Density of States and Critical Behavior of the Coulomb Glass

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(Received 29 May 2008; revised manuscript received 10 September 2008; published 12 February 2009)

We present zero-temperature simulations for the single-particle density of states of the Coulomb glass. Our results in three dimensions are consistent with the Efros and Shklovskii prediction for the density of states. Finite-temperature Monte Carlo simulations show no sign of a thermodynamic glass transition down to low temperatures, in disagreement with mean-field theory. Furthermore, the random-displacement formulation of the model undergoes a transition into a distorted Wigner crystal for a surprisingly broad range of the disorder strength.

DOI: 10.1103/PhysRevLett.102.067205 PACS numbers: 75.10.Nr, 05.50.+q, 64.60.−i, 75.40.Mg

The Coulomb glass (CG) is the earliest paradigm for understanding the effects of strong disorder in electronic systems with long-ranged interactions. Among its applications are the space-energy correlations in transistors, the magnetization-switched metal-insulator transitions in tunnel devices, the cotunneling magnetoresistance in ferromagnetic devices, the ambipolar gate effect, the huge magnetoresistance in semiconductor stacks, and the transparent refractory oxides, to name a few. In the CG, the Coulomb interaction remains long ranged because the disorder localizes the electrons and thus impedes screening. Therefore, the system forms its low-energy states by long-range configurational changes and avalanches. After some early approaches [1,2], Efros and Shklovskii (ES) argued that the stability of the low-energy states against the long-ranged single-particle dynamics requires the formation of a soft ''Coulomb gap'' in the single-particle density of states (DOS) of the form $\rho(E) \sim |E|^{\delta}$ with $\delta = D - 1$ as an upper bound and where the energy E is measured from the Fermi level [3], D being the space dimension. This Coulomb gap leads to a typical variable range hopping form of the low-temperature conductivity, i.e., $\sigma(T) = \sigma_0 \exp[-(T_0/T)^{-1/2}]$, σ_0 and T_0 constant.

There is considerable experimental evidence in support of these predictions from transport measurements of $\sigma(T)$ [4–7], as well as from tunneling conductance measurements of $\rho(E)$ [8–11]. However, subsequent theoretical considerations arrived at an exponential form of the DOS by considering multielectron ''polaronic'' processes: $\rho(E) \sim \exp[-(E_0/E)^{1/2}]$ [12,13], throwing the status of theoretical predictions for the DOS into question.

A large number of nonequilibrium glassy phenomena have been observed in disordered electronic systems. These include slow dynamics [14–17], aging, and memory effects [18–20], as well as changes in the noise spectrum [21]. However, the existence of a thermodynamic glass transition cannot be directly surmised from glassy dynamics. In fact, no well-defined thermodynamic glass transition has been found in association with these phenomena to date in three-dimensional (3D) systems.

These different theoretical predictions merged with the insight of Pastor and Dobrosavljevic, who described a disordered electron system with long-range interactions using the replica-based theoretical framework of glass physics [22,23]. Their work offered a unified platform to analyze both the DOS and the glassy characteristics of these systems. This programme was subsequently expanded by the work of Müller, Ioffe, and Pankov who included replica symmetry breaking technology into their calculations [24–26]. All these studies concluded that—within a mean-field approach—a soft Coulomb gap exists in the single-particle DOS at $T = 0$. Furthermore, for $T \leq T_c \sim W^{-1/2}$, where W is a measure of the disorder, the system freezes into a ''Coulomb glass'' state. Note that the Coulomb glass is analogous to a spin glass in a (random) field [27] which is known to not order.

The Coulomb glass has attracted considerable attention numerically as well. The initial work by Davies, Lee, and Rice reported the observation of a soft gap, but the data were not conclusive with respect to the detailed functional form of the DOS [28]. Subsequent numerical studies represented the disorder either by random site energies (CG) [29–34] or by random displacements (RD) between the sites [35–40]. While the CG and RD models have different symmetries (and thus possibly different universality classes [41]), it has nevertheless been argued that they both adequately capture the key aspects of the real electronic system [38]. Different studies of the DOS in 3D have reported a DOS vanishing at the Fermi level with $\rho(E) \sim |E|^{\delta}$ with $\delta = 2.1$–2.6 [29,30]. Even more surprising was the claim of a strongly disorder-dependent exponent δ [38]. Furthermore, studies attempting to locate a transition to a glassy state were only successful in the RD model [36,38–40].

The state of the field can be summarized as follows: A soft gap in the DOS has been widely confirmed, but the predicted ES exponent $\delta = D - 1$ is consistent only with experimental data, not with numerical simulations. A true finite-temperature transition to a glassy state has numerical support in the RD model but lacks evidence in the CG model and in experiments.

Our results show that in the 3D CG model, δ is close to 2 and weakly disorder dependent [25], and we find no signature of a finite-temperature glass transition. Furthermore, in the RD model, the low-temperature ordering is indicative of a distorted Wigner crystal.

Model and numerical details.—The Coulomb glass (CG) Hamiltonian is given by [3]

$$\mathcal{H}_{\mathrm{CG}} = \frac{1}{2}\sum_{i\neq j}(n_i - \nu)\frac{e^2}{\kappa r_{ij}}(n_j - \nu) + \sum_i n_i \varepsilon_i, \qquad (1)$$

where $n_i \in \{0, 1\}$ is the electron number at site i, ν the filling factor, and $e^2/\kappa r_{ij}$ the Coulomb repulsion. The sites lie on a three-dimensional lattice of size $N = L^3$, and the electron number is coupled to Gaussian-distributed random site energies ε_i with zero mean and standard deviation W, i.e., $\mathcal{P}(\varepsilon_i) = (2\pi W^2)^{-1/2}\exp(-\varepsilon_i^2/2W^2)$. In the RD model, instead of random site energies, the disorder is represented by Gaussian-distributed random displacements of the lattice sites with standard deviation $\sqrt{3}W$. The DOS is given by the disorder average of $\rho(E) = (1/N)\sum_i \delta(E - E_i)$ with $E_i = \sum_{j\neq i}(n_j - \nu)(e^2/\kappa r_{ij}) + \varepsilon_i$ the local single-particle energy [3].

For the simulations, we use particle-conserving dynamics and periodic boundary conditions. To cope with the long-range Coulomb interactions, we perform a resummation technique in which we sum all interactions over periodic images and renormalize the energy scales such that the nearest-neighbor distance is $a = 1$. To compute the ground-state DOS ($T = 0$), we use extremal optimization [42]. For the CG model, we perform $2^{19}N$ updates and study systems of up to $N = 14^3$ sites in 3D for $W = 0.2$ and 0.4 and average over 3000 disorder samples for $L \leq 12$ and 1800 (800) samples for $L = 14$ for $W = 0.2$ ($W = 0.4$). For the RD model, we study $N = 14^3$ sites and average over 100 disorder samples (fluctuations are small). For the study at finite temperatures, we use exchange Monte Carlo [43,44]. Equilibration is tested by a logarithmic data binning. Once the last three bins agree within errors, the system is in thermal equilibrium. Simulation parameters can be found in Table I.

Results for the density of states.—Figure 1 (top and center panels) shows the DOS at $T = 0$ for the 3D CG model for two disorder strengths close to the Fermi level ($E = 0$) at half filling ($\nu = 1/2$); the insets show the whole functional shape. The data can be fit very well with a form $\sim|E|^{\delta}$ with $\delta = 2.01(2)$ ($L = 14$) for $W = 0.2$ and $\delta = 1.83(3)$ ($L = 14$) for $W = 0.4$ (restricted to $|E| \leq 0.3$), which is close to the ES value of $\delta \approx D - 1$.

TABLE I. Top: Simulation parameters for the simulations of the 3D Coulomb glass model with Gaussian disorder of strength W at finite temperature. L is the system size, N_{sa} is the number of disorder samples, N_{sw} is the number of equilibration sweeps, T_{min} is the lowest temperature, $T_{\mathrm{max}} = 0.455$ the highest temperature, and N_{r} the number temperatures used in the exchange Monte Carlo method. Temperatures are measured in units of $e^2/\kappa a$, $a = 1$ being the lattice constant. Bottom: Parameters for the 3D RD model simulations.

W	L	N_{sa}	N_{sw}	T_{min}	N_r
0.20	6	4290	2^{18}	0.030	27
0.20	10	388	2^{18}	0.030	27
0.20	14	251	2^{18}	0.083	17
0.40	6	4955	2^{18}	0.030	27
0.40	10	148	2^{18}	0.030	27
0.40	14	98	2^{18}	0.083	17
W	L	N_{sa}	N_{sw}	T_{min}	N_r
0.10	8	173	2^{20}	0.030	27
0.20	8	133	2^{20}	0.030	27
0.40	8	93	2^{20}	0.030	27
0.80	8	143	2^{20}	0.030	27

Figure 1 (bottom) shows the DOS of the RD model for $L = 14$. The DOS shows a pronounced double-peak, the width of the peaks dependent on W. There is no sign of the characteristic Coulomb gap shape; moreover, the peaks at $|E| \sim 1$ are typical of a Wigner crystal (WC). Thus, the DOS of the RD model is indicative of the formation of a moderately distorted WC at $T = 0$.

Results at finite temperature.—At half filling ($\nu = 1/2$), the ground state of the *clean* system ($W = 0$) is a WC with a bipartite charge pattern. For a WC, the DOS is expected to be two delta functions, separated by a charge gap E_{WC}. The energy required to move a particle from a site on the occupied sublattice to a site on the unoccupied sublattice is $E_{\mathrm{WC}} \approx 2$ in units of $e^2/\kappa a$. Since the peaks of the DOS of the CG are approximately centered around $|E| \sim 1$ (Fig. 1, inset), it needs to be verified that the observed DOS is indeed representative of a glassy phase and not only that of a distorted WC. Therefore, we study the nature of the phase at finite T by computing both an order parameter for a glassy state,

$$q_{\mathrm{GL}} = \frac{4}{N}\sum_{i=1}^{N}(n_i^{\alpha} - 1/2)(n_i^{\beta} - 1/2), \qquad (2)$$

and an order parameter for the competing Wigner crystal

$$m_{\mathrm{WC}} = \frac{2}{N}\sum_{i=1}^{N}(-1)^i(n_i - 1/2). \qquad (3)$$

In Eq. (2), α and β refer to two copies of the system with the same disorder [45]. If the system forms a Wigner crystal, we expect $[\langle m_{\mathrm{WC}}\rangle]_{\mathrm{av}} \to 1$ for $T \leq T_c$, whereas if the system freezes into a glass, we expect $[\langle q_{\mathrm{GL}}\rangle]_{\mathrm{av}} \to 1$

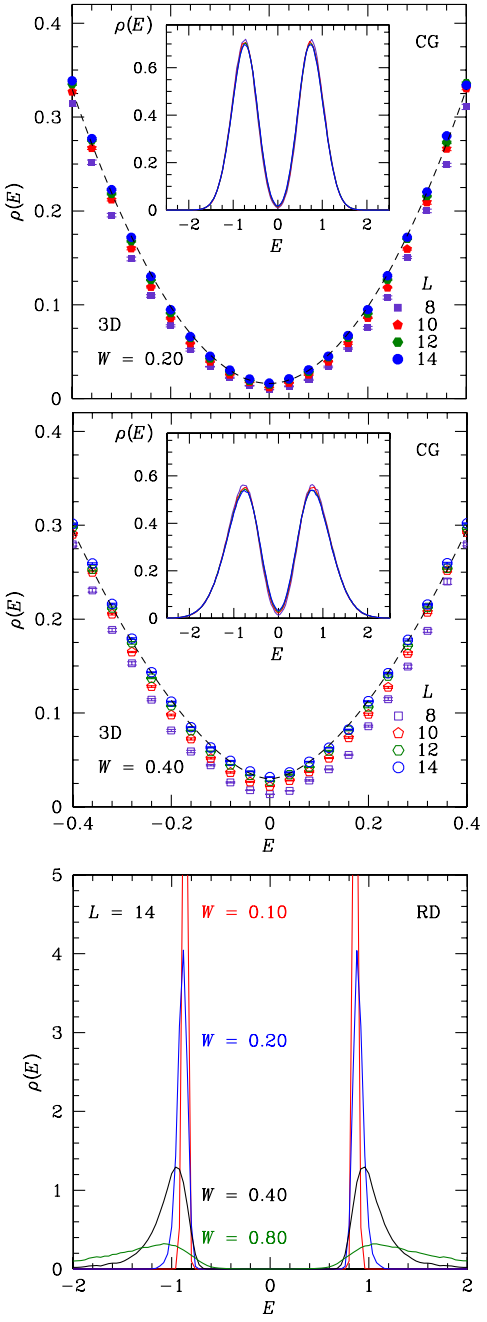

FIG. 1 (color online). Top: DOS for the 3D CG model for $W = 0.20$. The data are well fit by $\rho(E) \sim E^{\delta}$, $\delta \approx 2$ (dashed lines are a guide to the eye) around the Fermi level. Center: Same as in the top panel for $W = 0.40$. The insets show the full DOS. Both panels have the same horizontal range. Bottom: DOS for the 3D RD model. For all W studied, the data show a bimodal structure with peaks at $|E| \sim 1$ and a hard gap of size ~ 2, in stark contrast to the CG model.

and $[\langle m_{\mathrm{WC}} \rangle]_{\mathrm{av}} \to 0$ for $T \to 0$. Here, $[\cdots]_{\mathrm{av}}$ denotes the average over disorder and $\langle \cdots \rangle$ is a thermal average.

To locate the putative glass transition, we compute the two-point finite-size correlation length [46] given by

$$\xi_{\mathrm{GL}}(L,T) = \frac{1}{2\sin(|\mathbf{k}_{\mathrm{min}}|/2)}\left[\frac{\chi(\mathbf{0})}{\chi(\mathbf{k}_{\mathrm{min}})} - 1\right]^{1/2}, \quad (4)$$

where $\mathbf{k}_{\mathrm{min}} = (2\pi/L, 0, 0)$ is the smallest nonzero wave vector and $\chi(\mathbf{k})$ is the Fourier transform of the susceptibility $\chi = [\langle q_{\mathrm{GL}}^2 \rangle - \langle q_{\mathrm{GL}} \rangle^2]_{\mathrm{av}}$. We use four replicas to

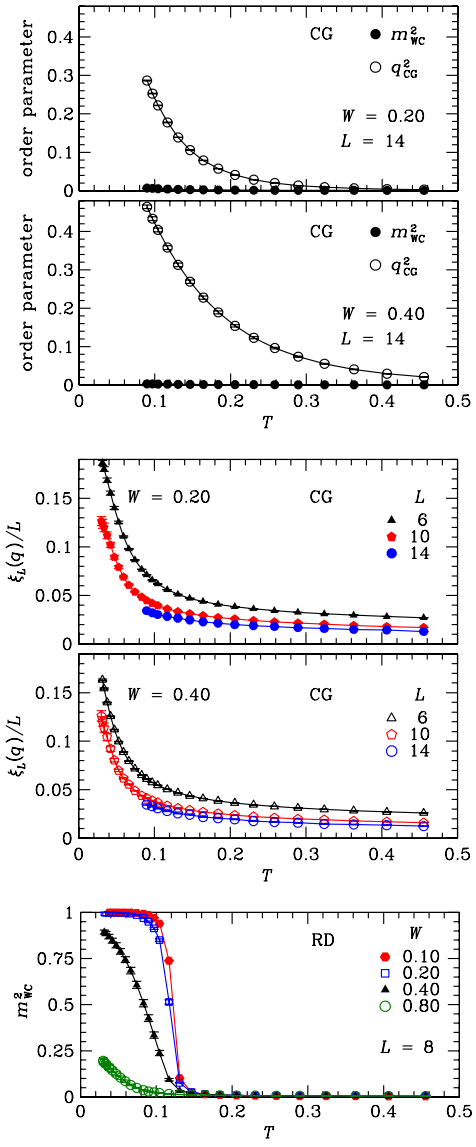

FIG. 2 (color online). Top: Wigner crystal order parameter $[\langle m_{\mathrm{WC}}^2 \rangle]_{\mathrm{av}}$ and glass order parameter $[\langle q_{\mathrm{GL}}^2 \rangle]_{\mathrm{av}}$ as a function of temperature T for different disorder strengths W for the CG model. In all cases, $[\langle m_{\mathrm{WC}}^2 \rangle]_{\mathrm{av}} \ll [\langle q_{\mathrm{GL}}^2 \rangle]_{\mathrm{av}}$. Center: Finite-size correlation length as a function of T for different disorder strengths and system sizes for the CG model. The data show no crossing, i.e., the absence of a thermodynamic transition for the studied temperature range. Bottom: Wigner crystal order parameter for the RD model ($L = 8$) as a function of temperature for different W. For $T \lesssim 0.1$, which quantitatively agrees with the critical temperatures estimated in Ref. [38], crystalline order emerges.

compute χ to avoid biases. Because $\xi/L \sim X[L^{1/\nu}(T - T_c)]$, a phase transition at T_c is signaled by the correlation lengths for different L's crossing at the same $T = T_c$.

Figure 2 (top panel) shows the $q^2_{\mathrm{GL}}(T)$ and $m^2_{\mathrm{WC}}(T)$ order parameters as a function of temperature for different disorder strengths in the CG model. The glass order parameter increases as the $T \to 0$, whereas the Wigner crystal order parameter does not exhibit any ordering tendency, $m_{\mathrm{WC}}(T)$ remaining $\sim$40 (140) times smaller than $q_{\mathrm{GL}}(T)$ for $W = 0.2$ ($W = 0.4$) at $T = 0.08$. Figure 2 (center panel) shows the correlation length for the glass order parameter as a function of T for the CG model. The data do not cross for the studied temperatures, and thus, there is no sign of a transition for $T \geq 0.03$, disagreeing with mean-field predictions [24,25]. The lack of a transition is mirrored by the small correlation length and the proximity to the ground-state energy (not shown).

In Fig. 2 (bottom panel), we show m^2_{WC} for the RD model for disorder strengths up to $W = 0.8$ covering the disorder range studied in Ref. [38]. For all W studied, m^2_{WC} rises noticeably (in contrast to the CG model). This further underlines that—for the studied disorder range—the phase transition in the RD model occurs into a surprisingly robust distorted Wigner crystal phase.

Conclusions.—We have analyzed the Coulomb glass at low and zero temperature and find that the gap exponent of the density of states is close to $\delta \approx D - 1$ in 3D systems. Furthermore, we find no evidence of a finite-temperature transition into a CG phase in 3D for $W = 0.2$ and 0.4. This suggests that the CG in 3D is at or below its lower critical dimension, which would explain the discrepancy with the mean-field results predicting a finite transition temperature. Finally, we have shown that in a broad disorder range, the random-displacement version of the CG model orders into a distorted Wigner crystal and not into a glassy state.

We thank S. Boettcher, V. Dobrosavljevic, E. Grannan, N. Jensen, M. Müller, M. Palassini, S. Pankov, D. Popovic, V. Oganesyan, M. Schechter, D. Sherrington, B. Shklovskii, T. Vojta, and A. P. Young for discussions. The simulations have been done on the ETH Zürich clusters. H. G. K. acknowledges support from the SNF under Grant No. PP002-114713.

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