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Dynamic approach to the two-dimensional classical lattice Coulomb gas of half-integer charges

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Abstract

The short-time dynamic behaviour of the two-dimensional classical Coulomb gas of half-integer charges on a square lattice is investigated using Monte Carlo simulations. We estimate the second-order phase transition temperature T_c and all the dynamic and static critical exponents z, β and ν. The value $\nu = 0.77(2)$ obtained is different from $\nu = 1$ in the pure two-dimensional Ising model, which provides evidence of a non-Ising exponent in the charge lattice melting transition. In addition, the dynamic critical exponent z is found to be 2.01(3), which is also different from the $z = 2.165(10)$ accepted generally in the pure two-dimensional Ising model.

1. Introduction

Statistical models known as the two-dimensional uniformly frustrated XY models [1] have attracted a lot of attention, mainly due to their physical relevance to Josephson-junction arrays in a transverse magnetic field. If the magnetic flux per plaquette is half of the flux quantum $\Phi_0 = h/2e$, the system is called fully frustrated (FF). The FFXY model displays rich low-temperature phase structures and critical phenomena. The FFXY model on a square lattice, for example, has a continuous $U(1)$ symmetry, corresponding to global rotation of the spins, and a discrete Z_2 symmetry, corresponding to long-range order of the ground-state vortex lattice [2–4]. In principle, the model has two kinds of phase transition, i.e. a KT phase transition (XY-like) for the $U(1)$ symmetry and an Ising-like continuous transition for the Z_2 symmetry.

Many authors argued that the nature of the Ising-like transition in the two-dimensional FFXY model differs from that in the pure two-dimensional Ising model [4–10]. They obtained the critical exponent $\nu < 1$ for the two-dimensional FFXY model and attributed it to the interaction between the XY and Ising critical excitations, because these two critical transitions occur close to each other. However, conflict on the determination of the value of ν still remains. For example, Olsson [11, 12] obtained $\nu = 1$, which is consistent with the pure two-dimensional Ising value, by calculating the chiral correlation function and its coherence length.

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A typical model in studying the nature of two-dimensional FFXY models is the square lattice FFXY model with cosine interaction through a periodic boundary condition (PBC) [4, 5]. However, it was claimed by the Umeå group in [13] and [14] that the PBC for the phase angles leads to a nonperiodic boundary condition for vortex interaction, so the natural condition should be a fluctuating twist boundary condition (FTBC) where the PBC for vortices is met. It is well known that in the lattice Coulomb gas (CG) context, the PBC is an extensively employed boundary condition where the vortex is undoubtedly periodic, so the debated boundary condition problem can be avoided in this model. Moreover, it has been argued that both the vortex interaction and the average vorticity at a plaquette are temperature dependent in the FFXY model with cosine interaction [11, 12], so it is difficult to include the effect of the spin wave in a entirely convincing manner. To avoid this kind of complicating factor one would rather have results from the CG model with half-integer charges, since both the average vorticity and the vortex interaction in this model are manifestly temperature independent.

In this paper we investigate numerically the dynamics of the square lattice CG model of half-integer charges by means of the short-time dynamics Monte Carlo (MC) method. The short-time dynamics MC method was proved to be a new way to determine the critical exponents and the critical temperature [15, 16]; for example, the critical temperature T_c, the static critical exponents β and ν and the dynamic exponent z can be determined easily and precisely. We concentrate our attention on the scaling behaviour of the chiral magnetization, and determine the critical temperature T_c and three critical exponents, β, ν and z of the Ising-like phase transition in the square lattice CG model of half-integer charges.

The paper is organized as follows: In section 2 we briefly introduce the lattice CG model and MC simulation method for the system. The results from our short-time dynamic scaling analysis are given in section 3. Finally, section 4 gives a short summary of our main conclusions.

2. Lattice CG model and MC method

The standard model to describe behaviour in a two-dimensional superconducting network is the two-dimensional uniformly frustrated XY model, given by the Hamiltonian [1]

$$H_{FXY} = J\sum_{\langle ij\rangle} U(\phi_{ij} = \theta_i - \theta_j - A_{ij}). \tag{1}$$

Here θ_i is the phase of the superconducting wavefunction at node i of the periodic network, the sum is over all nearest-neighbour bonds $\langle i\,j\rangle$ of the network, and

$$A_{ij} = \frac{2e}{\hbar}\int_i^j \boldsymbol{A}\cdot \mathrm{d}l \tag{2}$$

is the line integral of the magnetic vector potential $\boldsymbol{A}$ across the bond from i to j. For a uniform magnetic field $\boldsymbol{B} = \nabla \times \boldsymbol{A}$ applied transverse to the plane of network, the sum of the A_{ij} around any unit plaquette is

$$\sum A_{ij} = 2\pi f, \tag{3}$$

where the constant f is the density of magnetic flux quanta per plaquette. f is referred to as the 'uniform frustration', and the system of $f = \frac{1}{2}$ is called FF.

A possible choice for the interaction $U(\phi)$ is $U(\phi) = 1-\cos\phi$, and we obtain the ordinary frustrated XY model with Hamiltonian

$$H_{FXY} = -J\sum_{\langle ij\rangle} \cos(\theta_i - \theta_j - A_{ij}). \tag{4}$$

When the interaction $U(\phi)$ is the Villain function [17],

$$U(\phi) = -k_B T \ln \sum_{m=-\infty}^{\infty} e^{[-\frac{1}{2}(\phi - 2\pi m)^2 J/k_B T]}, \tag{5}$$

the Hamiltonian (4) can be mapped onto a *dual* 'CG' of interacting vortices [18, 19],

$$H_{CG} = \tfrac{1}{2} \sum_{i,j} (n_i - f) V(\boldsymbol{r}_i - \boldsymbol{r}_j)(n_j - f), \tag{6}$$

which yields the same partition function as that of Hamiltonian (4) at low temperature [20]. Here the sum is over all pairs of *dual* sites i, j, n_i is the integer vorticity on site i and the interaction V_{ij} is the two-dimensional lattice Green function which satisfies $\Delta^2 V(\boldsymbol{r}_i - \boldsymbol{r}_j) = -2\pi\delta_{ij}$, where Δ^2 is the discrete Laplacian. In this work, we restrict our interest to a square lattice. In this case, $V(\boldsymbol{r})$ is explicitly given by

$$V(\boldsymbol{r}) = \frac{1}{N} \sum_{k} e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \frac{\pi}{2 - \cos k_x - \cos k_y} \tag{7}$$

where $\boldsymbol{k}$ are allowed wavevectors with $k_\mu = (2\pi n_\mu / L)$, with $n_\mu = 0, 1, \ldots, L-1$. L is the length of the system, and $N = L^2$. For large r,

$$V(r) \sim \ln r. \tag{8}$$

Since $V(\boldsymbol{r} = 0)$ is divergent, the partition sum over n_i is restricted to neutral configurations where

$$\frac{1}{N} \sum_i n_i = f. \tag{9}$$

Thus the average density of vortices is equal to the density of flux quantum of the applied magnetic field.

The Hamiltonian (6), therefore, represents a density f of integer point charges, on a uniform compensating background charge $-f$, interacting with the two-dimensional Coulomb potential. For $f = \frac{1}{2}$, the ground state is an ordered chequerboard pattern with charges $\pm\frac{1}{2}$ on every other site.

The order parameter for the Ising-like phase transition is the chiral magnetization, which is defined as

$$M_I = \frac{1}{N} \sum_i q_i (-1)^{x_i + y_i}, \tag{10}$$

where $q_i = n_i - f$ and (x_i, y_i) is the coordinate of vortex i.

In order to investigate the phase transition of the CG model described above, we use MC simulations. Simulations are performed on a square lattice of size $L \times L$. At each step of the simulation we pick at random a pair of nearest-neighbour sites (i_0, i_1) and add a unit charge to site i_0 and subtract a unit charge from site i_1. In fact, for the $f = \frac{1}{2}$ case, we simply interchange the charges n_{i_0} and n_{i_1} at the two sites. This restricts configurations to those where half of the n_i are +1 and the other half are 0. Other values of charges n_i are not allowed, for they correspond to high-energy excitations. This excitation is then either accepted or rejected using the standard Metropolis algorithm: accept if $e^{-\Delta E/T} > r$, where r is a random number uniformly distributed in the interval [0, 1), and ΔE is the change in energy due to the excitation. $N = L^2$ steps of this process of updating the configuration are referred to as one MC step (MCS) (MCS is the time unit in this paper).

Since the interaction in the CG model is long range (equation (6)), the most time consuming procedure is to calculate energy ΔE. However, at low temperature ($T \approx T_c$ in this work), only a low rate of excitation is accepted. When this occurs, it is convenient to calculate ΔE without summing over all the sites. The method employed here is to store information on each

site in the system in the form of the potential table, which is updated for each site after each accepted excitation. The technique was discussed in detail by Lee and Teitel [18]. We find that the acceptance ratio near T_c is only about 0.04, thus this method improves running time on the order of tenfold.

3. Results and discussion

We have performed our simulation on a square lattice of size $L = 96$, starting with an ordered initial state. The magnetization M_I is calculated up to time $t = 1000$. We have simulated a total of 20 000 independent runs. Following the method of [5], the mean values and errors are obtained by dividing the whole sample into five subsamples, each containing 4000 independent runs. However, the data shown in the figures are averaged over all 20 000 runs.

In order to locate precisely the critical temperature T_c, MC simulations must be carried out within a very narrow temperature range bracketing the critical temperature. According to the previous calculations of the critical temperature $T_c = 0.1314(4)$ of [19] and $T_c = 0.1311(2)$ of [21] and our tentative simulations on a small system $L = 64$, we perform our MC simulation at temperatures $T = 0.130$, 0.131 and 0.132, which enclose the critical temperature T_c.

For a critical system with a second-order phase transition, the scaling form of the kth moment of the magnetization for the dynamic relaxation of a magnetic system starting from an ordered state is given by [5]

$$M^{(k)}(t, \tau, L) = b^{-k\beta/\nu} M^{(k)}(b^{-z}t, b^{1/\nu}\tau, b^{-1}L) \tag{11}$$

where $\tau = (T - T_c)/T_c$ is the reduced temperature, β and ν are the static critical exponents and z is the dynamic exponent. This scaling form is assumed to hold in the macroscopic short-time regime after a microscopic timescale t_{mic}. For sufficiently large system size L we can deduce the scaling behaviour for the magnetization M ($k = 1$ in equation (11))

$$M_I(t, \tau) = t^{-\beta/\nu z} G(t^{1/\nu z}\tau) \tag{12}$$

by setting the scaling factor b in equation (11) as $b = t^{1/z}$. Therefore, at T_c, i.e. $\tau = 0$, M_I shows a power-law decay with time. In figure 1, the time evolution of the magnetization $M_I(t)$ at different temperatures is plotted in a log–log scale. Data within the microscopic timescale $t_{mic} = 100$ are not included. The magnetization at a temperature between $T = 0.130$ and 0.132 can be obtained by quadratic interpolation. To determine the critical temperature T_c, we then calculate the deviation of $M_I(t)$ from the power law $y(t) = C_1 t^{-C_2}$ (C_1 and C_2 are fitting parameters), fitted in the time range $[t_1, t_2]$ using the least-squares method, for each temperature. The deviation is defined as the sum of square deviation of the data in the time range $[t_1, t_2]$ from the value power law given, i.e. $\sum_{t=t_1}^{t_2} [M_I(t) - y(t)]^2$. As suggested in [5], the temperature at which the magnetization has the best power law behaviour, i.e. the deviation is minimum, is the critical temperature T_c. In figure 2, the deviation of M_I from the power law, estimated in the time range (100, 1000), is plotted as a function of the temperature. We then obtain the critical temperature $T_c = 0.1309(2)$, which is consistent with those calculated from finite-size scaling analysis, $T_c = 0.1314(4)$ [19] and $T_c = 0.1311(2)$ [21]. In figure 1, the curve of $T_c = 0.1309$ derived from MC simulation is also plotted. Moreover, we have also compared two datum sets deduced from quadratic interpolation and calculated from MC simulation at the same temperature $T_c = 0.1309$. We find that these two sets of data are so close that it is difficult to identify them. For this reason, we only plot the curve of MC results. The slope of the curve obtained from MC simulation at T_c yields the critical exponent $\beta/\nu z = 0.0622(8)$.

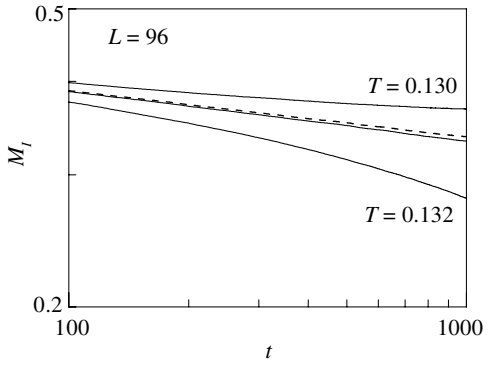

Figure 1. Log–log plots of the chiral magnetization $M_I(t)$ versus time t at different temperature. From above, the solid curves represent $M_I(t)$ at temperatures $T = 0.130$, 0.131 and 0.132, while the dashed curve is at the critical temperature $T_c = 0.1309$.

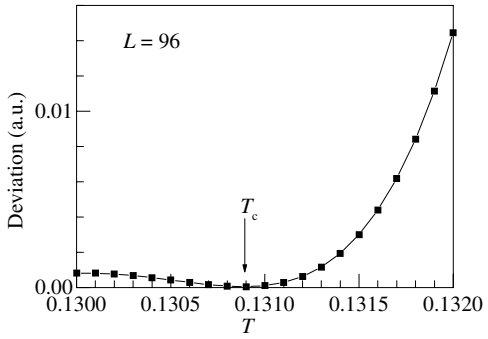

Figure 2. The deviation of $M_I(t)$ from the power law behaviour at different temperatures.

To extract the critical exponent $1/\nu z$, we calculate the differentiation of equation (12) that leads to

$$\partial\tau \ln M_I(t,\tau) = t^{1/\nu z}\partial\tau \ln G(\tau). \tag{13}$$

Therefore, $\partial\tau \ln M_I(t,\tau)|_{\tau=0}$ should also present a power-law behaviour at the beginning of the time evolution. In figure 3, $\partial\tau \ln M_I(t,\tau)$ at $T_c = 0.1309$ is plotted in a log–log scale. The power-law behaviour is clearly seen. The slope yields the critical exponent $1/\nu z = 0.644(9)$.

To calculate the dynamical critical exponent z, we use Binder's cumulant method. Thus, we calculate the cumulant $U = M_I^{(2)}/M_I^2 - 1$ for every MC step at T_c. In the short-time region, the cumulant shows a power-law scaling at the critical temperature [5]

$$U(t) \sim t^{d/z}. \tag{14}$$

In figure 4, the curve for $U(t)$ in log–log scale shows a nice power-law behaviour. The slope gives the critical exponent $d/z = 0.995(15)$. Since $d = 2$, then we can estimate the dynamic exponent $z = 2.01(3)$ from the Binder cumulant. With z in hand, we calculate the critical exponents $2\beta/\nu$ and ν from $\beta/\nu z$ and $1/\nu z$. We find the critical exponents $2\beta/\nu = 0.250(7)$ and $\nu = 0.77(2)$. Since ν is not close to unity, we conclude that the charge lattice melting transition is different from the pure Ising one.

In the ground state of the FFXY model, the vortices, which show up as charges $\pm\frac{1}{2}$ on the sites of the dual lattice, are ordered in a chequerboard pattern like that of the square lattice

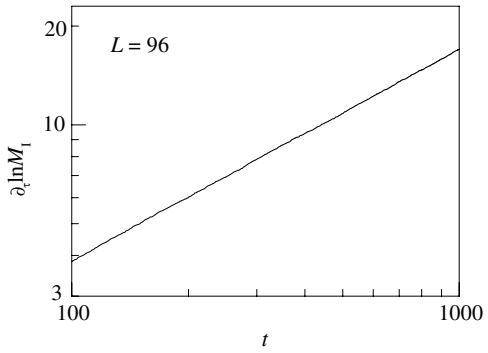

Figure 3. Log–log plot of the derivative $\partial\tau \ln M_I$ versus time t at the critical temperature $T_c = 0.1309$.

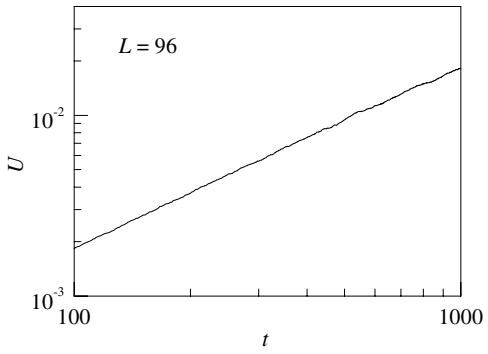

Figure 4. Log–log plot of the Binder cumulant U versus time t at the critical temperature $T_c = 0.1309$.

$f = \frac{1}{2}$ CG model. The ground state has twofold degeneracy, similar to the degeneracy of the antiferromagnetic Ising model, but unlike the Ising model the interactions in CG model are much more complex. Therefore, it is possible that the nature of the charge lattice melting transition in CG model is different from that of the ordinary Ising transition.

It is interesting to note that the dynamic critical exponent z is very close to two, which indicates simple diffusion in two dimensions. In the pure two-dimensional Ising model with local MC dynamics, it has been reviewed recently that the dynamic critical exponent z tends to converge at around $z = 2.165$ with uncertainty less than 2% [22–24]. Our finding $z = 2.01(3)$ in the CG model with half-integer charges is obviously different from that in the pure two-dimensional Ising model. It is to be noted that a dynamic short-time MC study of the FFXY model with a PBC gives a slightly larger value of $z = 2.17(4)$ [5], which may originate from the essential different boundary conditions. However, whether the PBC for the FFXY model is a natural boundary condition or not deserves further careful study.

We have also checked the finite-size effect on the determination of the critical temperature T_c. Figure 5 shows the time evolution of the magnetization $M_I(t)$ for system size $L = 32, 64, 96$ and 128 at temperature $T_c = 0.1309$. 20 000 independent runs are simulated for each system size. Only the smallest lattice size shows the finite-size effect, while the results for $L = 64$ and 96 coincide with the data of the largest lattice size $L = 128$ in the time interval $t = (1, 1000)$. Moreover, we also find no finite-size effect at other temperatures near T_c for

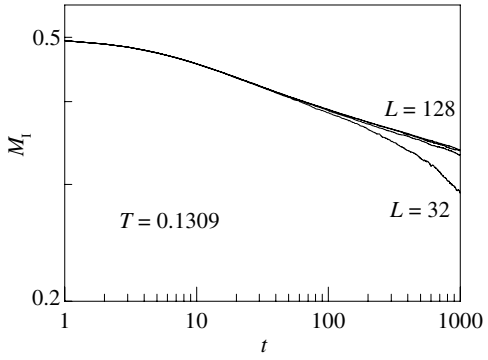

Figure 5. The time evolution of the chiral magnetization M_I for different system sizes at the critical temperature $T_c = 0.1309$. From bottom, the system size $L = 32, 64, 96$ and 128.

large system size, e.g. $L \geqslant 64$, in our simulation. This inconspicuous finite-size effect is in agreement with the character of the short-time dynamics [25]. In the short-time regime, both the chiral spatial correlation length ξ and the screen length λ associated with the KT transition are very small, so the conditions $L \gg \xi$ and $L \gg \lambda$ are easily satisfied. Therefore, we believe the system size of $L = 96$ is large enough to determine the critical temperature T_c as well as the critical exponents.

Finally, we point out that the simulation results of the short-time MC method do not suffer from large visible statistical or systematic errors. It has long been known that MC simulations are subject to both statistical and systematic errors [26–28]. In this work, since the short-time MC simulation starts from an initial ordered state, we find the statistical error is very small. Starting from an ordered state, the largest standard error of magnetism M_I is at the longest time $t = 1000$. However, for all 20 000 samples on the system $L = 96$, the largest standard error is about 10^{-3} of the dimension of M_I, smaller than the width of the curve plotted in figure 1, indicating that the statistical error is negligible. The systematic error often results from poor-quality random number generation (RNG). We have checked the statistical properties of our RNG[3] by dividing all 2×10^6 random numbers into 20 groups. We obtained the mean value $\langle r \rangle = 0.5002$ and $r^2 = 0.3334$, which are very close to the theoretical values 0.5 and 1/3, respectively, indicating that the RNG we used is good in randomness. In fact, the RNG has also been used in other fields, for example our previous MC simulation of thin-film growth [29], and always gave good simulation results. We believe therefore that, with the RNG, our simulation result only suffers from small statistical and systematic errors.

4. Summary

We have numerically investigated the short-time dynamic behaviour of the classical square lattice CG model of half-integer charges near its critical temperature. Based on the short-time dynamic scaling form, the critical temperature as well as critical exponents are determined. A more precise critical temperature T_c is found, $T_c = 0.1309(2)$. The estimated value $z = 2.01(3)$ is different from that of the pure Ising model, $z = 2.165(10)$ [22–24], generally accepted recently. The estimated value $\nu = 0.77(2)$ is also different from that of the pure Ising

[3] The code of the random number generator we used is $r = \text{seed1}^*\text{seed2}^*10^{-12}$; $r = r^*10^{-8} - \text{int}(r^*10^{-8})$; $\text{seed1} = 0.1^*\text{seed2}+r^*10^{11}+1.0987^*10^{11*}(1+r)+873\,476.509$; $\text{seed2} = r^*10^{11}+1.9877^*10^{11*}(1+r)+676\,4254.318$; where seed1 and seed2 are two seeds, and r is the random number.

model. The results reveal that the critical behaviour of the charge lattice melting transition is different from the pure Ising transition. It is shown in our simulation results that the short-time dynamic MC method is also very effective for the lattice CG model.

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