

Universal magnetic fluctuations with a field-induced length scale

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We calculate the probability density function for the order-parameter fluctuations in the low-temperature phase of the two-dimensional XY model of magnetism near the line of critical points. A finite correlation length ξ , is introduced with a small magnetic field h , and an expression for $\xi(h)$ is developed by treating nonlinear contributions to the field energy using a Hartree approximation. We find analytically a series of universal non-Gaussian distributions of the finite-size scaling form $P(m, L, \xi) \sim L^{\beta/\nu} P_L(mL^{\beta/\nu}, \xi/L)$ and present a function of the form $P(x) \sim \{\exp[x - \exp(x)]\}^{a(h)}$ that gives the probability density functions to an excellent approximation. We propose $a(h)$ as an indirect measure of the length scale of correlations in a wide range of complex systems.

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I. INTRODUCTION

There has recently been considerable interest in the fluctuations of a spatially averaged quantity in systems with correlations over a macroscopic length scale ξ [1–8]. The most accessible example from both an experimental and a theoretical point of view, is a critical system, where the divergence of the correlation length ξ is interrupted by the system size L . Here, the breakdown of Landau theory and the occurrence of a nonanalytic fixed point for the free energy in a renormalization group flow, tells one that the fluctuations will not be Gaussian. Even so, extending the scaling hypothesis to include the macroscopic scale L , one can deduce that the probability density function (PDF) for order-parameter fluctuations should have universal properties. Further, the PDF must be a homogeneous function of m , L , and ξ of the following form: [9]

$$P(m, L, \xi) \sim L^{\beta/\nu} P_L(mL^{\beta/\nu}, \xi/L). \quad (1)$$

Here, adopting the language of a magnetic phase transition, ν and β are the usual critical exponents relating to the divergence of the correlation length and the singularity in the magnetization m . The scaling hypothesis therefore predicts fluctuations of a universal form, independently of system size, for constant ratio ξ/L .

We study the low-temperature phase of the two-dimensional (2D) XY model, defined by the Hamiltonian

$$H = -J \sum_{\langle i, j \rangle} \cos(\theta_i - \theta_j) - h \sum_i \cos(\theta_i). \quad (2)$$

The exchange interaction and magnetic field are of strength J and h , and the angle θ_i gives the orientation of a classical spin vector of unit length, confined to a plane. We define the magnetization for a single configuration

$$m = \frac{1}{N} \sum_{i=1, N} \cos(\theta_i - \bar{\theta}), \quad (3)$$

where $\bar{\theta} = \tan^{-1}(\sum_i \sin \theta_i / \sum_i \cos \theta_i)$ is the instantaneous magnetization direction.

This is perhaps the simplest nontrivial system in which one can study critical phenomena. At low temperature and in zero field, there is a line of critical points, separated from the high-temperature paramagnetic phase by the Kosterlitz-Thouless-Berezinskii phase transition. The physics of this low-temperature phase is perfectly captured by a harmonic, or spin-wave Hamiltonian. That is, one can, without loss of generality, develop the cosine interaction to order $(\theta_i - \theta_j)^2$ and neglect the periodicity of θ_i . This Hamiltonian is diagonal in reciprocal space and can be solved straightforwardly. As a result, all critical phenomena can be calculated microscopically from Gaussian integration, without the need for either the scaling hypothesis, or the renormalization group. Along the line of critical points, the exponents β and ν are not individually defined, but their ratio is and the system has a single independent exponent $\eta = 2\beta/\nu = T/2\pi J$.

We have previously been interested in the zero field, or strongly correlated regime where the divergence of ξ is completely removed by the system size L , and P_L becomes a function of a single variable $mL^{\beta/\nu}$ [10]. We have found that P_L , when plotted as a function of $\mu = (m - \langle m \rangle) / \sigma$, is a universal function, not only of system size, but also of temperature and therefore of the critical exponent η . Here, $\langle m \rangle$ is the mean and σ the standard deviation of the distribution. This rather surprising result gives weight to our conjecture [3] that the critical fluctuations of systems in certain universality classes are captured, at least qualitatively by the fluctuations of the 2D XY model.

In this paper we generalize our previous results by introducing a second length into the problem with the aid of a magnetic field. The field breaks the symmetry moving the system into an ordered magnetic state with finite correlation length ξ . However, taking a van Hove type thermodynamic limit, with the ratio ξ/L constant, should lead to a family of limit functions, all with divergent correlation length, varying in form from the anisotropic limit (see Fig. 1) to a Gaussian function, as the ratio ξ/L falls to zero. In Sec. II, we develop a starting Hamiltonian that satisfies the requirements of the

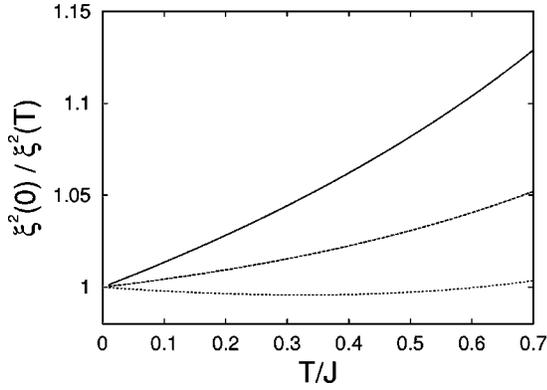


FIG. 1. $[\xi(0)/\xi(T)]^2$, as given by the Hartree approximations for, from bottom to top, $h/J=0.01, 0.05$, and 0.5 [Eqs. (9) and (10)] as a function of T/J .

scaling hypothesis, using a self-consistent Hartree approximation. In Sec. III we give theoretical results for the PDF for a finite field and compare our results with those from Monte Carlo simulation. In Sec. IV we fit the curve with a generalized form of Gumbel's first asymptote from extremal statistics.

II. HARTREE APPROXIMATION AND THE HYPERSCALING RELATION

Expanding the field energy in small angles, in the same way as the exchange term and Fourier transforming gives a convenient starting Hamiltonian

$$H = H_0 + \frac{J}{2} \sum_{q \neq 0} \left(\gamma_q + \frac{h}{J} \right) \phi_q^2, \quad (4)$$

where $\phi_q = \text{Re}[1/\sqrt{N} \sum_i \theta_i \exp(-i\vec{q} \cdot \vec{r}_i)]$ is the real part of the Fourier transformed spin variable. $\gamma_q = 4 - 2 \cos(q_x) - 2 \cos(q_y)$ and the sum $\sum_{\vec{q} \neq 0}$ is over the Brillouin zone for a square lattice with periodic boundaries, with \vec{q} taking on discrete values $q_x = (2\pi/L)n_x$, $q_y = (2\pi/L)n_y$, $n_x, n_y = 0, 2, \dots, \sqrt{N}$. Here and throughout the paper, we have set the nearest-neighbor distance on the lattice equal to unity. Expanding γ_q for small q we can write the Green's function propagator

$$G(q) \approx \frac{1}{q^2 + \xi^{-2}}, \quad \xi = \sqrt{J/h}; \quad (5)$$

the magnetic field indeed introduces a length scale ξ .

However, this naive starting point needs some development before proceeding with the calculation as, as it stands it does not satisfy the well-known hyperscaling relation. To see this, consider the following scaling argument [11]: at the critical temperature but in a finite field, the thermally averaged magnetization can be expressed in terms of both ξ and h :

$$\langle m \rangle \sim \xi^{-\beta/\nu} \sim \left(\frac{h}{J} \right)^{1/\delta}, \quad (6)$$

where δ is the usual critical exponent for the response in a finite field. Putting expression (5) for ξ in Eq. (6) leads to a relation between the exponents $\delta = 2\nu/\beta$, in disagreement with the hyperscaling relation $\delta + 1 = d\nu/\beta$, which should be valid for the 2D XY model [12]. The error comes from the development of the field term in small angles. Even at low temperature, when the nearest-neighbor differences $\theta_i - \theta_j$ are small, the deviations of θ_i from the fixed field direction are divergent in the thermodynamic limit. The development of the field term in small angles is therefore invalid. This problem can be dealt with in the low-temperature phase, in the absence of vortices, using the Hartree approximation introduced by Pokrovsky and Uimin [13]. Expanding $\cos(\theta_i)$ in powers of θ_i^2 , we make a mean-field decoupling

$$\theta_i^{2p} \rightarrow C_p \langle \theta_i^{2p-2} \rangle \theta_i^2, \quad (7)$$

where $C_p = (2p)!/2(2p-2)!$ is a binomial counting factor. As the underlying Hamiltonian (4) is quadratic, we can reduce $\langle \theta_i^{2p-2} \rangle$ using Wick's theorem, and after some resummation we eventually find

$$\cos \theta_i \approx 1 - \langle m \rangle \frac{\theta_i^2}{2}. \quad (8)$$

The field term in the Hamiltonian (4) then becomes

$$h \sum_i \cos(\theta_i) = Nh - \frac{1}{2} h_{eff}(T) \sum_{q \neq 0} \phi_q^2, \quad (9)$$

$$h_{eff}(T) = \langle m \rangle h.$$

Using the scaling relation $\langle m \rangle \sim (h/J)^{1/\delta}$, the effective field $h_{eff} \rightarrow h^{(\delta+1)/\delta}$ and the scaling argument, correctly yields the hyperscaling scaling relationship defined above. Note, however, that the scaling argument is valid in the thermodynamic limit, where $\xi/L \ll 1$ and the influence of the finite system size is negligible. In the crossover region that interests us, with $\xi/L \sim O(1)$ one cannot make this substitution, and in general one must explicitly work with expression (9).

The point of principle that poses the problem for the hyperscaling relation is that making the substitution $\cos(\theta_i) \approx 1 - (1/2)\theta_i^2$ results in an order-parameter conjugate to the field, $\langle m \rangle = \langle 1 - (1/2)\theta_i^2 \rangle = 1 - T/8\pi J \log(N)$ which diverges with system size, for any finite temperature. In order for the hyperscaling relation to hold, $\langle m \rangle$ must be a correctly defined intensive variable. For this to be so, the higher-order terms in the expansion of $\cos \theta_i$ must be retained, at least within the level of the approximation shown here. The calculation of Berezinskii [11] is consistent with this thermodynamic argument.

Still, in the absence of vortices, an effective coupling constant J_{eff} can be calculated in a similar manner. In zero field we did not need to account for this, as P_L for a quadratic Hamiltonian is independent of temperature throughout the low-temperature regime. However, as the correlation length depends on both the field and the coupling constant, we now have to calculate it if we are to have good agreement with numerical data. Expanding $\cos(\theta_i - \theta_j)$ in powers of the dis-

TABLE I. Variation of h_{eff} , ξ/L , a , and γ with field h for $L=32$ and $T/J=0.4$.

h	h_{eff}	ξ/L	a	γ
0.0	0.0	∞	1.5807	-0.89
0.001	0.001	0.987	1.611	-0.88
0.005	0.005	0.4407	1.7416	-0.844
0.01	0.0101	0.3111	1.903	-0.801
0.05	0.0512	0.1381	3.359	-0.583
0.1	0.1034	0.098	5.333	-0.463
0.5	0.523	0.0429	21.82	-0.23

crete difference operator $\vec{\nabla} \theta_i$ [11] and again using the decoupling (7) for $(\vec{\nabla} \theta_i)^{2p}$, we arrive at a self-consistent expression for $J_{eff}(T)$ [13,14]:

$$J_{eff} = J \exp\left(-\frac{T}{4J_{eff}}\right). \quad (10)$$

The Green's function we finally use for the calculation of the PDF is therefore of the form (5) but with the correlation length given in terms of the self-consistent effective field and coupling constant

$$\xi = \sqrt{\frac{J_{eff}}{h_{eff}}}. \quad (11)$$

The variation of ξ with temperature, for a fixed field is quite small throughout the range of fields that interests us. In Fig. 1 we show $[\xi(T)/\xi(T)]^2$ as a function of temperature for three different field strengths. Even for $h/J=0.5$, there is only a 10% variation, up to a temperature $T/J=0.7$, above which the Hartree approximation breaks down. As shown below, the temperature dependence of the resulting distribution function is even weaker than that for ξ/L , and for practical purposes it can be considered as temperature independent. The parameters h_{eff} and ξ/L can be found in Table I for a system of size $L=32$ at temperature $T/J=0.7$ and for field strength between $h=0.001$ and $h=0.5$. For a finite field the ratio ξ/L varies from $\xi/L=0.99$ to $\xi/L=0.043$.

III. THE PROBABILITY DENSITY FUNCTION IN A FINITE FIELD

We have previously developed [10,15] the following expression for the PDF:

$$P_L(\mu) = \int_{-\infty}^{\infty} \frac{dx}{2\pi} e^{ix\mu} \varphi(x), \quad (12)$$

$$\ln \varphi(x) = -ix \sqrt{\frac{1}{2g_2}} \sum_{\mathbf{q} \neq \mathbf{0}} \frac{G(\mathbf{q})}{N} - \frac{1}{2} \sum_{\mathbf{q} \neq \mathbf{0}} \ln \left[1 - i \sqrt{\frac{2}{g_2}} \frac{G(\mathbf{q})}{N} x \right],$$

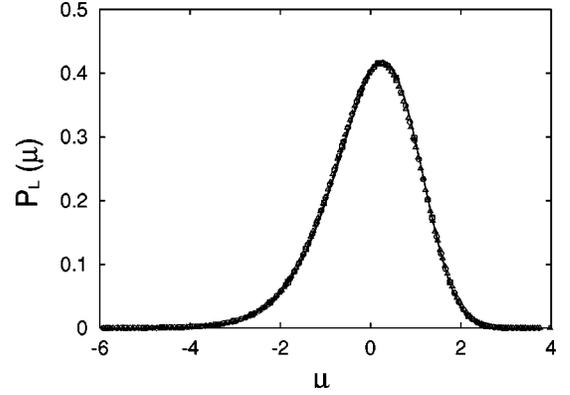


FIG. 2. Monte Carlo data for $P_L(\mu)$ for magnetic field $h/J=0.05$ and for $T/J=0.1, 0.4$ and 0.7 , using the Hamiltonian (2). The lines are for data generated from Eq. (12) (dotted) and for the function (15) (dashed).

where $g_k = 1/N^k \sum_{\mathbf{q}} \tilde{G}(\mathbf{q})^k$ and $\mu = (m - \langle m \rangle) / \sigma$. The PDF with a finite correlation length is calculated from the same expression by inserting the modified Green's function (5). The equivalence of Eqs. (1) and (12) is a result of the hyperscaling relation [10] and the functional dependence predicted by the scaling hypothesis (1) comes directly from dimensional analysis of Eq. (12). We note that the calculation can easily be extended to explore the non-Gaussian but noncritical behavior in all dimensions less than 4 [10]. Summing over the Brillouin zone for a large but finite system and performing a numerical Fourier transforms we generate the data shown in Figs. 2 and 3. Data is shown in Fig. 2 for $h/J=0.05$ ($\xi/L=0.138$ at $T/J=0.4$) and in Fig. 3 for $h/J=0.01, 0.05$, and 0.5 corresponding to $\xi/L=0.311, 0.138$, and 0.043 at $T/J=0.4$. It is compared with results from Monte Carlo simulation for a system of size $L=32$. In each case, theoretical and numerical data are shown for three temperatures: $T/J=0.1, 0.4$, and 0.7 . As in the zero-field case, which can be considered as the extreme non-Gaussian limit for such a system, the PDF's are characterized by an exponential tail for fluctuations below the mean and a double exponential above the mean [10]. Applying the field reduces the asymmetry and in a large field the data approach a Gaussian distribution.

Agreement between the theoretical calculation and the Monte Carlo simulation is generally extremely good, indicating that the Hartree approximations are accurate. In Fig. 2 all sets of data collapse, within numerical error, onto a single curve independently of temperature. This is the case for all field values chosen. When plotted on a logarithmic scale, temperature dependence is still not observable, but a difference between theoretical and numerical values can be observed along the exponential tail, for probability densities smaller than 10^{-4} . The discrepancy appears largest for fields around $h/J \sim 0.05$. This must indicate the limit of the ability of the Hartree approximation in dealing with the fluctuations. For a very small field, its effect is small and so errors are negligible, while for larger fields, critical fluctuations are smaller and one can imagine that the Hartree approximation becomes quantitatively very accurate. Only in the intermediate field range of $h/J \sim 0.05$, the combination of these two

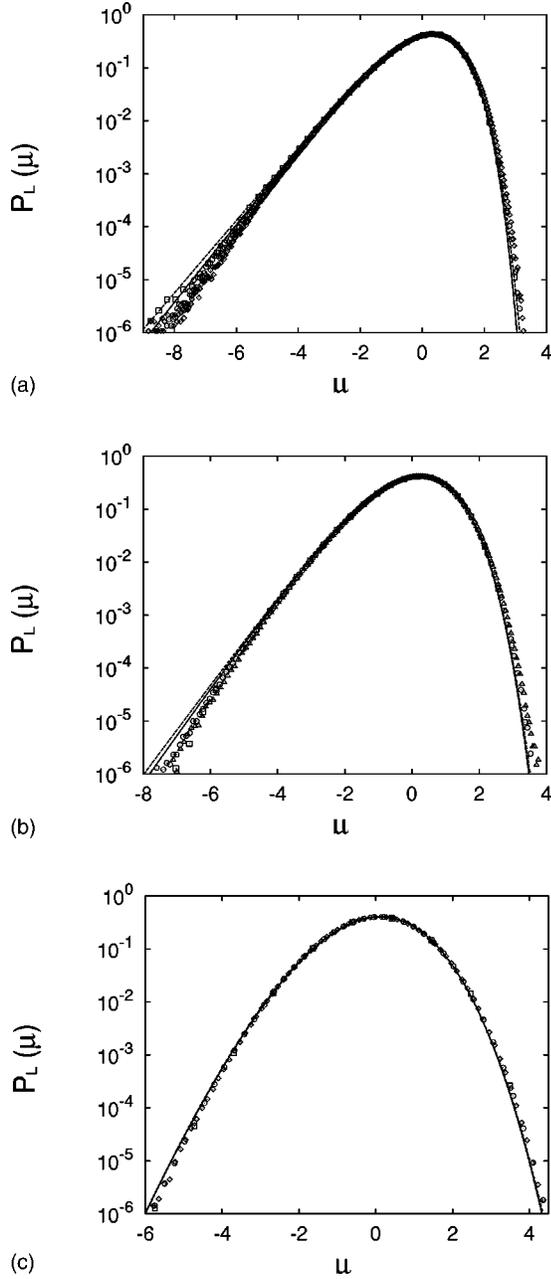


FIG. 3. Monte Carlo data for $P_L(\mu)$ for magnetic field (a) $h/J = 0.01$, (b) $h/J = 0.05$, and (c) $h/J = 0.5$ for $T/J = 0.1, 0.4$, and 0.7 . The lines are for data generated from Eq. (12) (full) and for the function (15) (dashed). Theoretical curves for different temperatures are superposed.

effects is sufficient to give the small deviation from the Monte Carlo data.

In all cases, both numerical and theoretical, the independence of the results on temperature is quite remarkable and it leads one to suggest that, as in the case of a zero field, the distribution is truly temperature independent throughout the range of temperature and system size for which the excitation of vortex pairs can be neglected. This point requires further study, but it is already clear that, from a pragmatic point of view, temperature dependence is not an observable phenomena.

Note that with the definition (3) we explicitly study the longitudinal magnetization, irrespective of its direction in space. This is the quantity that becomes critical at a phase transition in a system with continuous symmetry. The introduction of the magnetic field breaks the orientational symmetry in the thermodynamic limit and the variable conjugate to it is the projection of \vec{m} along the field direction. The fluctuations in these two quantities are different for a small field and in the crossover region, as $h \rightarrow 0$, the latter quantity becomes ill defined [16]. The two quantities become indistinguishable for $\xi/L \sim 0.1$.

The skewness $\gamma = \langle \mu^3 \rangle$, which parametrizes the asymmetry of the curve, varies from -0.89 in the extreme non-Gaussian limit to -0.23 for a ratio $\xi/L = 0.043$, and indeed goes smoothly to zero for $\xi/L \rightarrow 0$. Numerical values can also be found in Table I.

The origin of the skewness becomes clear if one considers the contribution made by the normal modes. The magnetization can be written

$$m = 1 - 1/2N \sum_{q>0} \phi_q^2 + \dots \quad (13)$$

To leading order in ϕ_q , m therefore consists of a sum over variables $m_q = (\phi_q^2/2N)$ which, within the spin-wave approximation, are statistically independent, with generating function

$$P(m_q) = \sqrt{\frac{\beta J q^2 N}{4\pi}} m_q^{-1/2} e^{-\beta J_{eff} N (q^2 + \xi^{-2}) m_q} \quad (14)$$

In zero field, the mean amplitudes $\langle m_q \rangle$ vary from a microscopic value $O(1/N)$ for modes on the zone edge through to a value of $O(1)$ for the long-wavelength modes at the zone center and the dispersion in the contributions is divergent in the thermodynamic limit. In two dimensions the density-of-states is linear in q , which is just what is required to engage the entire zone [10].

Violation of the central limit theorem therefore arises because the individual elements, although statistically independent, are not individually negligible. The modes of divergent amplitude near the Brillouin-zone center are responsible for the anisotropy, although all parts of the zone are required for a detailed reconstruction of $P(m)$. Introduction of the length scale ξ removes the divergence for $q \rightarrow 0$ and reestablishes the criterion that the statistically independent elements are individually negligible. In the limit that $\xi/L \rightarrow 0$ the distribution becomes Gaussian. If the thermodynamic limit is taken while keeping the ratio ξ/L constant, the amplitudes remains divergent, but the contribution from the zone center becomes progressively less, as the ratio ξ/L is reduced and the skewness falls to zero.

IV. FITTING WITH A GENERALIZED GUMBEL FUNCTION

In Refs. [10,15] we have compared the functional form of $P_L(\mu)$ with a series of standard expressions. Although none are exact solutions, they all give good fits to the data and

therefore offer very useful analytical functions as well as giving some insight into the physical processes responsible for the asymmetric PDF. Here, we only pursue one of these, the generalized Gumbel function for the statistics of extremes [17]

$$\sigma_z P_G(\mu_z) = w \exp[ab(\mu_z - s) - ae^{b(\mu_z - s)}], \quad (15)$$

which gives the a th largest or smallest values of a set of N random numbers z_i , in the limit that $N \rightarrow \infty$. For the smallest values, $\mu_z = (z - \langle z \rangle) / \sigma_z$. The constants w , b , and s depend on a through the three conditions of normalization, $\langle \mu_z \rangle = 0$ and $\langle \mu_z^2 \rangle = 1$ and one finds

$$w = \frac{a^a \alpha_a}{\Gamma(a)} \sigma_z,$$

$$b = \sqrt{\frac{1}{\Gamma(a)} \frac{\partial^2 \Gamma(a)}{\partial a^2} - \left[\frac{1}{\Gamma(a)} \frac{\partial \Gamma(a)}{\partial a} \right]^2}, \quad (16)$$

$$s = \frac{1}{b} \left[\log(a) - \frac{1}{\Gamma(a)} \frac{\partial \Gamma(a)}{\partial a} \right].$$

The function therefore has only one parameter, which is calculated by comparing the Fourier transform of Eq. (15) with $\Phi(x)$ of Eq. (12). Using the notation of Eq. (12) we have, for the Gumbel function,

$$\begin{aligned} \ln \varphi_G(x) = & \ln \frac{w \Gamma(a)}{s a^a} - ix \left(s + \frac{\Psi(a)}{b} - \frac{\ln(a)}{b} \right) - \frac{x^2}{2b^2} \Psi'(a) \\ & + i \frac{x^3}{6b^3} \Psi''(a) + \frac{x^4}{24b^4} \Psi'''(a) - i \frac{x^5}{120b^5} \Psi^{(4)}(a) \\ & + \dots, \end{aligned} \quad (17)$$

where $\Psi(z)$ is the digamma function $\Gamma'(z)/\Gamma(z)$. For Φ we have

$$\ln \varphi(x) = -\frac{1}{2}x^2 - i \frac{\sqrt{2}g_3}{3g_2^{3/2}}x^3 + \frac{g_4}{2g_2^2}x^4 + i \frac{2\sqrt{2}g_5}{5g_2^{5/2}}x^5 + \dots, \quad (18)$$

from which it follows that the constant a is implicitly given by

$$\frac{\Psi''(a)}{\Psi'(a)^{3/2}} = -2^{3/2} \frac{g_3^{3/2}}{g_2}. \quad (19)$$

For the zero field, the solution is $a \approx \pi/2$, rather than an integer value, showing $P(m)$ is not simply an extreme value distribution. This solution is an approximation although a good one, which can be seen by comparing the ratio of higher-order terms in the two expansions (17) and (18). These diverge slowly from unity [10]. Solving Eq. (19) for a finite field, gives a increasing with h . The subsequent curves are superimposed in Figs. 2 and 3, where one can see that the fitting function reproduces the results of the theoretical calculation to a good approximation. For a small field a very

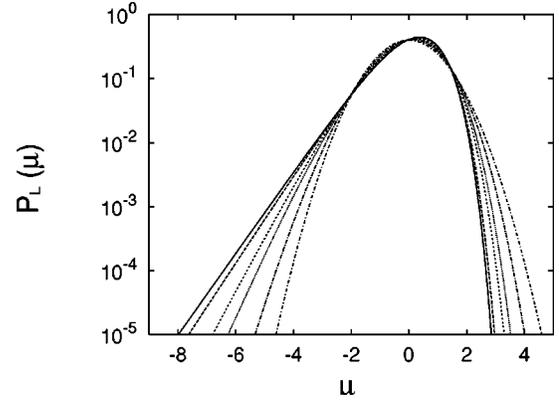


FIG. 4. Evolution of $P_L(\mu)$ from the function (15) with h/J . Moving from left to right for fluctuations below the mean, the data is for $h/J=0, 0.01, 0.05, 0.1, 0.5$, and ∞ .

small difference in the slopes of the exponential tails can be detected. However, this disappears with increasing h and the fitting function can be regarded as an excellent working tool for describing the data. In Fig. 4 we illustrate the evolution of the distribution from the anisotropic limit to the uncorrelated Gaussian limit as a function of field using Eq. (15). The values of $a(h)$ are shown in Table I. In terms of extremal statistics, the evolution of $a(h)$ means that we are describing the PDF of less and less extreme values, which becomes more and more normal.

For a strong field, one can solve Eq. (19) analytically. Evaluating g_2 and g_3 using a continuum approximation and using Stirling's formula, $\ln \Gamma(a) \approx a \ln a - a$, one finds

$$a \sim \frac{\pi}{2} \left[1 + \left(\frac{L}{2\pi\xi} \right)^2 \right]. \quad (20)$$

This simple expression gives a to a good approximation even outside the range of a values for which Sterling's formula is valid, and reproduces our previous result for $h=0$. It also allows one to see that a has a contribution coming from fluctuations within a correlated domain and a contribution coming from the fact that the system, with finite ξ , can be divided into a number $N_{eff} = (L/\xi)^2$ of statistically independent domains.

V. CONCLUSION

In conclusion, we have made a microscopic calculation of the generalized scaling function $P_L(mL^{\beta/\nu}, \xi/L)$ for order-parameter fluctuations near the line of critical points of the low-temperature phase of the 2D XY model. A Hartree approximation is used to treat the nonlinear corrections to a quadratic Hamiltonian. The approximation is necessary to ensure that the hyperscaling relation between critical exponents is satisfied. We show that the hyperscaling relation is a consequence of the nonlinearity necessary to ensure the correct system size dependence of the order parameter, conjugate to the applied magnetic field. This is a requirement of thermodynamics, rather than a general requirement for the observation of non-Gaussian fluctuations for global quantities. Indeed, observation of hyperscaling in nonthermody-

dynamic systems [18], could be taken as an indication that an equivalent phenomenology exists. For a fixed magnetic field, the correlation length is modified only slightly by thermal fluctuations and this manifests itself in the function P_L , which is essentially independent of temperature. The fact that the exponent $\beta/\nu=4\pi T/J$ is small and that $\delta=8\pi T/J-1$ is large, may be important for this observation. More work is required to clarify this point.

Finally, we propose that our fitting parameter $a(h)$ could be used as an experimental tool to estimate the correlation length scale in other correlated systems. We have previously made an empirical observation [3,15] that the fluctuation of global measures in other correlated systems, both in equilibrium and out of equilibrium, are very similar to those of the magnetization of the two-dimensional (2D) XY model in a zero field. We have proposed that these observations illus-

trate, at least qualitatively, universal features for correlated systems from different universality classes. This idea, as well as alternative interpretations [8,19], could be tested for example, in an enclosed turbulent flow using the experimental setup described in Refs. [1,5], by varying the ratio of the power injection length scale to the enclosure length scale.

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