Incommensurability and phase transitions in two-dimensional XY models with Dzyaloshinskii-Moriya interactions

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The Dzyaloshinskii-Moriya (DM) interaction in magnetic models is the result of a combination of superexchange and spin-orbital coupling, and it can give rise to rich phase-transition behavior. In this paper, we study ferromagnetic XY models with the DM interaction on two-dimensional $L \times L$ square lattices using a hybrid Monte Carlo algorithm. To match the incommensurability between the resultant spin structure and the lattice due to the DM interaction, a fluctuating boundary condition is adopted. We also define a different kind of order parameter and use finite-size scaling to study the critical properties of this system. We find that a Kosterlitz-Thouless-like phase transition appears in this system and that the phase-transition temperature shifts toward higher temperature with increasing DM interaction strength.

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I. INTRODUCTION

The XY model in two dimensions is a prototype model for magnetic spin systems that exhibit continuous symmetry and topological excitations. This model can describe superfluid films [1] and Josephson junction arrays [2] in two dimensions and undergoes a Kosterlitz-Thouless (KT) transition characterized by an exponentially divergent correlation length and in-plane susceptibility [3,4]. The KT transition is driven by the unbinding of pairs of vortices with opposite vorticity at a temperature T_{KT}.

The Dzyaloshinskii-Moriya (DM) interaction was first proposed by Dzyaloshinskii for explaining weak ferromagnetism in antiferromagnetic compounds [5], and the microscopic basis for this theory was later given by Moriya [6], who extended Anderson's superexchange theory [7] to include the spin-orbit interactions. Arising from the impurities in the system, this interaction is very important in low-symmetry crystals while it vanishes in high-symmetry crystals. The DM interaction exists in many materials and can lead to some special phenomena. In the superconductor $LaCu_2O_4$, this interaction induces a slight spin canting out of the CuO_2 plane [8]. It has been reported that the DM interaction can induce helical spin order in $Fe_xCo_{1-x}Si$ alloys [9] and the helix period is determined by the ratio of the DM interaction to the spin-exchange interaction. In Mn monolayers, the adjacent spins are not perfectly antiferromagnetic, but slightly canted, resulting in a spin spiral structure (with chiral order [10]) due to the DM interaction. This noncollinear, or spin spiral, order can be observed by using spin-polarized scanning tunneling microscopy, and *ab initio* calculations identify that this spin spiral order is stabilized by the DM interaction [11]. Using the polarized neutron diffraction method, a nonzero average chirality was obtained in Dy/Y multilayer films [12], which indicates that the DM interaction exists in this material. The chirality is due to the lack of the symmetry inversion on the interface. Since the DM interaction plays a key role in these materials, especially these helical magnetic systems, we simulate the 2D XY model with the DM interaction in order to understand the effects of their inclusion. We found that a kind of KT-type phase transition exists in this system when the DM interaction is small [13]. Monte Carlo (MC) simulations [14] provide us with a powerful tool for the study of such complicated systems. While the METROPOLIS "single spin-flip" algorithm [15] is used widely, there have been many high-resolution MC algorithms developed to improve upon and to speed up the original METROPOLIS algorithm, e.g., the Swendsen-Wang (SW) algorithm [16].

In this paper, we study the two-dimensional ferromagnetic XY model with DM interaction. This model has been recently treated in three dimensions by MC simulations using the standard single spin-flip METROPOLIS algorithm [17]. It has been shown that the second-order transition continuously transforms to a first-order transition by increasing the value of the DM interaction. This model has also been recently studied in two dimensions through a duality transformation and posterior RG analysis [18]. The system was mapped, in the low-temperature limit, into a two-dimensional Coulomb gas model of magnetic vortices with the DM interaction playing the role of an effective electric field. By applying RG analysis, it was claimed that the effective electric field affects the vortex-antivortex pairs and destroys the Kosterlitz-Thouless transition. In this work, we treat the same two-dimensional model by using a hybrid Monte Carlo algorithm, which combines the METROPOLIS algorithm and the Swendsen-Wang algorithm. The uniform magnetization, which is regularly regarded as the order parameter in the 2D XY model [19,20], disappears in the low-temperature

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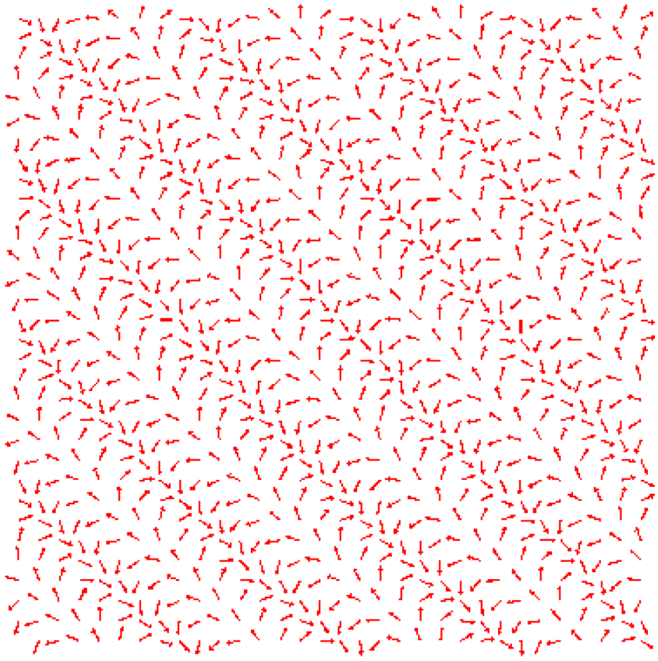

FIG. 1. Typical spin configuration at $T = 0.1$ and $d = 1$ for $L = 32$ with periodic boundary conditions. The arrows represent the spin orientations.

region because of the symmetric, undulating arrangement of the spin vectors induced by the DM interaction (see, e.g., Fig. 1). To describe this system in the low-temperature region, we define a different kind of order parameter and use a fluctuating boundary condition (FBC) [21] to match the incommensurability between the spin structure and the lattice size due to the DM interaction. By using finite-size scaling and the Binder (fourth-order) cumulant of the order parameter, we can determine the phase-transition temperature, and, contrary to the results of Proskurin *et al.* [18], we do find a Kosterlitz-Thouless transition as the DM interaction is varied.

This paper is organized as follows. In Sec. II, the two-dimensional XY ferromagnetic model with the DM interaction is introduced and the hybrid Monte Carlo algorithm is presented. We also introduce the fluctuating boundary condition briefly. In Sec. III, we first illustrate the incommensurability between the spin structure and the lattice due to the DM interaction, and we use the fluctuating boundary condition to match this incommensurability. Then, a different order parameter is defined, and we use the scaling of this order parameter with lattice size and the crossing of Binder cumulants to estimate the transition temperature. Section IV concludes the paper with a summary of our results.

II. MODEL AND METHOD

The XY ferromagnetic model with the DM interaction on the two-dimensional $L \times L$ square lattice can be written as

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j - \vec{D} \cdot \sum_{\langle ij \rangle} (\vec{S}_i \times \vec{S}_j) \tag{1a}$$

$$= -J\sqrt{1+d^2} \sum_{\langle i,j \rangle} \cos(\theta_i - \theta_j - \phi), \tag{1b}$$

where $\vec{S}_i$ is a two-component classical vector of unit length (also known as the planar rotator model), while the DM vector $\vec{D}$ is taken to be along the z axis. The constants J and D are positive and denote the strengths of the nearest-neighbor ferromagnetic coupling and the DM interaction, respectively. The angular brackets $\langle i, j \rangle$ mean that the corresponding sum is over the distinct nearest-neighbor pairs of the lattice.

In going from Eq. (1a) to Eq. (1b), one expands the spin dot product in the first sum, the cross product of the spin variables in the second sum, and, after taking the scalar product with the DM interaction, an additional canonical transformation is performed, namely

$$S_i^x = S_i^{x'} \cos\varphi_i - S_i^{y'} \sin\varphi_i,$$
$$S_i^y = S_i^{x'} \sin\varphi_i + S_i^{y'} \cos\varphi_i, \tag{2}$$

where φ_i is the rotational angle of the primed reference at the ith spin around the z $(= z')$ axis. The XY format of the Hamiltonian (1b) is eventually recovered by choosing for the nearest-neighbor rotational angle difference $\varphi_i - \varphi_j$ the value $\varphi_i - \varphi_j = \phi = \arcsin(d/\sqrt{1+d^2})$, with $d = D/J$ (a similar approach has been used in Ref. [22] in treating the quantum version of the system). In this case, we have a rescaled exchange interaction $J\sqrt{1+d^2}$. Note that here θ_i and θ_j in (1b) are, respectively, the spin angles of the ith and jth sites relative to the original x-axis direction.

To prepare for the simulations, a new transformation can be introduced, namely

$$\theta_i = \theta_i^0 - \frac{\pi}{2}(1 + \sigma_i), \tag{3}$$

where σ_i takes the values ± 1, and θ_i^0 denotes a trial angle at the site i. If $\sigma_i = -1$, θ_i just keeps the same value; if $\sigma_i = 1$, it means that θ_i is rotated by an angle of π. Combining Eqs. (1) and (2), we can obtain an Ising-type Hamiltonian

$$\mathcal{H} = -\sum_{\langle ij \rangle} J_{ij} \sigma_i \sigma_j, \tag{4}$$

where $J_{ij} = J\sqrt{1+d^2}\cos(\theta_i^0 - \theta_j^0 - \phi)$ is an effective nonuniform Ising coupling between spins. This transformation will be very useful for implementing the Swendsen-Wang algorithm to the model.

We use a hybrid Monte Carlo algorithm, which combines the standard METROPOLIS algorithm and the Swendsen-Wang algorithm to update the spins. At each site a new random orientation for the spin is chosen. The interaction energy between this spin and its nearest neighbors is calculated. If it is lower than the energy of the old state, the new state is accepted; otherwise, it is accepted only with a probability according to the standard METROPOLIS algorithm. To reduce the critical slowing down of the simulation, the Swendsen-Wang (SW) cluster algorithm is used here. In an initial spin configuration, we chose $\sigma_i = 1$ for all the sites. If $J_{ij} > 0$, we put a bond between the ith and jth sites with a probability $P(J_{ij}) = 1 - \exp(-2J_{ij}/k_B T)$, otherwise no bond is set up. After clusters are constructed by putting bonds between spins, every cluster has the same possibility to rotate an angle of π or just to keep the same value. One SW sweep related to Eq. (3) is followed after one METROPOLIS sweep related to Eq. (1).

To match the incommensurability due to the DM interaction, we adopt a fluctuating boundary condition [21]. It is described as follows: suppose there is a phase shift Δ across the boundary at the same row and column: $\Delta = \theta_{0,y} - \theta_{L,y}$ and $\Delta = \theta_{x,0} - \theta_{x,L}$ for $0 \leqslant x \leqslant L$ and $0 \leqslant y \leqslant L$. After a compound Monte Carlo sweep to update the spins described above while fixing Δ, we use the standard METROPOLIS algorithm to update Δ while fixing all the spins.

We perform Monte Carlo simulations on $L \times L$ lattices, with total sites $N = L^2$, to obtain the critical properties of the system. Typically, 10^4–10^5 hybrid MC steps are discarded for equilibration and 10^7–10^8 hybrid MC sweeps are then retained for averages. The sampling intervals for measuring system properties varied from 20 to 500 hybrid MC sweeps for different sizes. Multiple independent runs were used to compute statistical errors. Where not shown in the figures, error bars are smaller than the size of the symbols.

III. RESULTS

As we know, the DM interaction would result in nonzero chirality [12]. According to Eq. (1), there is an angular difference $\theta_i - \theta_j = \phi$ between the nearest-neighbor spins in the ground state, and ϕ is determined by the ratio of the DM interaction to the spin nearest-neighbor exchange coupling. The nearest-neighbor spins prefer to be parallel to each other in the ground state if there is only exchange coupling, while the DM interaction drives the nearest-neighbor spins to be perpendicular to each other in the ground state. So this angular difference ϕ results in the competition between the DM interaction and the spin-exchange coupling. To recognize the new order of this system at low temperatures, we pick up a random spin configuration when $d = 1$ at the low temperature $T = 0.1$ as Fig. 1 shows (the temperature here is measured in units of J/k_B, where k_B is the Boltzmann constant). It is obvious that this angular difference, whose value is close to ϕ, exists between the nearest-neighbor spins θ_i and θ_j both in the x and y directions. So the nearest-neighbor spins in the ground state would not be parallel to each other, as in the ground state of the XY model, but rotate through an angle ϕ per site both in the x and y directions if the spins are on the xy plane, just as Fig. 1 shows. Moreover, the spin arrangement is periodic from the left bottom to the right top, and the period is determined by the relative strength of the DM interaction d. This periodic spin arrangement leads to the magnetization being very small at low temperatures, even smaller than at high temperatures.

Moreover, this angular difference ϕ would lead to incommensurability of the system. After L sites, there is a phase shift $\Delta = L\phi$ across the boundary in the same row or column. If $\Delta = 2n\pi$, where n is an integer, it means that this phase shift is an integer multiple of 2π, the structure is commensurate with the lattice, and the periodic boundary condition is reasonable for this system; otherwise, the structure is incommensurate with the lattice. In the latter case, a periodic boundary condition (PBC) would introduce frustration and increase the energy of the system, or even result in choosing the wrong phase when the system is incommensurate. Thus, we consider a fluctuating boundary condition [21] to match the incommensurability.

How do we confirm the incommensurability of the system? As mentioned above, whether the system is incommensurate or not is dependent upon the lattice size L and the DM interaction d. For instance, when $d = 1$, $\phi = \pi/4$, and if L is a positive integral multiple of 8, e.g., 8, 16, 32, etc., the phase shift across the boundary Δ is also an integral multiple of 2π, so the structure is commensurate with the lattice, and the periodic boundary condition is suitable. But when $d = 0.5$, $\phi = 0.463\,648$, and even if L is also a positive integer multiple of 8, the system turns out to be incommensurate.

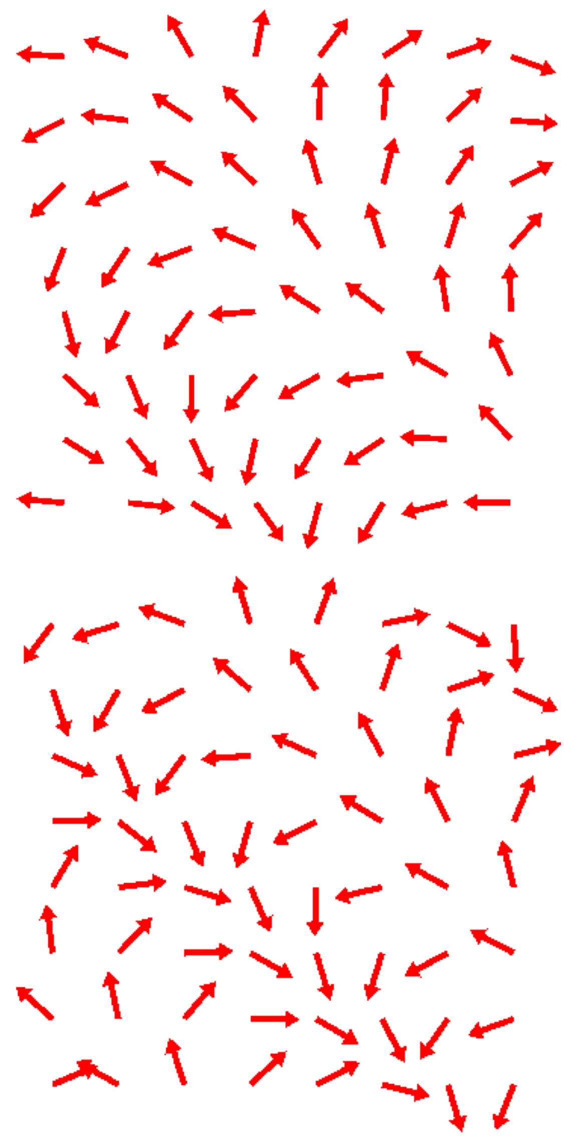

FIG. 2. Typical spin configurations at $T = 0.1$ and $d = 0.5$ for $L = 8$ with (top) fluctuating boundary conditions and (bottom) periodic boundary conditions. The arrows represent the spin orientations.

To make some sense of the incommensurability of the spin system, we first look at the spin configurations of the incommensurate system. Figure 2 (top and bottom) shows spin configurations of an incommensurate system for which $L = 8$, $d = 0.5$, and $T = 0.1$, resulting from the use of a fluctuating boundary condition (FBC) and a periodic boundary condition (PBC), respectively.

In fact, in Fig. 2 (top) the spin-variation wavelength is larger than the lattice size L but is allowed by the fluctuating

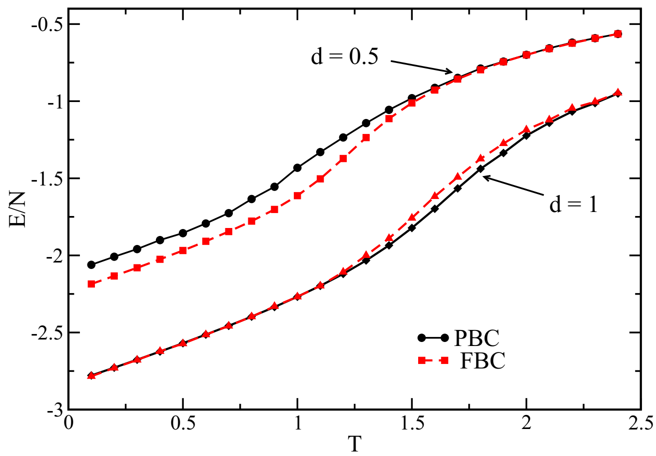

FIG. 3. Energy E/N, where $E = \langle \mathcal{H} \rangle$ and the angular brackets denote thermal average, vs temperature T for different DM interactions when $L = 8$ by using different boundary conditions. The errors are smaller than the symbol sizes. The lines are just guide to the eyes.

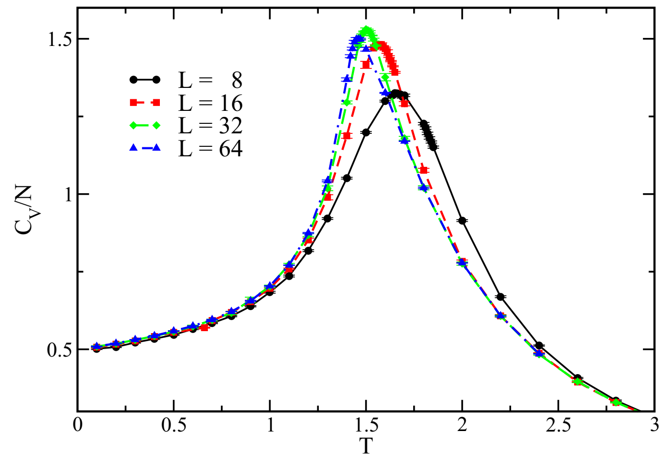

FIG. 4. Specific heat C_V/N vs temperature T for different lattice sizes when $d = 1$ by using periodic boundary conditions. The lines are just guide to the eyes.

boundary condition, and the system just chooses a phase shift across the boundary according to the balance between the spin structure and the lattice size. When using the periodic boundary condition, we force the spin wavelength to be an integer multiple of the lattice size L. For example, in Fig. 2 (bottom) the wavelength is forced to be equal to L, and Δ must then be equal to zero. So the periodic boundary condition would increase the energy of the incommensurate system. Figure 3 shows this in a plot of the energies versus temperature for different DM interaction and with different boundary conditions for $L = 8$. If $d = 0.5$, the system is incommensurate; the energy for PBC is larger than that found using FBC at low temperature. Consequently, FBC is better than PBC when the system is incommensurate. While the system is commensurate, such as $L = 8$ and $d = 1$, PBC and FBC give almost the same answer at low temperature, and PBC is suitable in order to reduce the fluctuation and save computing time. Thus, we use the periodic boundary condition if the system is commensurate, and we use the fluctuating boundary condition to simulate the incommensurate system.

We thus perform Monte Carlo simulations on $L \times L$ lattices with L ranging from $L = 8$ to 96. Figure 4 shows the specific heat versus temperature for $d = 1$ with PBC by using the dissipation fluctuation theorem. The values of specific heat are independent of lattice size and approach $1/2$ when the temperature T approaches zero. This is, in fact, expected on general grounds (equipartition theorem), since there is only a single degree of freedom for each spin in our 2D XY model. Moreover, a specific-heat peak appears near $T = 1.5$, while the corresponding transition temperature is near $T = 1.02$ in the 2D XY model [23]. (It is known that the specific-heat peak is above the transition temperature in the 2D XY model, and we shall see that the same holds true here.) This means that inclusion of the DM interaction drives the transition toward a higher temperature.

The peaks of the specific heat shown in Fig. 4 do not approach a constant value monotonically. After a given value of the lattice size, it starts decreasing. In fact, Fig. 5 shows the behavior of the maximum of the specific heat for larger values of the lattice size. The inset in this figure gives a finite-size approach of the form $C_v(\max) = C_v^\infty - A/L$, where $C_v^\infty = 1.426(8)$, comparable to the values obtained for the XY model through a fit $C_v(\max) = C_v^\infty - A/L^\alpha$ with $C_v^\infty = 1.44$ and $\alpha = 1.07$ [24]. A similar behavior of the specific-heat peak as a function of the lattice size has been recently obtained in the study of the two-dimensional XY vectorial Blume-Emery-Griffiths model [25].

Since the spins rotate along both the x and y directions at low temperature if the strength of the DM interaction is not very small, the magnetization, which is the regular order parameter in the 2D XY model [19,20], does not play the role of an order parameter in the system. This is because of the periodic, oscillating spin arrangement that results when the DM interaction is included. According to the spin arrangement

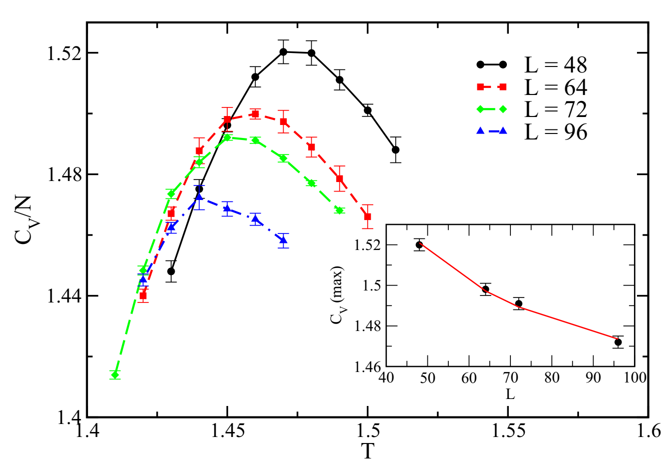

FIG. 5. Peaks of the specific heat as a function of temperature for larger lattice sizes when $d = 1$ by using periodic boundary conditions. The full line in the inset shows a corresponding fit of the data, as discussed in the text.

in the ground state, we define the order parameter as follows:

$$m = \frac{1}{L^2}\sqrt{\left(\sum_{i=1}^{L^2}\cos[\theta_i - (x_i + y_i)\phi]\right)^2 + \left(\sum_{i=1}^{L^2}\sin[\theta_i - (x_i + y_i)\phi]\right)^2}, \quad (5)$$

where (x_i, y_i) is the coordinate of the ith spin, and $x_i, y_i \in [0, L-1]$.

According to finite-size scaling theory [19,26], we can analyze the properties of finite systems near the critical temperature of the corresponding infinite system. Using the definition of the order parameter given above, we show plots of the order parameter versus the size L when $d = 0.5$ and 1 at different temperatures in Figs. 6 and 7. Both plots show power-law scaling behavior as $m \propto L^{-x}$ at $T \leqslant T_C$ with temperature-dependent exponent x, and there is no power-law behavior when $T > T_C$, in agreement with the behavior of a Kosterlitz-Thouless-type phase transition. In addition, the slopes of these straight lines at the "transition temperatures" are -0.125 in both plots. Exactly at the transition temperature $T = T_C$ the exponent x is equal to $\eta/2$ [19], where $\eta = 1/4$ is the critical exponent. In Fig. 6, when $T \leqslant 1.285$, all the plots are straight lines whose slopes are less than -0.125, while the plots are not straight lines when $T > 1.285$. It is clear that both of the phase transitions are Kosterlitz-Thouless-type and $x = 0.125$, and $T_C = 1.014 \pm 0.001$ for $d = 0.5$ and $T_C = 1.284 \pm 0.001$ for $d = 1$, respectively.

Examining the fourth-order cumulant of the order parameter, originally suggested by Binder to analyze Ising model critical properties [27], is an effective way to locate the critical temperature. The Binder cumulant of the order parameter is

$$U_4 = 1 - \langle m^4\rangle/3\langle m^2\rangle^2, \quad (6)$$

where the angular brackets denote a thermal average. As the system size L approaches infinity, $U_4 \to 0$ for $T > T_C$ and $U_4 \to 2/3$ for $T < T_C$. According to the renormalization-group theory, there is a "fixed point" in the U_4 curves that is independent of the system size L, and the location of the "fixed point" is the critical point. So, the Binder cumulants are scale-independent at the critical point, for large enough lattices, and we can use cumulant crossings for different system sizes to determine the phase-transition temperature T_C. Figures 8 and 9 show the temperature dependence of Binder cumulants for different lattice sizes for $d = 1$ and 0.5, respectively. It is obvious that at low temperature the values of U_4 for different sizes of the system rapidly approach the same value. As the temperature increases, however, the curves separate distinctly, especially for larger lattice sizes. Such behavior also coincides with the behavior of a Kosterlitz-Thouless-type phase transition.

One can also note in Figs. 8 and 9 that despite there being a scattering of the cumulant crossings, they are not simply random, with a clear tendency to move to lower temperatures, mainly for smaller systems. This means that the scaling behavior regime for U_4 should be valid for still larger lattices. However, an extrapolation scheme can be used to obtain the critical temperature, in the thermodynamic limit, by resorting to a fit of the data as a function of $1/L$ for smaller lattices, as was proposed in Binder's original paper for the spin-1/2 Ising model [27]. Using this convergence criterium for the temperatures of different lattices, in a similar way to that proposed in Ref. [27], we estimate that $T_C = 1.013 \pm 0.006$ for $d = 0.5$ and $T_C = 1.293 \pm 0.006$ for $d = 1$. These values agree with the results obtained by the power-law scaling of the order parameter with lattice size.

However, instead of the fits as a function of $1/L$, one can also use the scaling relation for the critical temperature itself (see, for instance, Ref. [28] for the two-dimensional Ising

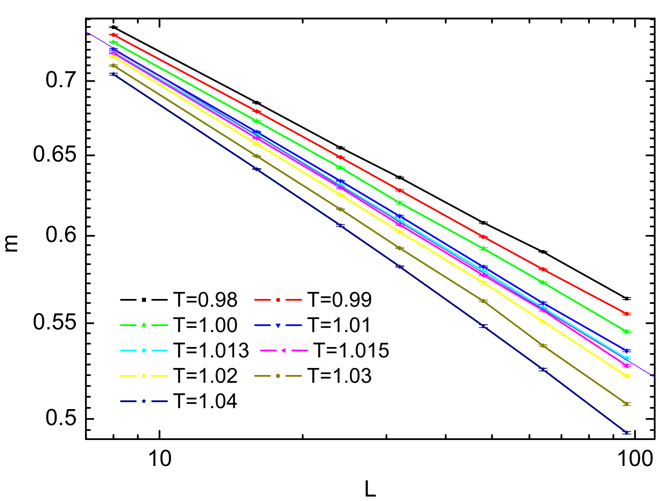

FIG. 6. Log-log plot of the order parameter m vs lattice size L for various temperatures near T_C when $d = 0.5$ using FBC. The lines are just a guide to the eyes. The longer curve corresponds to a straight line with slope -0.125.

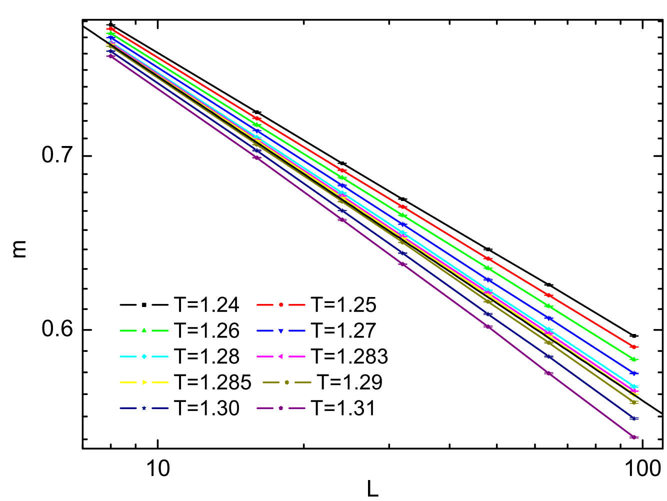

FIG. 7. Log-log plot of the order parameter m vs lattice size L for various temperatures near T_C when $d = 1$ using PBC. The lines are just a guide to the eyes. The longer curve corresponds to a straight line with slope -0.125.

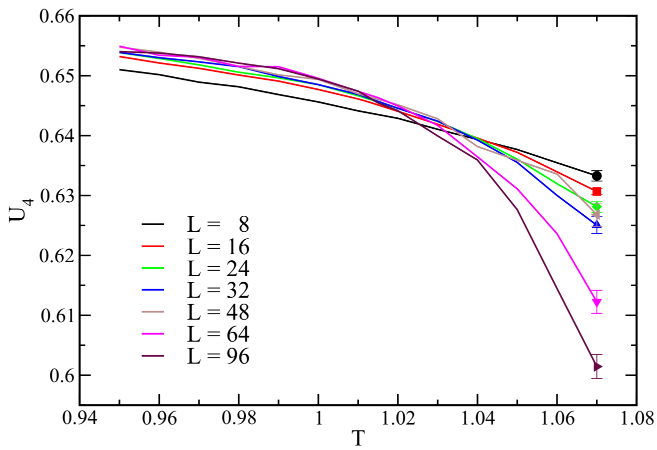

FIG. 8. Binder cumulant U_4 of the order parameter vs temperature T for different lattice sizes when $d = 0.5$ using FBC. The data symbols, with the corresponding error bars, have been omitted for clarity, except for $T = 1.07$, in order to give an idea of the error as a function of system size.

model). As an example, Fig. 10 shows the crossings with the smaller lattice size $L = 8$ and the second smallest $L = 16$, as a function of the system size, for $d = 1$ and 0.5. In the case of the Kosterlitz-Thouless transition, the corresponding finite-size scaling of the temperature crossings should behave as [14]

$$T_{\text{cross}} = T_C + B/(\ln L)^2, \tag{7}$$

where T_C is the transition temperature in the thermodynamic limit and B is a nonuniversal constant. The above relation comes from the fact that the correlation length in the infinite system behaves as $\xi = \exp[\pi/c(T - T_C)^{1/2}]$, where c is a nonuniversal constant, and at $T = T_{\text{cross}}$ one has $\xi \simeq L$. Fits of the data in Fig. 10 give, for $d = 1$, $T_C = 1.297(4)$, when the smallest lattice size is $L = 8$, and $T_C = 1.294(2)$ when

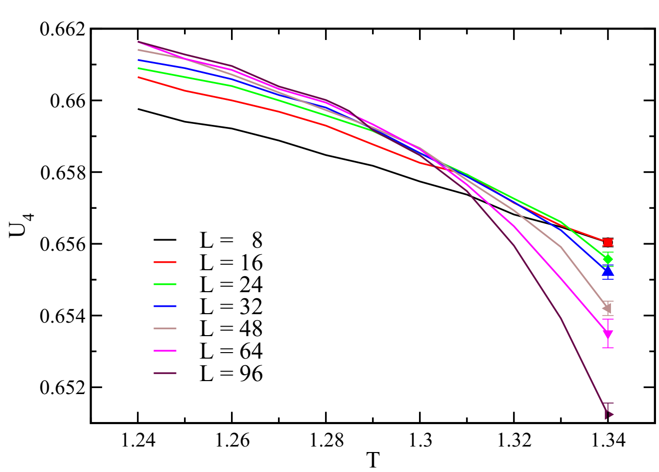

FIG. 9. The Binder cumulant U_4 of the order parameter vs temperature T for different lattice sizes when $d = 1$ using PBC. The data symbols, with the corresponding error bars, have been omitted for clarity, except for $T = 1.34$, in order to give an idea of the error as a function of system size.

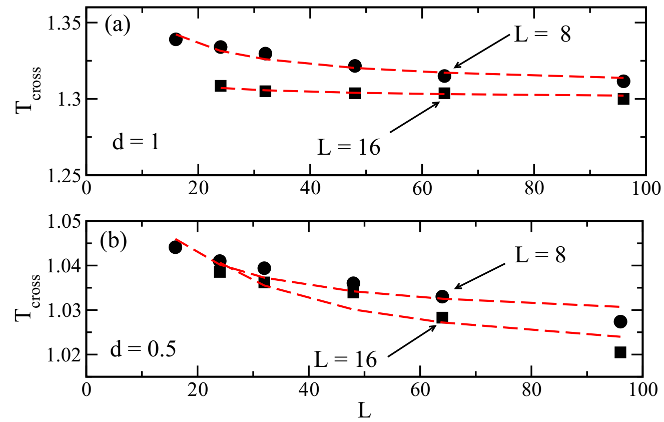

FIG. 10. Temperature of the crossings of the Binder cumulant of the order parameter as a function of different lattice sizes when $d = 1$ using PBC (a) and $d = 0.5$ using FBC (b). The data correspond to considering $L = 8$ and 16 as the smallest lattice. The dashed lines are a fit with Eq. (7). The error bars are smaller than the symbol sizes.

$L = 16$. For $d = 0.5$, we have $T_C = 1.022(9)$ with $L = 8$ and $T_C = 1.009(9)$ with $L = 16$. All the above values are in good agreement with the previous ones. We can thus overall estimate $T_C = 1.292(6)$ for $d = 1$ and $T_C = 1.013(4)$ for $d = 0.5$.

IV. SUMMARY

Using Monte Carlo simulations, we have studied the thermodynamics and critical properties of a 2D XY model with DM and exchange interactions. Since the DM interaction drives the nearest-neighbor spins to be perpendicular to each other, the spins rotate with respect to each other at low temperature. Hence, the magnetization does not play the role of an order parameter in the 2D XY model with the DM interaction. The spin rotation in the low-temperature regime induces incommensurability between the spin structure and the lattice. Therefore, a fluctuating boundary condition is adopted to match this kind of incommensurability, and a different kind of order parameter is defined to describe the phase transition. We use the power-law behavior of the order parameter with the lattice size and the crossing of the Binder cumulant to estimate the critical temperature. We have determined that there is a Kosterlitz-Thouless-type phase transition in the 2D XY model with the DM interaction, and the DM interaction can induce an increase in the Kosterlitz-Thouless transition temperature, contrary to what has been recently obtained by mapping the model to a two-dimensional Coulomb gas and by applying RG analysis [18]. We have not considered here the corresponding order parameter susceptibility because the size dependence of the susceptibility should really be the same as the size dependence of the order parameter, since they are computed from the same quantity.

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