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Phase transitions in the two-dimensional classical lattice Coulomb gas of half-integer charges

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We carry out Monte Carlo simulations of the two-dimensional (2D) classical lattice Coulomb gas of half-integer charges on a square lattice, which is believed to be in the same universality class as the fully frustrated 2D XY model, and find evidence for two transitions. At the lower temperature, we find a Kosterlitz-Thouless-type transition with a larger than universal jump in the dielectric constant ϵ^{-1}. At the higher temperature, we find a second-order charge lattice melting transition with a scaling behavior different from the pure Ising transition, in contrast to expectations from the symmetry analysis.

Statistical models known as the uniformly frustrated XY (FXY) models[1] have attracted a lot of attention, mainly due to their physical relevance to Josephson-junction arrays in a transverse magnetic field. The simplest case of such models is the fully frustrated XY (FFXY) model, which contains both a continuous symmetry, corresponding to global rotations of the spins, and a double discrete symmetry, corresponding to long-range order of the ground-state vortex lattice. Associated with this continuous symmetry, vortex excitations may appear as bound pairs at low temperatures. Unbinding of these bound vortex pairs with increasing temperature, may serve as a mechanism for the Kosterlitz-Thoules (KT) transition[2] as in the ordinary XY model. In such a case, the helicity modulus exhibits a discontinuous jump to zero from the universal Nelson-Kosterlitz value.[3] Proliferation of domain walls between the doubly degenerate ground-state vortex lattices may provide a mechanism for a continuous vortex-lattice melting transition as in an Ising transition.

Even in this simplest case there remain conflicting results about the nature of the phase transition. The first work of Teitel and Jayaprakash[1(a)] on this model suggested that there may be combined KT and Ising transitions at very close, if not equal, temperatures. The possibility of a larger than universal jump in the helicity modulus has also been suggested (see also Ref. 4). Subsequent numerical works[5] supported this picture, with some conflicting estimates on whether the two transitions should occur at the same critical or at different temperatures, with a slightly lower KT transition. The Ising critical behavior has usually been supported by observing logarithmic scaling[6] of the specific-heat peak with the system size. Grest[7] has studied the Coulomb gas (CG) model[8] of half-integer charges,[1(a)] which is believed to be in the same universality class as the FFXY model, and found two separate Ising and KT transitions, but with a nonuniversal KT jump. Very recently Lee, Kosterlitz, and Granato[9] have restudied the FFXY model using a new type of finite-size scaling analysis, and have claimed a single transition temperature with non-Ising-like critical behavior. This single transition picture was based on analysis of the Ising-like order parameter only. Their conclusion in favor of a single transition was based on the assumption that when the transitions are separate or decoupled, one should find a pure Ising transition; any non-Ising-like behavior should be taken as evidence for a single transition (see also Ref. 10). To support this single transition, however, an independent measure of the position of the KT transition is still essential. Therefore, the possibility of having two transitions at close but not equal temperatures may still have been left out. Recently Nicolaides[11] has studied correlation functions in this model using a large lattice of 128^2 sites, and found Ising and KT transitions at equal temperatures. Most recently, Ramirez-Santiago and José[12] have done a similar study as in Ref. 11, with even larger lattices of up to 240^2 sites. Similar non-Ising behavior was found as in Ref. 9, and a KT transition was found at the same temperature as the vortex-lattice melting transition, but with a nonuniversal jump in the helicity modulus.

Therefore, despite many reinvestigations, there still remain conflicting estimates as to whether the model has a single versus two transitions, as well as the nature of transition itself. To distinguish among these possibilities, we conduct extensive Monte Carlo (MC) simulations of the CG model of half-integer charges. We apply different finite-size scaling analyses from previous works, in order to determine the critical behavior and transition temperature(s) accurately.

In the Villain approximation[13] for the cosine potential in the XY model, the FXY model can be mapped into the fractional charge CG on the dual lattice of the XY model by the standard duality transformation,[14] yielding the Hamiltonian,

$$\mathcal{H}_{\rm CG}=\frac{1}{2}\sum_{ij}(m_i-f)G_{ij}(m_j-f)\ . \tag{1}$$

Here m_i corresponds to the integer vorticity of the phase at site i dual to the XY lattice,[2,14] f is the same as the uniform frustration in the FXY model, and the total charge is neutral, i.e., $\sum_i m_i=Nf$, where N is the number of all sites in the system. G_{ij} is the lattice Green's function which behaves logarithmically at large distances r_{ij}. The charges at site i are defined by $q_i=m_{i}-f$. For the fully frustrated case, $f=\frac{1}{2}$, the lowest magnitude charges are, thus, $\frac{1}{2}$ and $-\frac{1}{2}$. The ground state in this model con-

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sists of a lattice of charges $\frac{1}{2}$ and $-\frac{1}{2}$, which form a checkerboard pattern with the same symmetry as an Ising antiferromagnet.

In this model there can be two types of excitations.[1(a)] One is a KT-like excitation, which comes from the interchange of a given $+\frac{1}{2},-\frac{1}{2}$ pair with separation r, and gives an excitation energy proportional to $\ln r$ in the large r limit. The other is an Ising-like domain excitation, which results from the formation of oppositely ordered charge lattice domains, within the ordered phase.

To investigate the critical behavior of this model, we carry out extensive MC simulations on the square lattice of linear size L with periodic boundary conditions. Restricting the charges to be either $+\frac{1}{2}$ or $-\frac{1}{2}$ only, the new configuration is created by exchanging nearest-neighbor pairs. This change is then either accepted or rejected, using the standard Metropolis algorithm. The averages are taken using five independent runs which contain both heating and cooling. Typically, a total of 10^6 MC steps per charge are used for averaging, with an initial 10 000 MC steps at each temperature discarded for equilibration. Further details of the simulation method can be found in Ref. 15.

We first look at the charge lattice melting transition in this model by considering the dependence of the specific-heat peak on the system size, $C_{\text{peak}} \sim L^{\alpha/\nu}$. This charge lattice melting transition was originally suggested to be an Ising transition. In Fig. 1, we show our data for the specific-heat peak, which we plot on both a semilog and log-log scale. The semilog plot shows fair consistency with the logarithmic scaling behavior as in an Ising model, i.e., $\alpha=0$. A better fit, however, is obtained assuming a power-law divergence, at least for sizes $L \geq 12$, as seen on the log-log plot. This gives $\alpha/\nu=0.503\pm0.013$. Applying the hyperscaling law, this gives $1/\nu=1.251 \pm0.007$, which is different from the pure Ising value of 1. However, since the power-law scaling appears only marginally better than the logarithmic scaling, it may not be very persuasive to determine the nature of transition solely by this analysis.

As a better check, we analyze the charge lattice order parameter $M=(1/N)\sum_i q_i(-1)^{x_i+y_i}$. From the finite-size scaling theory,[6,16] the scaling of the singular part of the free energy $f \equiv -(1/N)\ln Z$ near a critical point is given by $f_s(t,h,L)=L^{-d}f_s(tL^{y_t},hL^{y_h})$, where $d=2$ is the dimensionality of the system, $y_t=1/\nu$ and $y_h=d-\beta/\nu$ are the eigenvalues of the scaling field t and h in the renormalization transformation. Since for any finite-size system L, the order parameter vanishes $\langle M \rangle=0$, we have for the scaling law of the order parameter squared, $M^2=L^{2(y_h-d)}f_h^{(2)}(tL^{yt},h=0)$, where $f_h^{(2)}$ is the second derivative of f_s with respect to h. To determine the critical exponent, we adopt Nightingale and Blöte's scheme[17] in analyzing our data for M^2. Taking the above equation for M^2, we can expand the scaling function $f_h^{(2)}$ about T_c, where $tL^{1/\nu}$ is small as follows:

$$M^2(T,L)=L^{-2\beta/\nu}[\Phi_0+\Phi_1 L^{1/\nu}(T-T_c) + O(L^{2/\nu}(T-T_c)^2)] \ . \tag{2}$$

Truncating this expansion at any finite order, we perform a χ^2 fit of our data M^2, using the Levenberg-Marquart method.[18] Here $2\beta/\nu$, $1/\nu$, T_c, Φ_0, etc., are unknown parameters to be determined by this fitting. Since the scaling form is supposed to hold in the large L limit, to check, whether we have reached this limit, we successively increase the seize of the smallest system included in our fit and repeat the fit. We continue this process until further increase in the size of the smallest system, or in the order of expansion of the scaling function does not change the parameter values obtained from this fit, within the estimated error. The error of the fitted parameters is estimated as in Ref. 15.

We show our data in Fig. 2 for lattice sizes from $L=6$ to $L=30$. From the second-order expansion of Eq. (2) for lattice sizes $L=10$–24, we find the critical exponents $\beta/\nu=0.1291\pm0.0184$, $1/\nu=1.1943\pm0.0728$, and $T_c=0.1314\pm0.0004$. The value of $1/\nu$ agrees with the re-

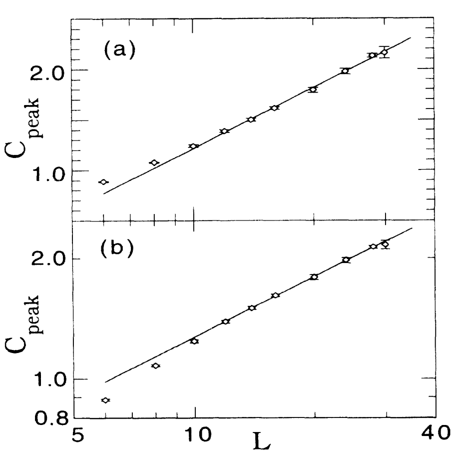

FIG. 1. Specific-heat peak as a function of lattice size L in (a) semilog and (b) log-log plot. The solid lines are least χ^2 fits to $L \geq 12$ data.

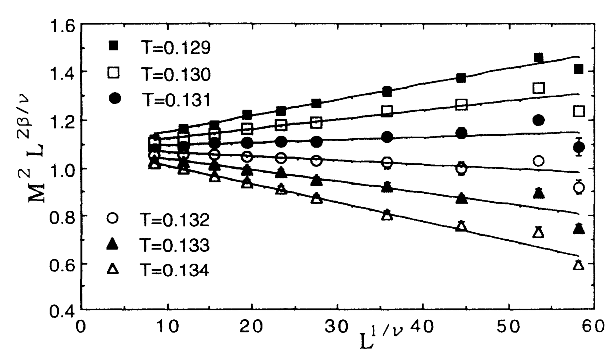

FIG. 2. The finite-size scaling behavior of the order parameter M^2. Symbols with error bars represent the MC data. From the left, the lattice sizes are $L=6$, 8, 10, 12, 14, 16, 20, 24, 28, and 30. The solid lines represent the result of fitting Eq. (2) to a second-order expansion in $T-T_c$, using data from $L=10$–24. The fitted values of $1/\nu=1.1943$ and $\beta/\nu=0.1291$ were used in making the axes of the plot. 10^6 total MC steps per charges were used.

sult from the specific heat. These values may be compared with those obtained in Ref. 9, $\beta/\nu=0.155\pm0.015$ and $1/\nu=1.1765\pm0.0353$, and those in Ref. 12, $\beta/\nu=0.1106\pm0.0065$ and $1/\nu=1.143\pm0.040$. In Fig. 2, we notice that data for sizes $L=28$ and 30 show the most deviation from the fitted curves. We believe that this deviation is attributed to the poor statistics of the data, rather than a systematic change in the scaling of the data as L increases. These poor statistics may have been caused by the familiar critical slowing down near T_c, which usually affects the large system more seriously than the small system. We have tried to fit our data including these two largest sizes, and found, within estimated error, the same values as above only with a substantially increased χ^2 error of the fit.

As another method of analysis, we use Binder's cumulant method.[19] Adopting the free block version of this method, we calculate the cumulant $U(T,L)=1-\langle M^4\rangle/3\langle M^2\rangle^2$ in each lattice of size L. In the large L limit above T_c, U tends to zero. Below T_c, U approaches the nonzero value of $\frac{2}{3}$, since the system orders at either $+M$ or $-M$. Using $f_h^{(4)}(t,h=0)=N^3(\langle M^4\rangle-3\langle M^2\rangle^2)=L^{4y_h-d}f_h^{(4)}(tL^{y_t},\,0)$ where $f_h^{(4)}$ is the fourth derivative of f_s with respect to h, and the scaling equation for M^2, one finds that $U(T,L)=\phi(tL^{1/\nu})$, where ϕ is a scaling function. Therefore, right at T_c, where $t=0$, U should become the nontrivial universal value, $\phi(0)$ for all L. This behavior of U can be seen in our data shown in Fig. 3 for system sizes $L=6$–30, suggesting $T_c\approx0.132$. We can also apply the same scheme as in the analysis of M^2, expanding the scaling function ϕ near T_c, where $tL^{1/\nu}$ is small as follows:

$$U(T,L)=\phi_0+\phi_1L^{1/\nu}(T-T_c)+O(L^{2/\nu}(T-T_c)^2)\ . \quad (3)$$

Here $1/\nu$ is the only exponent to be determined. From a fit to a fourth-order expansion of Eq. (3) for lattice sizes $L=10$–24, we find the critical exponent $1/\nu=1.1954\pm0.0394$, and $T_c=0.1315\pm0.0003$. These values are consistent with those obtained from the fit of M^2. Again, the data for the sizes $L=28$, and 30 scatter around the fitted curve. Therefore, from the results of our

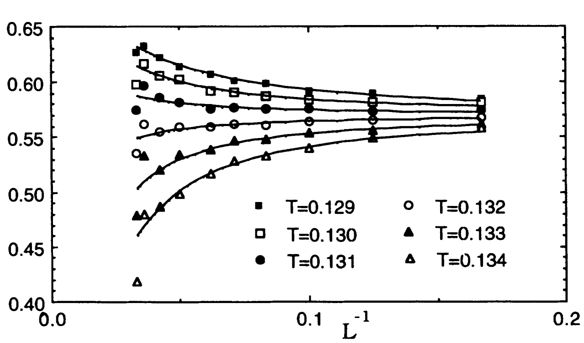

FIG. 3. The finite-size scaling behavior of the Binder cumulant U. Symbols represent the MC data, and error bars are not shown for clarity of the figure. The same lattice sizes as shown in Fig. 2 are used. The solid lines represent the result of fitting Eq. (3) to a fourth-order expansion in $T-T_c$, using data from $L=10$–24 and the fitted value of $1/\nu=1.1954$. 10^6 total MC steps per charges were used.

analysis of both M^2 and U, we conclude that the charge lattice melting transition is different from the pure Ising transition.

To check whether this non-Ising behavior can be attributed to neglecting corrections to scaling from slow irrelevant variables, we try to fit our data for U to an expansion of a scaling function including a correction to scaling:[6]

$$U=\phi(tL^{1/\nu},gL^{x})\ , \quad (4)$$

where g is the irrelevant scaling field and x is the correction-to-scaling exponent, $x<0$. Expanding Eq. (4) for small t and g, we fit our data to determine the unknown parameters as was done before. First, we fix $1/\nu$ to the Ising value of 1. Finding stable values for the remaining parameters would mean that the correction to scaling is significant and the transition should be taken as Ising. However, we find that the fitted values x, and the polynomial coefficients [i.e., ϕ_i's in Eq. (3)] are unstable, and the χ^2 errors of the fit are almost doubled compared to the previous fit. We also see that the coefficients of the terms in g grow rapidly in magnitude and suffer from big fluctuations as we increase the order of expansion. This may mean that the correction terms from g are free to change and are not playing any significant role. Repeating the same fit with $1/\nu$ as a free parameter, we now find a stable fit for the coefficients of the terms in t, and the same value of $1/\nu$ as in the previous result ignoring g, with the same χ^2 errors. The same behavior in the coefficients of g is seen as above. Therefore, we believe that the critical behavior is not attributed to neglecting corrections to scaling, and is truly non-Ising-like.

To determine the behavior of the KT-like transition independently, we measure the inverse dielectric constant, given by standard linear response theory[7,20] as

$$\epsilon^{-1}(T,L)=\lim_{k\to0}\left\{1-\frac{2\pi}{k^2TN}\langle q_kq_{-k}\rangle\right\}\ , \quad (5)$$

where $q_k\equiv\sum_i q_i e^{-i\mathbf{k}\cdot\mathbf{r}_i}$ is the Fourier transform of the charge density. ϵ^{-1} maps onto the helicity modulus of the FFXY model.[1(a),20,21]. In our simulations, ϵ^{-1} is approximated by averaging over the two smallest allowed wave vectors $(2\pi/L)\hat{x}$, $(2\pi/L)\hat{y}$ for each system size. An instability criterion, based on the Kosterlitz-Thouless argument, requires that ϵ^{-1} jumps discontinuously to zero at $T_{\rm KT}$, bounded by $\epsilon^{-1}(T_{\rm KT})\geq4T_{\rm KT}$. This holds as an equality in the KT analysis, giving a universal jump prediction $\epsilon^{-1}(T_{\rm KT})/T_{\rm KT}=4$. More generally, it can serve as giving an upper bound on $T_{\rm KT}$, $T_{\rm KT}\leq\epsilon^{-1}(T_{\rm KT},L)/4$, or equivalently a lower bound on the jump in ϵ^{-1}, $4\leq\epsilon^{-1}(T_{\rm KT},L)/T_{\rm KT}$. In Fig. 4, we plot $\epsilon^{-1}(T,L)$ vs T for various lattice sizes L. Intersection with the dashed line $4T$ gives the KT upper bound on $T_{\rm KT}$. From the intersection with the largest size $L=30$, we see that $T_{\rm KT}\approx0.1297$, which is slightly lower than that found for the charge lattice melting transition, $T_c\approx0.1315$. We note that when we estimate $T_{\rm KT}$ from the smaller size $L=24$, where the statistics are better than for $L=30$, we see that $T_{\rm KT}$ is still slightly lower than T_c (around a 1%

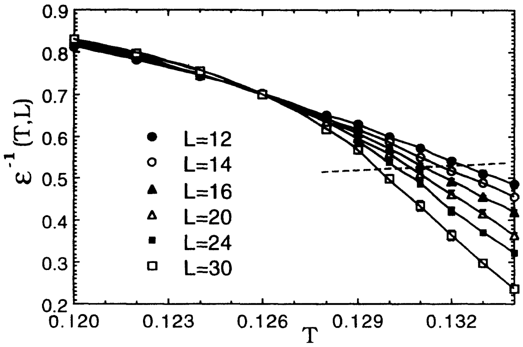

FIG. 4. Inverse dielectric function $\epsilon^{-1}(T)$ for various square lattice sizes L. The common intersection of the curves for different L approximates T_{KT}. Intersection with the dashed line $4T$ gives the KT bound $\epsilon^{-1}(T_{\mathrm{KT}}) \geq 4T_{\mathrm{KT}}$. 10^6 total MC steps per charges were used.

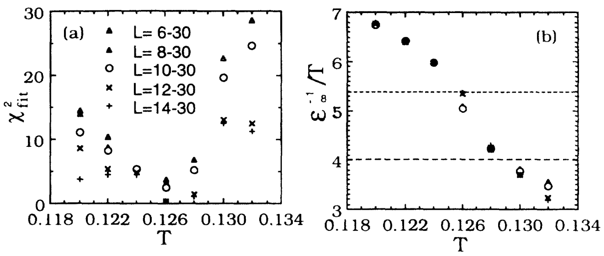

Fig. 5. (a) The χ^2_{fit} error for a fit to Eq. (6) as a function of T, and (b) corresponding fitted value of ϵ_∞^{-1}/T for different sequences of L. $L=6, 8, 10, 12, 14, 16, 20, 24, 30$ have been used.

difference). Since this application of the universal KT bound gives an estimation of T_{KT} which is very close to T_c, considering statistical errors, this analysis alone may not give a definitive conclusion. We, therefore, use another analysis to estimate T_{KT}.

For a more precise location of T_{KT}, and estimate of the jump in $\epsilon^{-1}(T_{\mathrm{KT}})$, we use finite-size scaling. From the identification of ϵ^{-1} with the helicity modulus, we expect that the finite-size behavior at T_{KT} should follow the Josephson scaling relation,[22] $\epsilon^{-1}(T,L) \sim L^{2-d}H[L/\xi(T)]$, where ξ is the correlation length which diverges at T_{KT}. Since $d=2$, we might expect that $\epsilon^{-1}(T_{\mathrm{KT}},L)$ is independent of L. Therefore, all the curves for different sizes L should intersect at the same point T_{KT}. Using this criterion, and the data of Fig. 4, we estimate $T_{\mathrm{KT}} \approx 0.126$.

To estimate both T_{KT} and the jump in $\epsilon^{-1}(T_{\mathrm{KT}})$, we follow Weber and Minnhagen's finite-size scaling analysis,[23] including leading logarithmic corrections to the Josephson scaling law. Based on the Koserlitz recursion equations, they find

$$\epsilon^{-1}(T_{\mathrm{KT}},L) = \epsilon_\infty^{-1}\left[1 + \frac{1}{2\ln L + c}\right], \qquad (6)$$

where for the universal KT transition, one has $\epsilon_\infty^{-1} \equiv \epsilon^{-1}(T_{\mathrm{KT}},\infty) = 4T_{\mathrm{KT}}$. Following their approach, we do a least χ^2 fit of the MC data at each temperature, to the form (6), with ϵ_∞^{-1} and c as free parameters. The temperature at which the χ^2 error is smallest, we identify as the transition T_{KT}, and the fitted parameter ϵ_∞^{-1} gives the jump in ϵ^{-1}. In Fig. 5, we plot χ^2_{fit} and the fitted ϵ_∞^{-1}/T versus T, using different ranges of lattice size L. The transition temperature as given by the minimum χ^2_{fit}, is $T_{\mathrm{KT}}=0.126$. We find that at this temperature $\epsilon^{-1}(T_{\mathrm{KT}}/T_{\mathrm{KT}}) \approx 5.35$, larger than the KT universal value of 4. This value is slightly bigger than the value of 5.21 found in Ref. 12. This may also be compared with the result of Grest,[7] $\epsilon^{-1}(T_{\mathrm{KT}})/T_{\mathrm{KT}} = 4.88 \pm 0.31$ with $T_{\mathrm{KT}} = 0.129 \pm 0.002$. We note here that for $T \leq 0.126$, our fitting yields $c \gtrsim 50$, giving only very small corrections to Eq. (6), while for $T > 0.126$, our fitting yields $c \lesssim 0.1$, which would imply larger corrections.

In conclusion, we have found two transitions at close but clearly separated temperatures, rather than a single transition. We remark that the naive application of the universal KT bound gives an estimation of $T_{\mathrm{KT}} \approx 0.1297$, which is very close to the lattice melting transition temperature $T_c \approx 0.1315$) (1% difference). When T_{KT} is estimated using finite-size-scaling analysis, we find $T_{\mathrm{KT}} \approx 0.126$, giving a 4% difference. At the lower temperature, we found a KT-like transition, with a larger than universal jump in ϵ^{-1}. At the higher temperature, we found a continuous charge lattice melting transition which belongs to a different universality class than the Ising transition, in contrast to expectations from the symmetry analysis. Similar results were found for closely related CG models in our earlier work.[15,24] However, how the pairwise KT excitations couple to the Ising-like domain excitations, remains fundamentally not understood.

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