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Geometrically-frustrated pseudogap phase of Coulomb liquids

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ABSTRACT

We study a class of models with long-range repulsive interactions of the generalized Coulomb form $V(r) \sim 1/r^{\alpha}$. We show that decreasing the interaction exponent in the regime $\alpha < d$ dramatically depresses the charge ordering temperature T_c in any dimension $d \geq 2$, reflecting the strong geometric frustration produced by long-range interactions. A nearly frozen Coulomb liquid then survives in a broad pseudogap phase found at $T > T_c$, which is characterized by an unusual temperature dependence of all quantities. In contrast, the leading critical behavior very close to the charge-ordering temperature remains identical as in models with short-range interactions.

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1. Introduction

The phenomenon of screening has long been known in presence of long-range Coulomb interactions, and it is generally expected to render the observed behavior very similar to that of systems with short-range interactions. Indeed, recent computational work has investigated the critical behavior close to charge ordering in lattice Coulomb systems [1], suggesting the Ising universality class. In addition, analytical arguments have been presented [2] supporting this view, for a broad class of lattice models with the generalized Coulomb interaction of the form $V(r) \sim 1/r^{\alpha}$ in $d \geq 2$ dimensions. We should mention, however, that long-range interactions are generally expected to produce mean-field like critical behavior for $d < \alpha < d^*$, while for $d < d^* < \alpha$ one expect short-range critical behavior. The nontrivial effect of long-range interactions upon the critical behavior is possible only for $\alpha > d$, because in this regime the interaction is "integrable" (no neutralizing background is needed), and screening becomes inoperative.

Should one expect any interesting or novel physics in Coulomb-like models ($\alpha < d$), in comparison to the short-range situation? Our work confirms that these models indeed feature conventional critical behavior in the narrow critical region $T \approx T_c$. We show, however, that a striking new behavior is uncovered in a broader temperature interval, reflecting strong geometric frustration inherent to such long-range interactions. First, we find a dramatic decrease of melting temperature of lattice Coulomb gas as a result of the level of frustration in the system. This can be easily understood by noting that our lattice Coulomb gas maps into an antiferromagnetic Ising model with long-range interactions. Here, all the spin tend to anti-align with all other spins, but this cannot be achieved for very long interactions ($\alpha < d$), resulting in very low melting temperature. Indeed, for half-filled Coulomb systems ($\alpha = 1$), the melting temperature T_c is one order of magnitude smaller [3] than the generalized Coulomb energy $E_c = e^2/a$, where a is the lattice constant. Continuum models [4–6] show an even more dramatic behavior, with the melting temperature being as much as two orders of magnitude smaller then the Coulomb energy. This striking behavior, although well documented in several model studies, is not widely appreciated or understood in simple terms.

The second robust feature of these models, which has only recently been discovered [7], is the emergence of the "pseudogap phase". This pseudogap phase is a specific feature of long-range type interaction with $\alpha < d$, and is observed in a broad temperature range $T_c < T < T^*$ (see Fig. 1), where T^* is the pseudogap temperature where the gap in the single particle density of state (DOS) starts to open. We show that the physical Coulomb interaction ($\alpha = 1$) lays deep in the regime of very long range interaction $\alpha \to 0$, the regime where our analytical "extended dynamical mean-field theory" (EDMFT) approach becomes is asymptotically exact [7]. This observation explains the surprising accuracy of this analytical scheme both when applied to clean models [7], and in previous applications to Coulomb glasses [8].

2. Model and EDMFT approach

Our model is described by the Hamiltonian of particles living on a half-filled hypercube lattice (lattice spacing a) that interact via Coulomb-like interaction $V(R_{ij}) \sim (R_{ij}/a)^{-\alpha}$,

$$H = \frac{1}{2}\sum_{ij} V(R_{ij})(n_i - \langle n \rangle)(n_j - \langle n \rangle). \quad (1)$$

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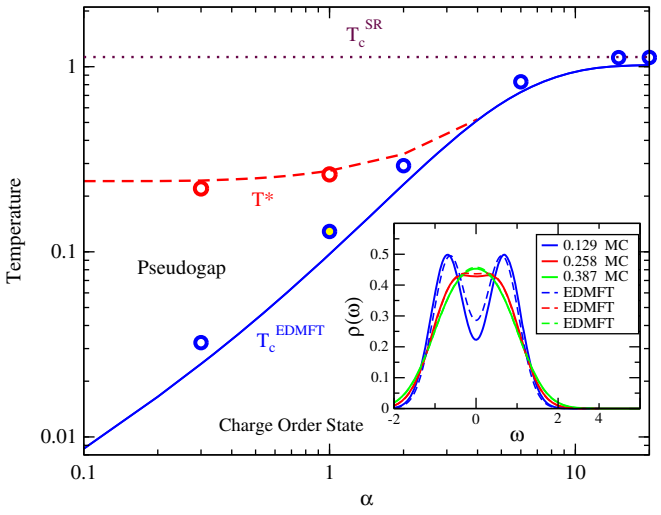

Fig. 1. Phase diagram of the half-filled classical $D=3$ lattice model with interactions $V(R)=R^{-\alpha}$. The charge ordering temperature $T_c(\alpha)\sim\alpha$, as obtained from EDMFT theory (full line) and Monte Carlo simulations (open symbols). The pseudogap temperature T^* (dashed line) remains finite as $\alpha\to 0$; a broad pseudogap phase emerges at $\alpha\le d$. We also show $T_c^{SR}\approx 1$ for the same model with short-range interactions (dotted line). The inset shows corresponding single particle density of state (DOS) for different temperatures. The EDMFT results (dashed line) show excellent agreement with Monte Carlo simulation (solid line) above the melting temperature T_c [7,8].

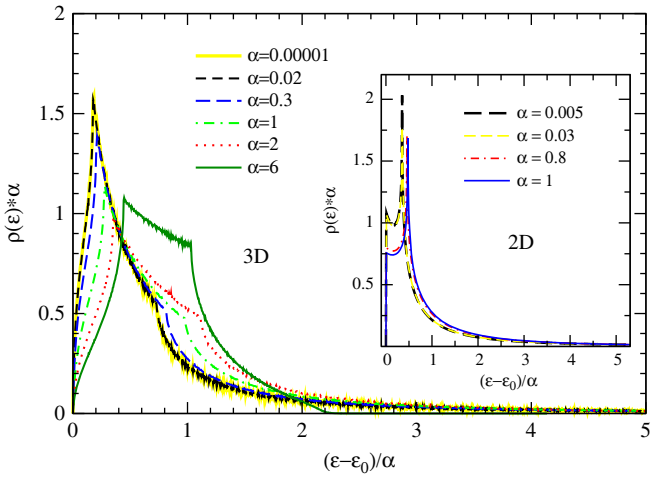

Fig. 2. Scaling behavior of the spectral density $v(\varepsilon)$ of plasmon modes on a 3D hypercubic lattice. The low-energy branch of the spectrum, which describes the "sheer" charge fluctuations close to the ordering wavevector, features an α-dependent energy scale, one that sets the melting temperature $T_c\sim\alpha$. The scaling becomes exact for very long interaction range $\alpha\ll 1$, but is approximately valid for all $\alpha\le 1$, explaining the simple α-dependence of all quantities.

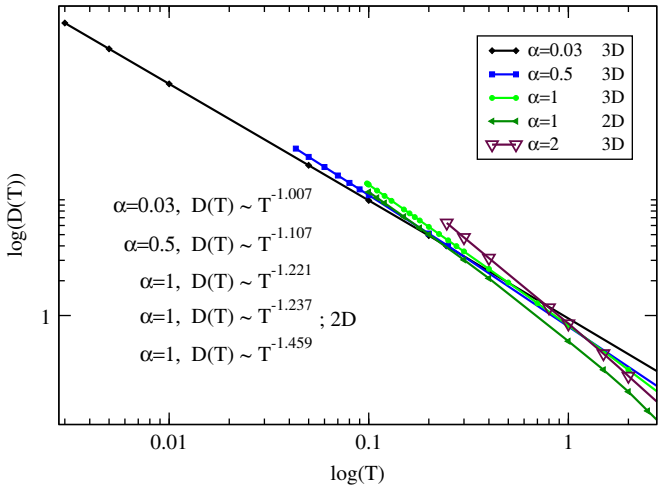

Fig. 3. The power law behavior of $D(T)$ for different interaction range α. In the limit of $\alpha\to 0$, we find parameter $D(T)\sim T^{-1}$, both in $d=2$ and $d=3$.

Here R_{ij} is the distance between lattice sites i and j expressed in the units of the lattice spacing. In general, our unit of energy the nearest-neighbor repulsion $E_c=V(1)$. We focus on the half-filled system $\langle n\rangle=1/2$ that maps the problem into "antiferromagnetic-like" Ising model. In addition to numerically exact (classical) Monte Carlo simulations, we also utilize an analytical approach, the so-called extended dynamical mean field theory (EDMFT) [9,10] which is expected [7] to be accurate for very long interaction ($\alpha\ll 1$), where the effective coordination number becomes very large. The inter-site charge correlations are included in this approach, and are treated on the same footing as the local ones [10]. Here, the lattice problem is mapped into an effective impurity problem embedded in a self-consistently determined bath containing both fermionic and bosonic excitations [9,10]. In our case, this bosonic bath describes the plasmon excitations induced by the inter-site charge correlations.

In this paper, we focus on the classical limit, where the origin of the pseudogap phase is most pronounced and the accuracy of the EDMFT can be tested directly with simple classical Monte Carlo simulations. Here, the density–density correlation function becomes

$$\chi(k)=(4+D+\beta V_k)^{-1} \tag{2}$$

and the self-consistent condition

$$\frac{1}{4}=\int d\varepsilon v(\varepsilon)(4+D+\beta\varepsilon)^{-1}, \tag{3}$$

where we define the classical plasmon-mode spectral density (Fig. 2) $v(\varepsilon)=\sum_k\delta(\varepsilon-V_k)$. By solving numerically the self-consistent condition in Eq. (3) using the spectral density $v(\varepsilon)$, the T dependence of dimensionless parameter $D(T)$ is found to be power-law dependent (Fig. 3). The analytic solution can be derived at the limit of $\alpha\ll d$, spectral density becomes $v(\varepsilon)\backsimeq\delta(\varepsilon-\varepsilon_0)$, where $\varepsilon_0=V_Q$ ($Q=(\pi,\pi)$ in 2D, and $Q=(\pi,\pi,\pi)$ in 3D) is the minimum energy in momentum space (center of Brillouin zone). By solving Eq. (2) at this limit, we find the analytic solution $D(T)\sim T^{-1}V_Q$. The result qualitatively holds all the way to $\alpha\sim d$ as shown in Fig. 3.

The charge ordering temperature $T_c(\alpha)$ is defined by the $\chi(k)\to\infty$ at the corresponding ordering wave vector $k=Q$; in $d=3$ the system forms a BCC structure, and a checkerboard patter in $d=2$. The depression of melting temperature as a function of interaction parameter $\alpha\ll 1$ can be understood in simple way by noting that the spectral density $v(\varepsilon)$ has a simple scaling form

$$v(\varepsilon)=\alpha^{-1}\tilde{v}\{(\varepsilon-\varepsilon_0)/\alpha\} \tag{4}$$

as shown in Fig. 2. The sharp peak of $(\varepsilon-\varepsilon_0)$ below characteristic energy scale $\varepsilon^*(\alpha)\sim\alpha$, physically correspond to "sheer" plasmon modes with wave vector $k\approx Q$ [5,11]. This energy scale plays a role of an effective Debye temperature. This tells us why the ordering temperature decreases

$$T_c(\alpha)=\alpha\int d\varepsilon\tilde{v}(\varepsilon)/\varepsilon\sim\varepsilon^*(\alpha)\sim 0.1\alpha \tag{5}$$

in agreement with the estimation of Lindermann criterion applied to the sheer mode. At the lowest energy near ε_0 the dispersion relation assumes the standard form $v(\varepsilon)\sim\varepsilon^{(d-2)/2}$, same as for short-range interactions. This can also be understood from the