

Critical behavior of the two-dimensional uniformly frustrated charged Coulomb gas

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The nature of the phase transition for the two-dimensional Coulomb gas on the square lattice in the presence of a uniform frustration f is studied by Monte Carlo simulation. We present evidence for a nonuniversal Kosterlitz-Thouless (KT) jump for the inverse dielectric constant ϵ_0^{-1} for $f = \frac{1}{2}$, $\frac{1}{3}$, and $\frac{1}{4}$. For the fully frustrated case $f = \frac{1}{2}$, two distinct transitions, one KT-like and the other Ising-like, is observed in contrast to earlier studies for the XY model, which suggested only one transition, even though both models are believed to be in the same universality class.

I. INTRODUCTION

The uniformly frustrated XY model¹⁻¹⁵ has been studied extensively in recent years as a model for 2D coupled arrays of Josephson junction and superconducting wires in a transverse magnetic field. Unlike the unfrustrated XY model which cannot exhibit long-order order at finite temperatures, the frustrated XY model is expected to display different critical behavior. In addition to the underlying continuous $U(1)$ symmetry, there exist a discrete symmetry, which leads to the possibility of long-range order in two dimensions.

While there have been several analytic,⁷⁻¹² and numerical studies^{3,13-15} of the phase transition for the frustrated XY model for rational f , a number of unsettled issues still remain including the nature of the transition. At low temperatures, it has been well established³⁻¹⁵ that long-range order exist, associated with the discrete symmetry of the ground states. For rational filling factors $f = \Phi/\Phi_0 = p/q$ (Φ is the average flux through an elementary plaquette, $\Phi_0 = hc/2e$ is the flux quantum), the ground state^{4,5} is periodic with a unit cell of size $q \times q$. The ground-state energy $E_0(f)$ has been determined for a number of lattices^{4,5} and $E_0(f)$ is a nonmonotonic function of $f \in [0, \frac{1}{2}]$ with sharp features at several f . For the fully frustrated case $f = \frac{1}{2}$, which has a doubly degenerate ground state, it is still not clear whether there exist only one transition⁶⁻¹⁵ at the critical temperature T_c which is a combination of a Kosterlitz-Thouless^{16,17} (KT)-like one for spins and an Ising-like one for chirality or two successive transitions,^{11,12} in which the KT transition temperature is different from the Ising-like one. While several recent analytic studies⁹⁻¹¹ are in favor of the former case, Granato and Kosterlitz¹¹ point out this special case is not very amenable to theoretical analysis. Also, in each of these analytic studies, the models have a symmetry which is different than the fully frustrated XY model and they do not allow fractional vortices which are believed to be important at the transition. Another point at issue is whether the jump in the helicity modulus^{3,6,18} at the KT transition is universal or not. Minnhagen¹⁹ has argued that there are two classes of possible KT transitions for the XY models, one associated with a universal

jump²⁰ from $\Upsilon(T_c) = 2k_B T_c / \pi$ to zero at T_c and one associated with a larger, nonuniversal jump whenever T_c is below a critical value T_c^* . While some simulations^{21,22} and at least one experiment²³ suggest that the $f = \frac{1}{2}$ frustrated XY model belongs to the second of these classes, the observed size of the nonuniversal jump is only slightly larger than the universal value $2k_B T_c / \pi$. Since a nonuniversal jump also had been predicted by Choi and Stroud⁹ for $f = \frac{1}{2}$ due to the effect of the Ising excitations on the transition, the available data cannot be used to test Minnhagen's predictions.

The occurrence of a Kosterlitz-Thouless transition in combination with an Ising transition has been suggested by Lee *et al.*²⁴ for the antiferromagnetic XY model on the triangle lattice in zero external magnetic field. Because of the breaking of a discrete symmetry, the system exhibits an additional discrete order parameter, the staggered helicity. Miyashita and Shiba²⁵ found distinct Ising and KT transitions that were within 2% of each other and argued that is likely that there is an intermediate phase between them. Lee *et al.*²⁴ however, argued using finite size scaling analysis on larger systems that the two transitions were at same temperature and that the spinwave-stiffness constant at T_c was consistent with the universal jump predicted by Nelson and Kosterlitz.²⁰

To address these questions in greater detail, I have carried out Monte Carlo simulations and finite size scaling on the square lattice for several values, $f = 0, \frac{1}{2}, \frac{1}{3},$ and $\frac{1}{4}$. However, instead of working with the usual frustrated XY model, I studied the fractionally charged Coulomb gas (CG), which is believed to be in the same universality class.^{1,2,17} While the interaction range is long range in contrast to the XY model, one only has to deal with discrete integer variables not continuous spins. This model has the advantage that the usual Gaussian spin waves which are present in the XY model have been eliminated, leading to more rapid equilibration. The price one pays is that the interaction is long range. However because of access to modern supercomputers, this is no longer a serious difficulty. Working directly with the CG model it is also straightforward to check Minnhagen's predictions¹⁹ for nonuniversal jumps at the KT transition, since it is for this model that the calculations were

actually performed and, his prediction can simply be stated. When the transition temperature T_{CG} is between $\frac{1}{4}$ and T_{CG}^* (≈ 0.1436), the jump in ϵ_0^{-1} is exactly $4T_{CG}$, where ϵ_0^{-1} is the inverse dielectric constant. For $T_{CG} < T_{CG}^*$ the jump is larger and nonuniversal. Since no simulations for the Coulomb gas model were available, Minnhagen²² used an approximate scaling relation^{21,25} between T_{CG} and the XY temperature T to show that some previous Monte Carlo results for the helicity modulus T appeared to have a nonuniversal jump. In this paper, I present results for the jump in ϵ_0^{-1} for several values of f which test Minnhagen's predictions directly in the Coulomb gas model.

II. MODEL AND METHOD

The Hamiltonian for the charged Coulomb gas model is^{15,17}

$$H = -2\pi J \sum_{l,m} q_l G_{l,m} q_m, \quad (1)$$

where $G_{l,m}$ is the 2D lattice Green's function and the sum is over all pairs of sites (lm) . The "charge" $q_l = n_l - f$, where n_l is an integer variable. As a consequence of charge neutrality, $\langle n_l \rangle = f$. Though a direct simulation of Eq. (1) is possible,¹⁵ the interaction $G_{l,m}$ falls off only logarithmically in 2D and one would need to carry out the equivalent of an Ewald sum to avoid introducing large truncation errors. An alternate, yet equivalent procedure for carrying out the numerical simulations is to first rewrite Eq. (1) in a more convenient form.²⁷ To motivate this alternative formulation, consider a superconducting network where each node is connected to exactly four others. In an external field the fluxoid (the circulation of the phase gradient) must be quantized:

$$\oint \nabla \phi \cdot dl = \frac{4\pi}{c\Phi_0} \oint \lambda^2 \mathbf{J} \cdot dl + \frac{2\pi}{\Phi_0} \oint \mathbf{A} \cdot dl = 2\pi n, \quad (2)$$

where \mathbf{A} is the vector potential, λ is the penetration depth, and \mathbf{J} is the screening current. This condition must be satisfied for every closed loop. For the square lattice, with lattice spacing $l=1$, define \mathbf{J} in each link in terms of a new set of variable $F_{i,j}$ for plaquette (i,j) such that \mathbf{J} in the vertical direction equals $F_{i,j} - F_{i+1,j}$ and $F_{i,j} - F_{i,j+1}$ in the horizontal direction as shown in Fig. 1. Note that these differences carry with them a sign reflecting the direction in which the current flows. Equation (2) can then be written as

$$= q_{ij}, \quad (3)$$

where $F_{i,j}$ is in units of $c\Phi_0/2\lambda^2$, n_{ij} is the number of fluxoids in area $a_{ij}=1$, and $\langle n_{ij} \rangle = f$. If we use periodic boundary conditions and take the Hamiltonian as the square of the current in each link²⁸

$$H = \pi \sum_{ij} (F_{i,j} - F_{i+1,j})^2 + (F_{i,j} - F_{i,j+1})^2 \quad (4)$$

it is easy to show that Eq. (4) can be transformed into Eq.

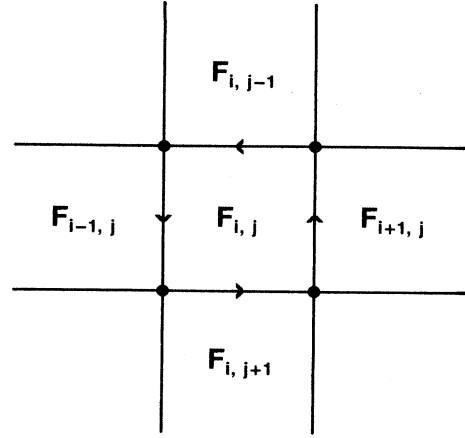


FIG. 1. Diagram of square lattice showing new variables F_{ij} .

(1). Note that Eqs. (3) and (4) can easily be generalized to arbitrary lattices including quasiperiodic and disordered lattices in which the length of wires between nodes may not be equal.

The advantage of Eq. (4) over (1) can be seen as follows. First, rewrite Eq. (3) in the form of a matrix, $\underline{A}\mathbf{F}=\mathbf{q}$ when \mathbf{F} and \mathbf{q} are 1D vectors of length L^2 , the number of plaquettes. \underline{A} can be inverted to determine \mathbf{F} , by adding a small amount ϵ to each zero element of \underline{A} . I used $\epsilon=10^{-9}$ and checked that for all $\epsilon < 10^{-3}$, the results are independent of ϵ . Even though \underline{A} is large, size $L^2 \times L^2$, the inversion need only be done once, since \underline{A} depends only on the connectivity of the lattice.²⁹ Standard Monte Carlo techniques were then used to find the equilibrium "charge" configurations. A plaquette was chosen at random and a unit of "charge" was added to q_l and subtracted from one of the eight nearest or next nearest neighbor plaquettes, also chosen at random. Since for each exchange only two values of q_l were changed, the new values of \mathbf{F} could be determined directly from the old ones without having to recalculate $\underline{A}\mathbf{q}$. These new \mathbf{F} 's were then inserted into Eq. (4) to determine the change in energy ΔE . The move was then accepted with probability $\exp(-\Delta E/kT)/[1 + \exp(-\Delta E/kT)]$.

The simulations were carried out for several lattice sizes from $L=12 \rightarrow 50$ on a square lattice with periodic boundary conditions for $f=0, \frac{1}{2}, \frac{1}{3}$, and $\frac{1}{4}$. L was always chosen to be commensurate with f . Away from the critical temperature runs were typically of length $1-2 \times 10^4$ "charge" exchanges per plaquette, while near the critical temperature, this number was increased to between 4 and 20×10^4 . The average energy, specific heat, and the inverse dielectric constant defined by^{3,18}

$$\epsilon_0^{-1} = 1 - \frac{2\pi J}{k_B T} \lim_{k \rightarrow 0} \frac{\langle n_k n_{-k} \rangle}{k^2}, \quad (5)$$

where $n_k = 1/N \sum_{ij} n_{ij} \exp(ik \cdot \mathbf{r}_{ij})$ were measured after the system was equilibrated. ϵ_0^{-1} was evaluated by averaging over the five smallest allowed k vectors for

each size system. In addition, for $f = \frac{1}{2}$, the staggered magnetization M_s and susceptibility χ_s was also determined. Most runs were made on heating from low temperature in increments of $T/\pi = 0.001$. In addition, near the transition results were also obtained on cooling from above the transition temperature to check that the system was equilibrated. For large L , smaller increments were needed to determine the position of transition temperature accurately.

III. RESULTS

As a check of the procedure described above, I first considered the case $f = 0$. Results for the specific heat C and inverse dielectric constant ϵ_0^{-1} for the $f = 0$, unfrustrated CG are shown in Fig. 2 for three values of L . The solid line in Fig. 2(b) is $\epsilon_0^{-1} = 4T$. The simulation results cross this line at $T_{CG} = 0.220 \pm 0.005$, which is in excellent agreement with the results of Saito and Müller-Krumbhaar³⁰ who found $T_{CG} = 0.215$ from their simulations on the discrete Gaussian model. As expected, the peak in C is considerably above T_{CG} , just as found for the XY model.³¹

Consider next the fully frustrated case, $f = \frac{1}{2}$. Results for C , M_s , and ϵ_0^{-1} are presented in Fig. 3 for five values of L . The peak value of the specific heat C_{max} is plotted versus $\log L$ in Fig. 4. The linear dependence of C_{max} on

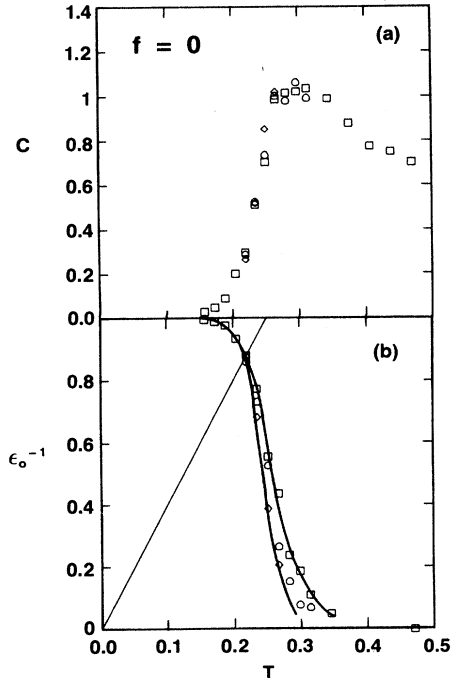


FIG. 2. Specific heat C and inverse dielectric constant ϵ_0^{-1} vs temperature T for $f = 0$ for three values of L , $L = 20$ (\square), 30 (\circ), and 40 (\diamond). The solid line in (b) corresponds to the prediction of Ref. 18 for the universal value of $\epsilon_0^{-1} = 4T$ at the transition. Below this line $\epsilon_0^{-1} = 0$ for $L \rightarrow \infty$. The smooth curves through the points for ϵ_0^{-1} for $L = 20$ and 40 are a guide to the eye and not a fit.

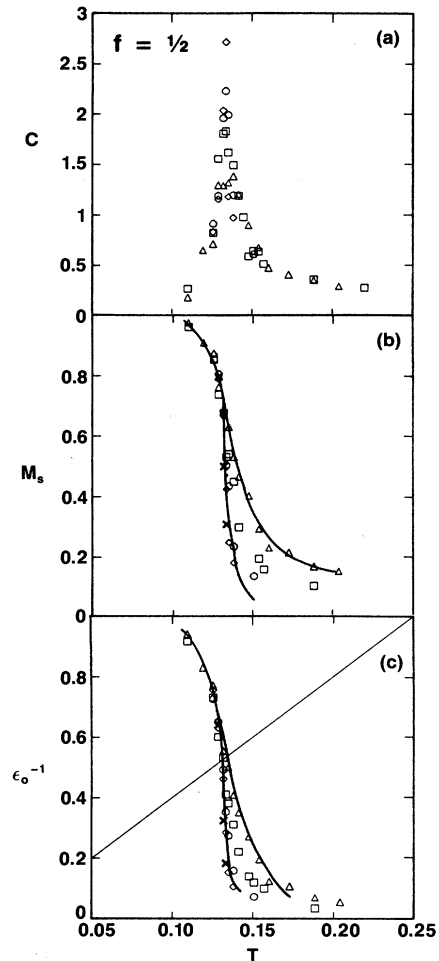


FIG. 3. Specific heat C , staggered magnetization M_s and inverse dielectric constant ϵ_0^{-1} vs T for $f = \frac{1}{2}$ for $L = 12$ (\triangle), 20 (\square), 30 (\circ), 40 (\diamond) and 50 (\times). The solid line in (c) is $\epsilon_0^{-1} = 4T$, while the smooth curve through the points for $L = 12$ and 40 are only a guide to the eye.

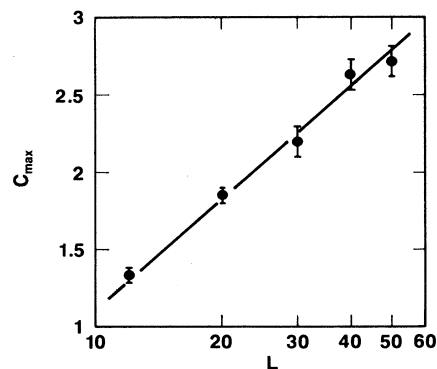


FIG. 4. Maximum in specific heat C_{max} vs $\log_{10} L$ for $f = \frac{1}{2}$.

$\log L$ indicates a critical exponent $\alpha=0$ which is characteristic of the Ising transition, in agreement with earlier results for the XY model.^{3,13} The peak in both C and χ_s (not shown) occurs at a temperature $T_I=0.133\pm 0.001$, independent of L for $12\leq L\leq 50$, in contrast to the XY model³ in which T_C varied significantly with L over a comparable range of L . This is also in contrast to earlier work of Thijssen and Knops¹⁵ on the CG who found the peak position varied significantly more for $16\leq L\leq 30$ than found here. While Thijssen and Knops¹⁵ did not specify precisely how they cut off the logarithmic interaction between vortices in Eq. (1), the differences in the position of the specific heat peak are probably related to differences in how the interactions were truncated. In the present formulation Eq. (4) there are no problems with truncating the interaction. They found that $T_I=0.130\pm 0.001$. To check whether the KT-like transition occurs at the same temperature, consider the results for ϵ_0^{-1} . For $T\geq 0.133$, a finite size scaling analysis shows that $\epsilon_0^{-1}\rightarrow 0$ as $L\rightarrow\infty$. Results for $T=0.132$ are decreasing strongly with L but do not follow a clear L^{-1} (see Fig. 5) or $1/\ln L$ dependence. However at $T=0.132$, ϵ_0^{-1} for $L>20$ is well below the Nelson-Kosterlitz²⁰ value of 0.53, and appears to vanish as $L\rightarrow\infty$. For $T\leq 0.129$, there is no systematic dependence of ϵ_0^{-1} on L , indicating the KT transition occurs at $T_{KT}=0.129\pm 0.002$, below the Ising-like transition. Thijssen and Knops¹⁵ find $T_{KT}=0.132\pm 0.001$ and no evidence for a nonuniversal jump in ϵ_0^{-1} . However as seen from Fig. 5 at 0.132, $\epsilon_0^{-1}\rightarrow 0$ as $L\rightarrow\infty$. From Figs. 3(c) and 5 we see that the jump in $\epsilon_0^{-1}(T_{KT})$ is 0.63 ± 0.03 , greater than the universal value 0.52 and in agreement with Minnhagen's result,¹⁹ 0.646. The argument could also be turned around by assuming that Minnhagen is correct, in which case $T_{KT}=0.129$.

This is the first numerical evidence for two distinct transitions, the lower one of the KT type and the higher one Ising like. Teitel and Jayaprakash³ carried out the first simulations for the fully frustrated XY model but found significant finite size effects for both the position of

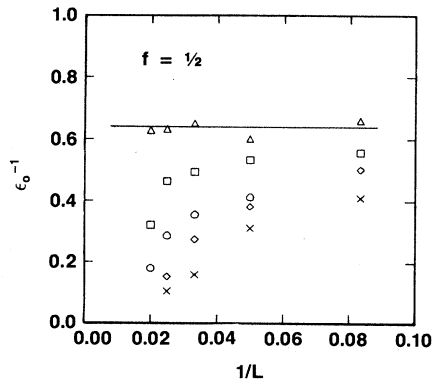


FIG. 5. Finite size scaling analysis for the inverse dielectric constant ϵ_0^{-1} vs $1/L$ for $12\leq L\leq 50$ for $T=0.138$ (\times), 0.135 (\diamond), 0.1335 (\circ), 0.132 (\square), and 0.129 (\triangle).

the specific heat peak and for the helicity modulus Υ . They were unable to distinguish whether there was one or two transitions. The best numerical simulations for the fully frustrated XY model are by Berge *et al.*¹³ who suggested that both transitions occur at the same temperature. However they did not measure the helicity modulus Υ , and thus is not possible to determine from their data precisely where the KT transition really is. Instead they determined the phase diagram¹³ from the locus of specific heat maxima for a model in which one bond per plaquette had a negative strength $-\eta J$. In this model $\eta=1$ corresponds to the fully frustrated model $f=\frac{1}{2}$. For $\eta\neq 1$ they found two peaks in the specific heat but only one for $\eta=1$, which they interpreted as evidence for a single transition. However for $\eta\neq\pm 1$, their Hamiltonian does not have the same symmetry of the fully frustrated model. Also since they do not have an independent measure of the position of the KT transition, their simulations cannot unambiguously determine whether one or two transitions occur. Clearly, it would be of interest to determine Υ and carry out detailed finite size scaling of $T_I(L)$ for the fully frustrated XY model to test the results presented here.

In Figs. 6 and 7, we present results for C and ϵ_0^{-1} for the cases $f=\frac{1}{3}$ and $\frac{1}{4}$. Clearly in both cases, there is no singularity in the specific heat and $\alpha<0$. The peak occurs at $T=0.075\pm 0.03$ for $f=\frac{1}{3}$, while for $f=\frac{1}{4}$, a peak position is difficult to determine. For $f=\frac{1}{3}$, results for $T\geq 0.075$ clearly fall below the Nelson-Kosterlitz²⁰

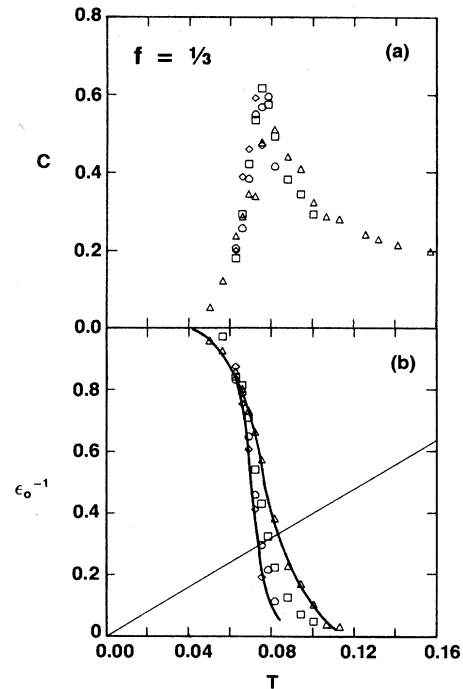


FIG. 6. C and ϵ_0^{-1} vs T for $f=\frac{1}{3}$ for $L=12$ (\triangle), 21 (\square), 30 (\circ), and 39 (\diamond). Solid line in (b) is $\epsilon_0^{-1}=4T$.

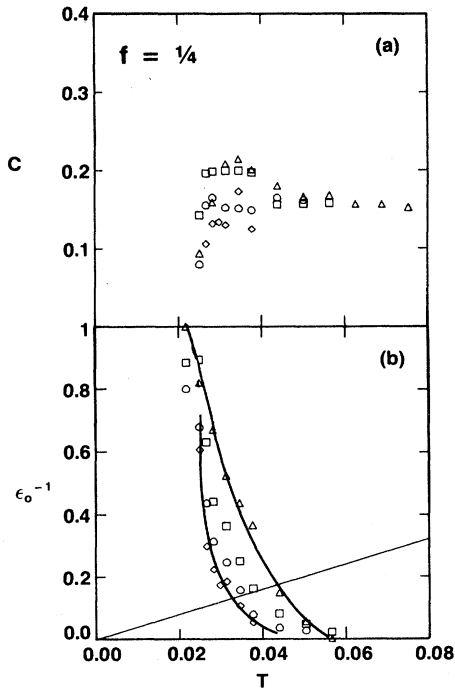


FIG. 7. C and ϵ_0^{-1} vs T for $f = \frac{1}{4}$ for $L = 12$ (Δ), 20 (\square), 32 (\circ), and 40 (\diamond). Solid line in (b) is $\epsilon_0^{-1} = 4T$.

line for the largest systems studied. Results for ϵ_0^{-1} for $T = 0.069$ and 0.072 show significant finite size effects, while for $T \leq 0.066$, ϵ_0^{-1} becomes nearly independent of L , suggesting $T_{CG} \sim 0.066$. The jump in ϵ_0^{-1} at T_{CG} would then be approximately 0.78 ± 0.05 compared to the universal value of 0.26 . While the data seem to strongly suggest a large nonuniversal jump in ϵ_0^{-1} at a temperature significantly less than where the peak in the specific heat occurs, I cannot rule out the possibility that ϵ_0^{-1} decreases rapidly for $T > 0.066$ to a nonzero value and then has a universal jump at $\epsilon_0^{-1} = 4T$ or a smaller nonuniversal jump. The systems are not large enough to obtain a good asymptotic estimate of ϵ_0^{-1} as $L \rightarrow \infty$ for $T = 0.069$ and 0.072 to determine if they truly vanish or not. I tried finite size scaling analysis on $\epsilon_0^{-1}(L)$ as a function of both L^{-1} and $1/\ln L$ for these two temperatures and could not obtain a particularly good fit. A similar analysis for $f = \frac{1}{4}$ suggests $T_{CG} < 0.025$. For large L and low T , it is very difficult to equilibrate the system for $f = \frac{1}{4}$ and precise determination of T_{CG} is not possible for this case. The jump in ϵ_0^{-1} at T_{CG} in this case is clearly nonuniversal and seems to be quite large, approximately 0.90 . Minnhagen²⁰ predicts a smaller jump (≈ 0.60 for $T_{CG} \approx 0.066$ and 0.55 for $T_{CG} \approx 0.025$) than found here. The difference could be a result of the approximations used in the theory breaking down at low temperatures. However, it is also possible that even where I observe a significant finite size dependence in ϵ_0^{-1} , as $L \rightarrow \infty$, ϵ_0^{-1} is actually nonzero, resulting in a smaller jump at T_{KT} . It

is not possible to determine at present which of these two are correct.

From the available data, it is also possible to check the approximate Coulomb gas scaling used in Refs. 21 and 22. Their relation between the CG temperature T_{CG} and the XY temperature T is

$$T_{CG} = \frac{T_{CO}}{2\pi\Upsilon_0} \frac{T}{T_{CO} - T}, \quad (6)$$

where close to $T = 0$, the helicity modulus has the form $\Upsilon = \Upsilon_0(1 - T/T_{CO})$. For the square lattice²² $T_{CO} = 4$ for $f = 0$ and 2 for $f = \frac{1}{2}$, while $\Upsilon_0 = -(1/2N)\langle H \rangle / T = 1$ for $f = 0$ and $\sqrt{2}/2$ for $f = \frac{1}{2}$. For $f = 0$, recent very accurate estimates for the XY model³² give $T_{KT} = 0.887J$. Equation (6) then gives $T_{CG} = 0.181$, significantly below the value 0.22 found here and in Ref. 30. For $f = \frac{1}{2}$, Teitel and Jayaprakash³ and Berge *et al.*¹³ find $T_C \approx 0.45J$ from the position of maximum in specific heat. This would give $T_{CG} = 0.131$ from Eq. (6), which is in good agreement with the value, 0.129 , found here.

Lee *et al.*²⁴ suggest that the Ising and KT transitions occur at one temperature with a universal jump in the helicity modulus for the antiferromagnetic XY model on a triangle lattice. In the present case, I am suggesting two transitions and a nonuniversal jump in ϵ_0^{-1} at T_{KT} . It is interesting to consider the possibility that the existence of two distinct transitions is related to the fact that the discontinuity in ϵ_0^{-1} is nonuniversal whereas the two transitions are congruent when the jump is universal. Additional simulations for other models which have both a discrete and continuous symmetry are needed to test this possibility.

In conclusion, I have presented for the first time, detailed Monte Carlo simulations for the uniformly frustrated charged Coulomb gas. The results suggest two distinct transitions for $f = \frac{1}{2}$, the lower one KT like and the higher one Ising like with a nonuniversal jump in ϵ_0^{-1} at T_{KT} . This is in contrast to earlier simulations on the fully frustrated XY model¹³ and the CG¹⁵ model. Several recent analytic predictions⁹⁻¹¹ suggest a single transition. Even though the interaction is long ranged for the Coulomb gas model, the advantage over XY simulations is that the variables are discrete integers instead of continuous spin variables. It turned out that for the CG model, the Ising-like transition temperature T_I showed negligible finite size corrections, allowing for an accurate determination of $T_I(\infty)$. This coupled with results for the inverse dielectric constant ϵ_0^{-1} gave the first numerical evidence for two transitions. Comparable numerical results for the fully frustrated XY model, which determine simultaneously $T_I(\infty)$ and the helicity modulus Υ have not been carried out.

I also presented evidence for a nonuniversal jump in the inverse dielectric constant ϵ_0^{-1} for $f = \frac{1}{2}$, $\frac{1}{3}$, and $\frac{1}{4}$. While the nonuniversal jump for $f = \frac{1}{2}$ may or may not be associated with the nearby Ising transition,⁹ the results for $f = \frac{1}{3}$ and $\frac{1}{4}$ clearly support Minnhagen.¹⁹

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²⁸Note that while Eq. (4) has the same form as the discrete Gaussian (DG) model, which is dual to the CG, it is very different. In the CG the F_{ij} 's are constrained by Eq. (3), while in the DG the F_{ij} 's can take on any integer values. For a review on the DG model, see J. D. Weeks, in *Ordering in Strongly Fluctuating Condensed Matter Systems*, edited by T. Riste (Plenum, New York, 1980).
²⁹Since the storage requirement for \underline{A} grows as L^4 , it is clear that in many cases computer memory limitations may significantly restrict the size of L . This problem can be alleviated by reducing the size of A , which can be done by reducing the number of independent variables F_{ij} . On the square lattice, one can eliminate from Eq. (3) all F_{ij} 's which are on the black squares of the checkerboard and thereby reduce the size of \underline{A} by four. Repeated application of this procedure could be used to reduce the size of A further. For $f = \frac{1}{4}$, $L = 40$ the program ran at a speed of 4.15 steps/sec with the full matrix \underline{A} and 2.54 steps/sec for A reduced in size by 4 on the Exxon Cray XMP 14se. Thus while the memory requirements for A can be reduced, there is a cost in CPU time.
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