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Dimensional Crossover in the XY Model*

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We use the single-cluster Monte Carlo algorithm to simulate the periodic Gaussian XY model on $L^2 \times N$ lattices of film geometry ($L \gg N$) with up to $N = 16$ layers, imposing free boundary conditions at the bottom and top layer. Based on measurements of the specific heat, the spin-spin correlation function and the susceptibility in the high-temperature phase we study the crossover from three- to two-dimensional behaviour as criticality is approached. For the transition temperatures, determined from Kosterlitz-Thouless fits to the correlation length and susceptibility, we observe a pronounced scaling behaviour with N, but find an associated critical exponent that deviates from theoretical expectations. More qualitatively, we further investigate the shapes and distribution of vortex loops in the crossover region.

1. INTRODUCTION

According to the concept of universality qualitative properties of systems with short-range interactions exhibiting continuous phase transitions should depend only on the spatial dimension and on the symmetry of the order parameter. Strictly speaking, in determining the spatial dimension only those directions count in which the system extends to infinity. For films of finite thickness we therefore expect a phase transition (if at all) that can be classified according to the two-dimensional (2D) universality class. More precisely we expect a crossover from three-dimensional (3D) bulk to 2D behaviour as soon as the correlation length ξ of the system approaches the order of the film thickness. Since ξ diverges at a continuous phase transition, this is always the case in the vicinity of the transition point.

In a numerical simulation on present day computers the area L^2 of the film can never be really large and additional care is necessary to disentangle the dimensional crossover from finite-size effects in L. And far away from the transition point the correlation length is so small that non-universal lattice corrections become important and modify the universal 3D bulk behaviour. Thus altogether there are three types of crossover involved which must be carefully distinguished. It is therefore necessary to simplify the models as much as possible. Some time ago the Ising model has been investigated by Binder and Hohenberg [1] as the typical example for a system with a one-component order parameter. Here we report results for the XY model as the generic model with a two-component order parameter.

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2. THE MODEL

The partition function of the periodic Gaussian XY model is given by

$$Z = \prod_{\boldsymbol{x}} \left(\int_{-\pi}^{\pi} \frac{d\theta(\boldsymbol{x})}{2\pi} \right) \times \sum_{\{n_i(\boldsymbol{x})\}} \exp\left(-\frac{\beta}{2} \sum_{\boldsymbol{x},i} (\nabla_i \theta - 2\pi n_i)^2 \right), \quad (1)$$

where $\nabla_i \theta(\boldsymbol{x}) \equiv \theta(\boldsymbol{x}+\boldsymbol{i}) - \theta(\boldsymbol{x})$ are the lattice gradients in the $\boldsymbol{i}$ direction of the lattice, the integer variables $n_i(\boldsymbol{x})$ run from $-\infty$ to ∞, and $\beta \equiv J/k_B T$ is the (reduced) inverse temperature. Our choice of the periodic Gaussian formulation is motivated by the fact that, in contrast to the "cosine formulation" (with $\exp(\beta \cos(\nabla_i \theta))$, eq. (1) can exactly be rewritten in terms of topological defects with long-range interactions of the

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Coulomb type [3]. In 2D this is the starting point of the renormalization group treatment of Kosterlitz and Thouless [2] (KT). Physically the defects can be interpreted as the vortex excitations invoked in the description of liquid helium [3, 4].

Films of increasing thickness were simulated by stacking $N = 1, 2, 3, 4, 6, 10$, and 16 layers of size $L \times L$ with $L \gg N$ on top of each other along the z-direction. The ferromagnetic coupling J was taken to be isotropic. Within each layer we took periodic boundary conditions in order to reduce finite-size effects in L as much as possible, while at the top and bottom layer we imposed free boundary conditions in the z-direction.

The limiting cases $N = L$ (3D) and $N = 1$ (2D) have been investigated by a variety of approaches. In 3D, analyses of high-temperature series (HTS) expansions [5], resummations of field theoretic perturbation series [6], and recent Monte Carlo (MC) simulations [7, 8] are all compatible with a conventional power-law behaviour $\xi \propto (1-\beta/\beta_c)^{-\nu}$ and $\chi \propto (1-\beta/\beta_c)^{-\gamma}$ with critical exponents $\nu = 0.670$ and $\gamma = 1.316$. In 2D, however, the situation has been quite controversial. While the KT theory predicts an exponentially diverging correlation length,

$$\xi \propto \exp[b(1-\beta/\beta_c)^{-\nu}], \qquad \nu = 1/2, \tag{2}$$

and susceptibility $\chi \propto \xi^{2-\eta}$ with $\eta = 1/4$, alternative considerations [9] suggested a conventional power-law behaviour with non-trivial critical exponents ν and γ. To clarify this point analyses of extended HTS expansions [10] and MC studies [11] of the "cosine formulation" were performed, and the results were interpreted in favor of the KT scenario. Since we decided to investigate the dimensional crossover effects for the periodic Gaussian formulation we first studied the 2D limit with great care and found from high-statistics simulations on large lattices of sizes up to 1200^2 also in this formulation (an even stronger) evidence for the KT predictions [12, 13].

3. RESULTS

In our MC simulations [13, 14] we worked with the single-cluster (1C) update algorithm [15], slightly adapted to the periodic Gaussian formulation (employing the Z_n approximation with $n = 100$). To get an overview we measured the specific heat C, although it is well known that in 2D the peak location does not coincide with the transition point but is displaced by about 25% to higher temperatures. The interesting question was how this would change with increasing thickness N of the film. The main results are based on analyses of the spin-spin correlations, $g(\boldsymbol{x}, \boldsymbol{x}') \equiv \langle \vec{s}(\boldsymbol{x}) \cdot \vec{s}(\boldsymbol{x}')\rangle$, and the susceptibility, $\chi \equiv V\langle[\frac{1}{V}\sum_{\boldsymbol{x}} \vec{s}(\boldsymbol{x})]^2\rangle$, in the high-temperature phase, using for the measurements variance reduced "cluster observables" [16]. To reduce finite-size effects in L, we always took care that $L \approx 6-8\xi$. Extensive tests for the pure 2D model showed that this is a save condition [12, 13].

To determine the transition point $\beta_c(N)$ for each film thickness N, we first located the onset of the two-dimensional KT behaviour via goodness-of-fit analyses. As a general rule we find that this is the case for $\xi > N/2$. Only for the thickest film with $N = 16$ layers we start seeing a region with 3D bulk behaviour; see Fig. 1. It is tempting to identify this 3D region with $\xi < N/10$, but even for $N = 16$ layers this is of course still perturbed by non-universal lattice corrections. Having determined the region of 2D behaviour, we

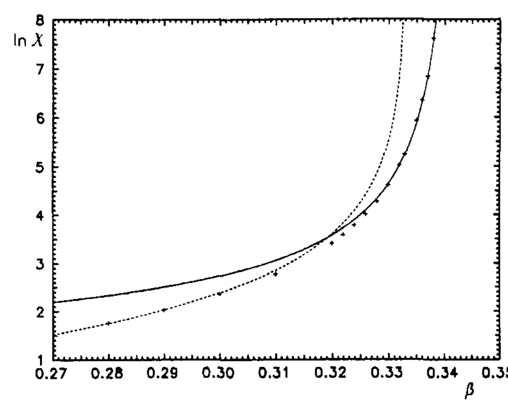

Figure 1. Crossover from 3D power-law behaviour (dashed line, using $\gamma_{3D} = 1.316$) to 2D KT behaviour (solid line) of the susceptibility for $N = 16$ layers.

then fitted the data for ξ and χ to the KT prediction (2) and the corresponding formula for χ, respectively. As a test for systematic errors we also used (2) rewritten as a function of T. Depending on N, the number of data points included in the fits was 5 or 6, with a maximal correlation length between 26 and 46, requiring layer sizes of the order of 200^2 to 400^2. For each film thickness N these fits provided us with four estimates of $\beta_c(N)$, which according to Fisher's scaling prediction [17] should scale asymptotically as

$$\beta_c(N) = \beta_c(\infty) + cN^{-\lambda}, \tag{3}$$

with

$$1/\lambda = \nu_{3D} = 0.670 \pm 0.002. \tag{4}$$

Here $\beta_c(\infty) \equiv \beta_c^{3D}$ is the critical coupling of the 3D bulk system and ν_{3D} is the bulk correlation length exponent. The results of three-parameter fits to (3) for each of the four sets of $\beta_c(N)$ values (labeled according to the type of KT fit used to determine $\beta_c(N)$) are collected in Table 1. In Fig. 2 we plot $\beta_c(N) - \beta_c(\infty)$ with $\beta_c(\infty) = 0.334$ vs N on a log-log scale. We see that the critical couplings do indeed scale quite nicely down to remarkably small values of N. The solid curve is a straight line corresponding to the exponent

$$1/\lambda = 0.71 \pm 0.01. \tag{5}$$

This value is significantly larger than the theoretical prediction (4). For this comparison, however, it should be kept in mind that (3) is only valid asymptotically for large N. We have checked for a systematic trend in our data by discarding more and more points for small N in the fits. As a result we observe only a slight trend to smaller values of $1/\lambda$, which is hardly significant in view of the increasing error bars. After completion of this work we received a preprint [18] in which $1/\lambda = 0.70(8)$ was found from an independent simulation of the "cosine formulation". Clearly, the only way to clarify this discrepancy is to perform further simulations for much larger systems.

Table 1
Three-parameter fits $\beta_c(N) = \beta_c(\infty) + cN^{-\lambda}$.

fit	χ^2	Q	$\beta_c(\infty)$	$1/\lambda$
$\xi(T)$	7.21	0.07	0.3343(9)	0.706(19)
$\xi(\beta)$	8.24	0.04	0.3344(10)	0.703(20)
$\chi(T)$	3.86	0.28	0.3336(4)	0.725(8)
$\chi(\beta)$	2.02	0.57	0.3334(4)	0.721(9)

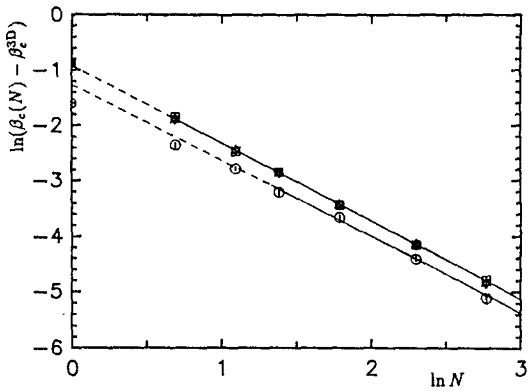

Figure 2. Scaling of $\beta_c(N)$ with N, calculated from KT fits to $\xi(T)$ (+), $\xi(\beta)$ (□), $\chi(T)$ (△), and $\chi(\beta)$ (▽). Also shown are the peak locations of the specific heat (o).

In Fig. 2 we also show the scaling of the peak locations $\beta_{\max}(N)$ of the specific heat. We see that the absolute distance from $\beta_c(N)$ decreases with increasing N. Assuming that also $\beta_{\max}(N)$ scales according to (3), a three-parameter fit gives an even larger exponent of $1/\lambda \approx 0.8$ and favors a value of $\beta_{\max}(\infty) \equiv \beta_{\max}^{3D} \approx 0.331$ that is slightly smaller than $\beta_c^{3D} \approx 0.334$. Recalling that also in 3D the specific-heat peak is finite (the critical exponent $\alpha = 2 - D\nu \approx -0.01$ is slightly *negative*), we are not aware of any argument enforcing the equality of β_c^{3D} and $\beta_{\max}^{3D}$.

Let us finally discuss the topological defect structure in the film geometry. Since geometrically the films are 3D, the topological excitations are vortex *lines*. On the other hand one expects that near criticality these lines should behave effectively like the vortex *points* invoked in the KT picture. One possible scenario advanced in the literature [19] is that near criticality these lines degenerate to rod-like objects in z-direction, such that the projection onto the xy-plane should look like a gas of vortex points (with the correct

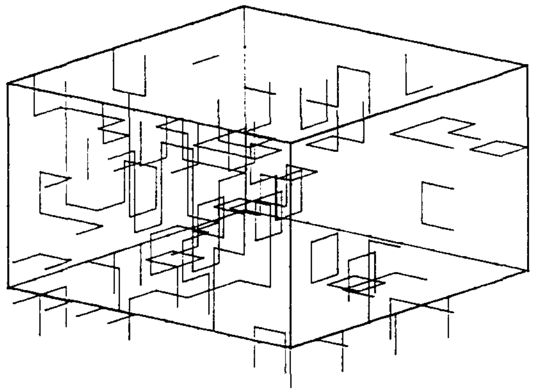

Figure 3. Vortex lines in a 6×10^2 section of a 6×200^2 lattice at $\beta = 0.355$ ($\xi \approx 19$).

logarithmic long-range interaction derived from a summation over the $1/r$ interactions between all line elements, similar to the treatment of parallel currents in electrodynamics). The vortex line distribution displayed in Fig. 3 clearly shows that this explanation does not work. In fact, corresponding plots for the pure 3D case [20] look quite similar. And it is straightforward to show that due to the finite number of layers the interaction potential must become anisotropic with logarithmic terms. To understand the entropic contributions, however, is a difficult problem which is not yet solved.

To summarize, for films of XY spins in the periodic Gaussian formulation with up to $N = 16$ layers and free boundary conditions in the z-direction we observe a pronounced scaling of the critical couplings with N. The associated critical exponent, however, is not in agreement with theoretical expectations.

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