binder's g [4, 5]:

$$g = \frac{1}{2}\left(3 - \frac{[\langle q^4\rangle]}{[\langle q^2\rangle]^2}\right) \tag{2}$$

Binder's g provides a way to monitor the phase transition. Since g is dimensionless, we expect that it should satisfy a scaling form

$$g(L,T) = \hat{g}(L^{1/\nu}(T - T_C))\,. \tag{3}$$

Thus at the critical temperature, $g(L,T_C)$ should have the same value independent of the system size L (as long as L is sufficiently large for finite size scaling to apply) [4, 5]. We have determined the critical exponent ν and the transition temperature T_C as a function of the disorder σ through the finite size scaling of $g(L,T)$ [5, 6]. In Fig. 1 we plot $g(L=8,T)$ versus T for various values of σ.

Notice that the transition region moves to lower temperatures with increasing disorder. This reflects the decrease in T_C with increasing σ. The transition temperature corresponds to the temperature where the curves of $g(L,T)$ versus T for all sizes cross.

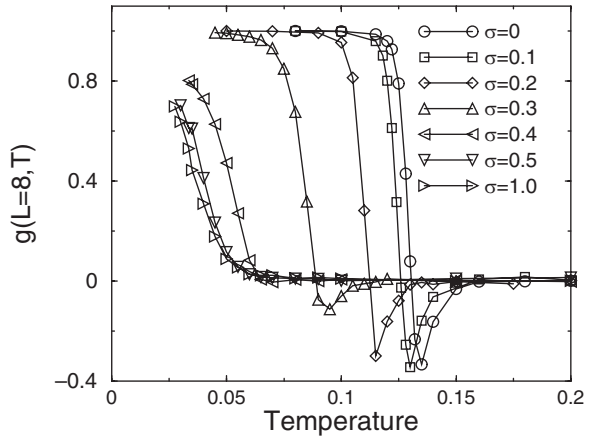

Fig. 1 $g(L=8,T)$ vs. T for $\sigma=0$ (45 runs), $\sigma=0.1$ (10 runs), $\sigma=0.2$ (5 runs), $\sigma=0.3$ (15 runs), $\sigma=0.4$ (115 runs), $\sigma=0.5$ (45 runs), and $\sigma=1$ (108 runs). The number of runs in parentheses is the number of runs that were averaged to obtain the data.

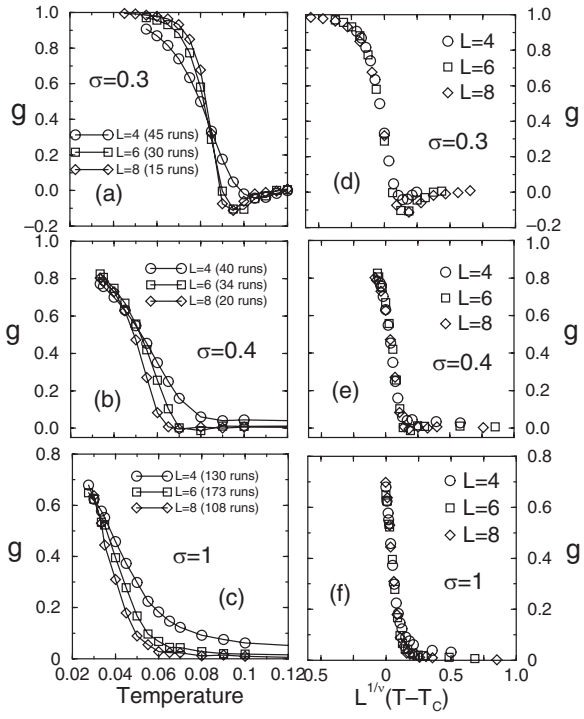

Fig. 2 a)–c) $g(L,T)$ versus T for $\sigma = 0.3$, 0.4, and 1.0 at $L = 4$, 6, and 8. The solid lines are guides to the eye. ($g(L = 8, T)$ vs. T is virtually identical.) The number of runs in parentheses is the number of runs that were averaged to obtain the data. d) $g(L,T)$ for $\sigma = 0.3$ scaled using $\hat{g}\big(L^{1/\nu}(T - T_C)\big)$ with $T_C = 0.085 \pm 0.002$ and $\nu = 0.071 \pm 0.02$. e) $g(L,T)$ for $\sigma = 0.4$ scaled using $\hat{g}\big(L^{1/\nu}(T - T_C)\big)$ with $T_C = 0.045 \pm 0.001$ and $\nu = 1.05 \pm 0.05$. f) $g(L,T)$ for $\sigma = 1$ scaled using $\hat{g}\big(L^{1/\nu}(T - T_C)\big)$ with $T_C = 0.028 \pm 0.001$ and $\nu = 1.30 \pm 0.1$.

To more accurately determine T_C, we use the scaling hypothesis to collapse the data for a given value of σ onto a single curve as shown in Fig. 2. T_C and ν are used as adjustable parameters to collapse the data. We can estimate the errors in the critical temperature and the critical exponent ν by how well the curves can be made to collapse. The values of ν and T_C at various values of σ are given in table 1. In Fig. 3 we plot T_C and ν versus σ.

We can see that the transition temperature decreases from $T_C = 0.128 \pm 0.001$ at $\sigma = 0$ to $T_C = 0.028 \pm 0.001$ at $\sigma = 1$. ν increases from $\nu = 0.55 \pm 0.05$ at $\sigma = 0$ to $\nu = 1.30 \pm 0.10$ at $\sigma = 1$.

It is interesting that T_C is much lower than the characteristic energies of the system which are of order unity. This is especially true for large values of the disorder. The reason for this was given by Grannan and Yu [6] and is as follows. At the temperatures of our simulations, nearby pairs of sites will with high probability consist of an occupied and an unoccupied site. Since these strongly coupled pairs of sites are close together, they are guaranteed to have small dipole moments. Therefore, they will interact weakly with the rest of the system, remaining active down to temperatures much lower than the bare interaction energy.

To summarize, we have performed a Monte Carlo study of a classical three dimensional Coulomb system of electrons at half filling. We systematically increase the positional disorder by introducing deviations from positions in a cubic lattice. We start from a completely ordered system and gradually transition to a Coulomb glass. The phase transition as a function of temperature is second order for all values of disorder. We use finite size scaling to determine the transition temperature T_C and the critical exponent ν. We find that T_C decreases and that ν increases with increasing disorder.

Table 1 The values of T_C and ν for different valuse of σ.

σ	T_C	ν
0.0	0.128 ± 0.001	0.55 ± 0.05
0.1	0.123 ± 0.001	0.57 ± 0.05
0.2	0.110 ± 0.001	0.61 ± 0.05
0.3	0.085 ± 0.002	0.71 ± 0.02
0.4	0.045 ± 0.001	1.05 ± 0.05
0.5	0.030 ± 0.001	1.35 ± 0.05
1.0	0.028 ± 0.001	1.30 ± 0.10

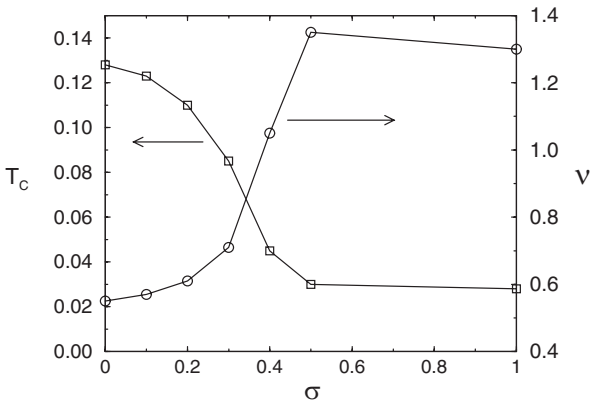

Fig. 3 The transition temperature T_C (□) and the critical exponent ν (○) versus the disorder σ.

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