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Relevance of soft modes for order parameter fluctuations in the two-dimensional XY model

B Portelli and P C W Holdsworth

Laboratoire de Physique, Ecole Normale Supérieure de Lyon, 46 Allée d'Italie,
F-69364 Lyon Cedex 07, France

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Abstract

We analyse the spin wave approximation for the two-dimensional XY model, directly in reciprocal space. In this limit the model is diagonal and the normal modes are statistically independent. Despite this simplicity non-trivial critical properties are observed and exploited. We confirm that the observed asymmetry for the probability density function for order parameter fluctuations comes from the divergence of the mode amplitudes across the Brillouin zone. We show that the asymmetry is a many-body effect despite the importance played by the zone centre. The precise form of the function is dependent on the details of the microscopic generating function for the modes. We discuss the relevance of this to more complex or non-equilibrium systems where similar distributions are observed.

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1. Introduction

Order parameter fluctuations in critical systems are known to be non-Gaussian [1] and the form and universal nature of the fluctuations have been studied from a field-theoretic and renormalization group point of view [2–6]. More recently, a surprising and more pragmatic motivation has come from the experimental observation that the probability density for fluctuations of global measures in correlated, but non-equilibrium systems, such as energy injected into a closed turbulent flow, or global measures of self-organized criticality can be of the same form as those for order parameter fluctuations in a critical system [7–11]. In this context, we have made a series of studies of order parameter fluctuations in the low temperature phase of the two-dimensional (2D) XY model [12–14]. This is arguably the simplest system in which one can study critical phenomena as in zero field a continuous line of critical points stretches from the Kosterlitz–Thouless–Berezinskii phase transition [15], T_{KT} , to zero temperature. Therefore, the critical behaviour occurs even at temperatures where a harmonic approximation to the starting Hamiltonian is valid. Further, it follows from a renormalization group analysis [16] that the behaviour at all temperatures below T_{KT} is perfectly captured at

large length scales by a harmonic Hamiltonian with effective coupling. As a result, we have been able to calculate the probability density function $P(m)$ for all temperatures below which vortices make a measurable contribution, without either invoking the scaling hypothesis or using renormalization group theory [13, 14].

In this paper, we take further advantage of the simplicity of the model, making a study of $P(m)$ directly in Fourier space. The harmonic Hamiltonian is diagonalized in reciprocal space and the problem becomes one of a set of statistically independent normal modes. One can thus study the contribution to $P(m)$ from different parts of the Brillouin zone (BZ). In section 2 we show that it is essentially the soft modes near the zone centre which are responsible for the asymmetric non-Gaussian form for $P(m)$. However, we show further that a complete and detailed description of the $P(m)$ requires many modes and the problem remains intrinsically a many-body one.

In section 3 we discuss our results in relation to extremal statistics. We have previously fitted $P(m)$ to a function reminiscent of Gumbel's first asymptote from extremal statistics. With this description in terms of normal modes we are in a position to study the contribution from the mode with the largest amplitude in each configuration. We confirm that it is not sufficient to keep the largest of the statistically independent modes and conclude that, if extremal statistics are relevant for the description of the global measure, then they must be applied to composite correlated structures and not to the most fundamental excitations of the problem.

In section 4 we study the effect of changing the form of the microscopic generator for the normal modes. We show that changing from the Gibbs measure to an arbitrary form does change the final outcome for the global fluctuations. We generalize the Gibbs measure analytically using a $\chi^2(\nu)$ distribution for the contribution from each mode. This function gives the probability for a composite variable constituting a sum of ν statistically independent degrees of freedom. We show that the global measure becomes Gaussian as ν becomes large and give a physical interpretation for this. Some conclusions are presented in section 5.

2. Description of the two-dimensional XY model in Fourier space

2.1. Framework of the study

In the 2D XY, or plane rotator, model classical spins of unit length, confined to a plane in spin-configurational space, interact via the Hamiltonian

$$H = -J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j = -J \sum_{\langle i,j \rangle} \cos(\theta_i - \theta_j) \quad (1)$$

where the orientation of the spin vector is given by the angle θ_i . J is the exchange constant, the sum is over nearest neighbours and here we consider spins on sites of a square lattice with periodic boundaries and lattice spacing of unit length.

At low temperature the harmonic, or spin-wave, Hamiltonian can be written as

$$H = \frac{1}{2} \sum_{\text{BZ}} J \gamma_q \varphi_q^2 \quad (2)$$

where $\varphi_q = \text{Re}[1/\sqrt{N} \sum_i \theta_i \exp(-i\vec{q} \cdot \vec{r}_i)]$ and $\gamma_q = 4 - 2 \cos(q_x) - 2 \cos(q_y)$. Here φ_q takes on values between $\pm\infty$ as we have neglected the periodicity of the original spin variables. The sum is over the $N - 1$ modes of the BZ neglecting the Goldstone mode at $q = 0$. The latter is a purely diffusive mode contributing zero energy. As discussed below we find that we can replace $\gamma_q = q^2$ without introducing an error in the calculated distribution function.

In principle, this Hamiltonian correctly describes the critical behaviour throughout the low-temperature phase as bound vortex pairs are renormalized away at very large length scale.

In practice, this is true for the finite system sizes studied here only as long as no vortex pairs are excited. However, as vortices only appear in a relatively small range of temperature close to the KTB transition [18], there remains a large range of temperature over which the behaviour is correctly described by a Hamiltonian of this form. Within this regime non-linear but analytic terms in the expansion of $\cos(\theta_i - \theta_j)$ are accounted for perfectly by an effective coupling constant [13, 16].

Thus, at low temperature, the 2D XY model can be viewed as a poly-disperse perfect gas of particles of ‘mass’ $J\gamma_q$. The probability function for each mode is therefore a Maxwell–Boltzmann distribution

$$P(\varphi_q) = \sqrt{\frac{\beta J \gamma_q}{2\pi}} \exp\left(-\frac{\beta J \gamma_q \varphi_q^2}{2}\right) \quad (3)$$

depending explicitly on the vector \vec{q} .

The aim of this paper is to show that this dispersion of mass, associated with a Gibbs measure, is the motor leading directly to the asymmetry of the probability density function (PDF) for the magnetic order parameter. Given the separable nature of the problem, we are able to do this by performing numerical simulation and analytic work directly in Fourier space, without referring to the spins in real space. The order parameter m for a single configuration can be defined as

$$m = \frac{1}{N} \sum_{i=1}^N \cos(\theta_i - \bar{\theta}) \quad (4)$$

where

$$\tan \bar{\theta} = \frac{\sum_i \sin \theta_i}{\sum_i \cos \theta_i} \quad (5)$$

is the instantaneous magnetization direction. With this definition, m is a scalar quantity giving the length of the magnetization vector independent of its direction in the spin plane.

In a previous paper [13], we have calculated the PDF for a large, but finite size, system, as a function of the reduced variable $\mu = (m - \langle m \rangle)/\sigma$, where $\langle m \rangle$ and σ are the mean and the standard deviations of the distribution:

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

$$\ln \psi(x) = -ix \sqrt{\frac{1}{2g_2}} \sum_{\text{BZ}} \frac{G(\mathbf{q})}{N} - \frac{1}{2} \sum_{\text{BZ}} \ln \left[1 - i \sqrt{\frac{2}{g_2}} \frac{G(\mathbf{q})}{N} x \right] \quad (6)$$

where $P_L(\mu) = \sigma P(m)$, $G(\mathbf{q}) = \gamma_q^{-1}$ and $g_k = \sum_{\text{BZ}} G(\mathbf{q})^k / N^k$. The sum over \mathbf{q} and the integral over x , in (6), are performed numerically and $P_L(\mu)$ approaches a (thermodynamic) limit function rapidly for $N > 100$ spins. Surprisingly this function, shown in figure 1 and discussed in detail below, is independent of temperature and therefore of critical exponent $\eta = T/2\pi J$ along the line of critical points.

Expanding (4) in small angles, keeping only the leading terms and Fourier transforming, one can write

$$m \approx 1 - \frac{1}{2N} \sum_{\text{BZ}} \varphi_q^2 = 1 - \sum_{\text{BZ}} m_q \quad (7)$$

where $m_q = \frac{1}{2N} \varphi_q^2$ has the normalized distribution

$$P(m_q) = \sqrt{\frac{\beta J \gamma_q N}{\pi}} m_q^{-1/2} e^{-\beta J N \gamma_q m_q}. \quad (8)$$

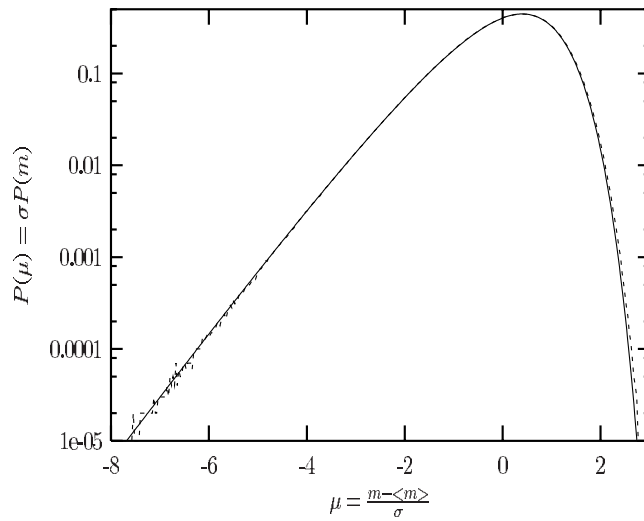


Figure 1. The PDF in two dimensions ($L = 32$) at temperature $T = 1$. The continuous line is the fast Fourier transform, equation (6). The dotted line is for \mathbf{q} -space Monte Carlo.

While this expansion is strictly valid for first order in T and for finite systems only, we have previously shown that the PDF for the fluctuations in m , given by (7), is identical to that for m given by (4), even outside the range of T for which the expansion is valid. For this linear development of the order parameter, the critical exponent, $\eta = 0$. There are a number of subtle points associated with this result; most notably, the violation of the hyperscaling relation between critical exponents if definition (7) is used. These points will not be discussed further here; rather, we refer the reader to [11, 13, 14] where they are discussed in detail. However, the important point for this paper is that the magnetic fluctuations of the entire low-temperature phase can be characterized by the harmonic Hamiltonian (2) and the linearized order parameter (7) and the problem can be analysed entirely in Fourier space, with statistically independent harmonic degrees of freedom.

2.2. Simulations in Fourier's space

We first test these ideas by comparing the PDF, as generated by [6], against Monte Carlo simulation performed directly in \mathbf{q} -space. We take the real part of the Fourier transformed spin variable as the independent degree of freedom on each point in the Brillouin zone and define the quarter of the zone with q_x and q_y positive. Points with $q_x \neq 0$ and $q_y \neq 0$ have a four-fold degeneracy, points on the axis, with $q_x = 0$ or $q_y = 0$, have a two-fold degeneracy and the origin is excluded, giving the total of $N - 1$ points. For each configuration, amplitude φ_q is generated using (3). The results of the simulation are compared in figure 1 with the theoretical result given by equation (6). Data are shown for 10^8 configurations. The agreement is quite excellent, showing clearly that the model of statistically independent variables and the calculation leading to (6) are consistent and that they correctly describe the fluctuations in the low-temperature domain. The PDF is asymmetric, with a quasi-exponential tail for fluctuations below the mean, and with a much faster double exponential fall off for fluctuations above the mean [13].

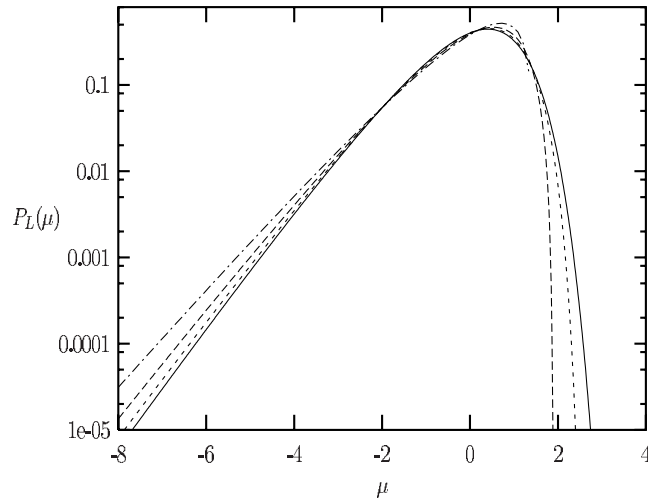


Figure 2. PDF generated from the first shell (four modes, dotted–dashed line), one shell (eight modes, long dashed line), two shells (24 modes, short dashed) and full Brillouin zone (solid line). All results are generated from equation (6) for $L = 100$.

2.3. Relevance of soft modes

Our aim is now to study the effect on the PDF coming from different parts of the BZ and in particular the contribution from the soft modes, near the zone centre. We should be able to do this by restricting the summations in equation (6) to the desired part of the zone only. We define shells moving out from the zone centre: the first contains only the four softest modes. The subsequent shells are squares of length $\frac{2\pi}{L}n$ and unit thickness, containing $(2n + 1)^2 - 1$ modes. We have tested the PDF generated from equation (6), with restricted sums over the shells defined above, against Monte Carlo data taken for modes in the same shells. We again found essentially perfect agreement giving confidence in the theoretical result for both complete and partial sums over the Brillouin zone. In the following analysis we need to make no further reference to numerical simulation and can restrict ourselves to the analytic result of equation (6). Some initial steps in this approach were taken in [17] for the PDF of height fluctuations in models of interface growth.

Results are shown in figure 2 for summations over varying numbers of shells in the Brillouin zone and in figure 3 for a calculation including all modes except the four softest modes. One can see that the asymmetry comes explicitly from the soft modes near the zone centre. The exponential tail is reproduced to a first approximation with only the first four modes, while excluding them from the distribution gives a nearly symmetric distribution.

The reason for this is the dispersion in the typical amplitudes for modes over the Brillouin zone. For small q values $\gamma_q \sim q^2$, which means that the average value, $\langle m_q \rangle$, is of order $O(T/J)$ at the zone centre, while $\langle m_q \rangle \sim T/NJ$ on the zone edge. The dispersion in contributions, therefore, diverges with system size. The magnetization is the sum over variables $m_q \sim \varphi_q^2$, not φ_q themselves and the distribution for m_q (equation (8)), therefore has exponential tails. If terms in the sum are not individually negligible, as is the case here, the distribution for the global measure is consequently asymmetric. However, it is not the case that the global PDF is reproduced quantitatively by softest modes by themselves. More modes are required for a quantitative fit and one must include more than the four shells shown in figure 2 for a good fit to the eye.

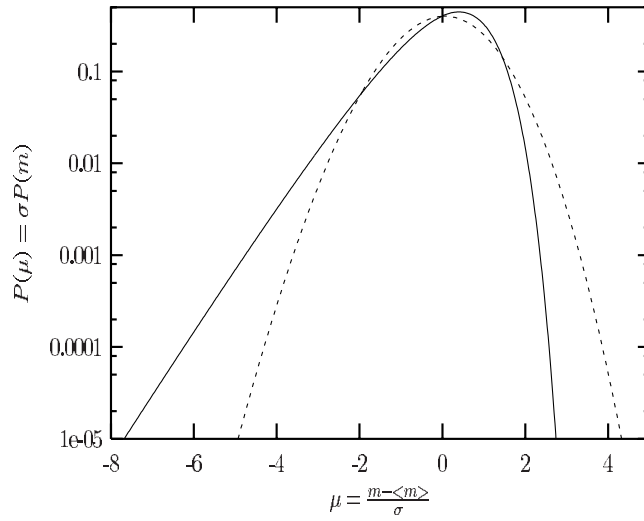


Figure 3. PDF generated from all but the first shell ($N - 5$ modes, short dashed line) and full Brillouin zone (solid line). All results are generated from equation (6) for $L = 100$.

The contribution to the PDF from any set of N_g modes with fixed q is that for an ideal gas of N_g identical particles; the so-called χ^2 distribution

$$f(x) \sim x^{(N_g/2)-1} \exp(-\beta x). \quad (9)$$

Writing the χ^2 distribution in terms of μ one finds

$$P_L(\mu) = \mathcal{N}(s - \mu)^{(N_g/2)-1} \exp(b(\mu - s)) \quad (10)$$

where

$$\mathcal{N} = \left(\frac{\alpha\sigma}{T}\right)^{N_g/2} \frac{1}{\Gamma\left(\frac{N_g}{2}\right)} \quad (11)$$

$$s = \frac{1 - \langle M \rangle}{\sigma} \quad b = \frac{\alpha\sigma}{T} \quad \alpha = 8\pi^2 J \quad \sigma = \frac{1}{\alpha} \sqrt{\frac{N_g T}{2}}.$$

The PDF is, therefore, a convolution over χ^2 distributions with varying particle number and ‘mass’. Once the discrete nature of the lattice is lost the number of particles for each value of q is proportional to the density of states, $n(q) \sim q^{d-1}$. For numerical simplicity we have defined square shells but our findings are compatible with this continuum description. Note that the PDF coming from the four softest modes only is cut off just to the right of the maximum (see figure 2). This corresponds to $\mu = s$, $m = 1$ and the distribution is not defined for larger fluctuations above the mean. The constraint $m \leq 1$ does not come into play for the distributions with larger numbers of modes, within the observed range of fluctuations.

We study the goodness of fit for n shells, in figure 4, where we plot the error function

$$\delta(\mu, N/N_{eff}) = \frac{P_L(\mu, N_{eff})}{P_L(\mu, N)} \quad (12)$$

with $N_{eff} = (2n + 1)^2 - 1$, for $N = 10^4$ sites. The further out in the wings one goes, the more shells one has to include in order to get a required value of δ . For large μ and $N \gg N_{eff}$ we find

$$\delta(\mu, N_{eff}) \sim 1 + \mathcal{C}(\mu) \frac{1}{N_{eff}} \quad (13)$$

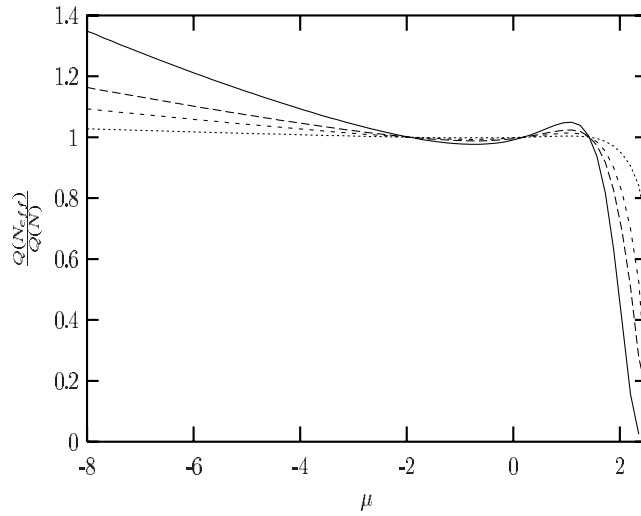


Figure 4. $\delta(\theta) = \frac{Q(N_{eff}, \theta)}{Q(N, \theta)}$ for a given size N and for different N_{eff} (different fractions). From top to bottom on the left of the figure, the curves are for 4, 8, 25 and 48 modes.

independently of N . The many-body nature of the distribution is confirmed by the fact that δ only goes to zero as N_{eff} diverges.

We have previously argued [13] that the critical nature of the 2D XY model is epitomized by the fact that all length scales from the microscopic to the macroscopic are important. For example, calculation of the mean magnetization $\langle m \rangle$ involves an integral of the form $\int_{2\pi/L}^{\pi} (1/q) dq \sim \log(L)$ where both limits of integration come into play. One could argue that the above result, with δ becoming independent of N in the limit $N \gg N_{eff} \gg 1$, is not quite in agreement with this discussion as only the zone centre is important in this limit. However, exactly the same would be true for a situation where the central limit theorem is satisfied, that is, with zero dispersion in the spin wave stiffness of the modes; here one would build a Gaussian distribution by adding the modes from different shells and in the above limit, this would be attained with arbitrary accuracy by increasing N_{eff} independent of the value of N . The latter is realized in the presence of a strong magnetic field [14] where the dispersion in spin-wave stiffness is removed by the finite magnetic correlation length. The above analysis is not, therefore, the most sensitive measure of criticality, although it does clearly show that the global measure is the result of many-body contributions, while at the same time showing why no error is incurred when replacing γ_q by q^2 in the various summations.

2.4. Comparison with the three-dimensional XY model

Criticality can be seen more clearly by comparing with the magnetic fluctuations in the low-temperature phase of the three-dimensional XY model. Here there is broken symmetry and long-range magnetic order, although the longitudinal susceptibility remains weakly divergent in the ordered phase and temperature is a dangerously irrelevant field near $T = 0$ [19, 20]. As a result the PDF for the magnetic fluctuations is weakly asymmetric [13] as shown in figure 5. Equation (6) is easily extended to three dimensions, and the same partial summations over the BZ can be performed. Included in figure 5 are the PDFs calculated from the softest modes only and from all but the softest modes. As one can see, the form of the curve is well reproduced

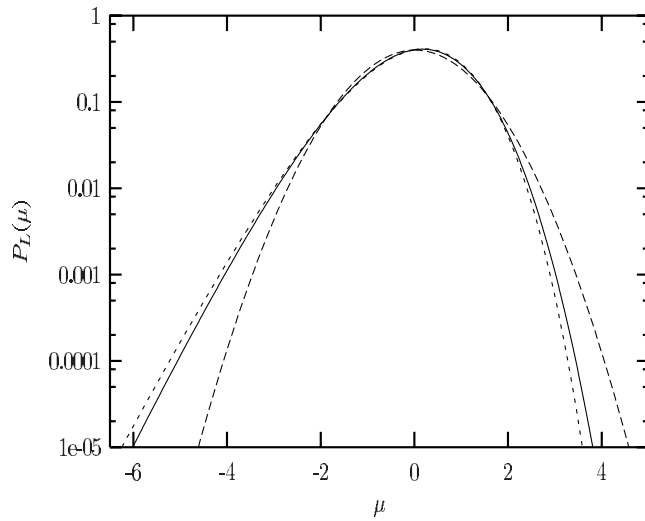


Figure 5. PDF for the 3D XY model for the first shell (six modes, short dashed), all modes except the first shell (long dashed) and full Brillouin zone (solid line). All results are generated from equation (6) for $L = 100$.

by the first shell. This should be compared with the two-dimensional case where many more modes were required for an equivalent description.

This can be seen in more detail by considering the evolution of the asymmetry of the distribution through the skewness γ [13]

$$\gamma = \langle \mu^3 \rangle = \sqrt{\frac{8g_3^2}{g_2^3}}, \tag{14}$$

as one consecutively removes shells around the zone centre from the summations in g_k . That is, we now sum over the BZ except for an ever increasing number of shells around the zone centre. The results are shown in figure 6 for two and three dimensions. Clearly, it is necessary to remove fewer shells in three dimensions than in two dimensions, before $\gamma \rightarrow 0$ and the distribution becomes Gaussian.

3. Link with extreme statistics

In [10, 13], it was shown that the analytic expression for the PDF $P_L(\mu)$ is extremely well represented by a function reminiscent of Gumbel’s first asymptote for the statistics of extremes [21]

$$P_G(\mu) = w(e^{b(\mu-s)} - e^{b(\mu-s)})^a, \tag{15}$$

where

$$\begin{aligned} w &= \frac{a^a b}{\Gamma(a)}, \\ b &= \sqrt{\frac{1}{\Gamma(a)} \frac{\partial^2 \Gamma(a)}{\partial a^2} - \left[\frac{1}{\Gamma(a)} \frac{\partial \Gamma(a)}{\partial a} \right]^2}, \\ s &= \frac{1}{b} \left[\log(a) - \frac{1}{\Gamma(a)} \frac{\partial \Gamma(a)}{\partial a} \right]. \end{aligned} \tag{16}$$

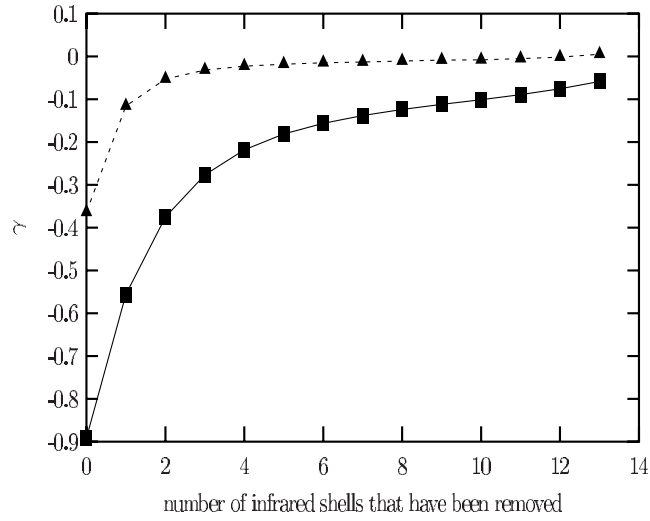


Figure 6. Evolution of the skewness γ as a function of removed infrared shells. Study in two (full line) and three (dashed line) dimensions.

The function therefore has a single independent parameter a . When a is an integer, equation(15) gives the PDF for the a th smallest value from a set of N random numbers in the limit $N \rightarrow \infty$. We have made a comparison between the function ψ of equation (6) and the characteristic function for P_G

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

where $\Psi(z)$ is the digamma function $\Gamma'(z)/\Gamma(z)$. Expanding ψ and equating the first four terms we find an implicit equation

$$\frac{\Psi''(a)}{\Psi'(a)^{3/2}} = -2^{3/2} \frac{g_3}{g_2^{3/2}}. \quad (18)$$

Solving for a and hence for the other constants we find $a = 1.58$, $b = 0.93$, $s = 0.37$, $w = 2.16$. This does not represent the exact solution for P_L ; higher order terms in the expansion of the two functions are not the same and their ratio diverges slowly from unity with increasing order.

Although [15] is not the exact solution, merely a good approximation, and the best fit value $a \approx \pi/2$ is non-integer, it is still interesting to search for a concrete link with extremal statistics. As we have reduced our model to one of the statistically independent Gaussian variables the obvious question seems to be: is the PDF of the dominant mode the same as that of the global measure? We define a magnetization $m = 1 - m_{max}$, where m_{max} is the largest of m_q . We compare, in figure 7, the PDF for this quantity with that for the full magnetization. The difference between the two distributions is not very great, but they are certainly not the same and we confirm what we have seen in the previous section, that the correct distribution comes from an ensemble of statistically independent objects and not a single mode. The extreme values are well described by the Gumbel function with $a = 1$, despite the dispersion in the spin wave stiffness. The diverging dispersion means that the largest mode is always one of only a few modes near the zone centre and it is by no means clear whether Gumbel's asymptote should apply here.

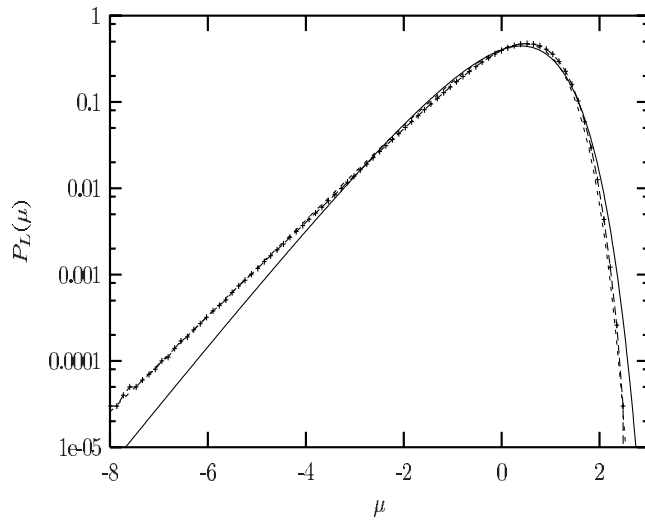


Figure 7. Contribution from the Fourier mode of extreme amplitude (dashed line) and comparison with the PDF generated from equation (6) (solid line) and the Gumbel asymptote, $\alpha = 1$ (dotted line).

We can conclude therefore that an extremal description is not applicable to the fundamental excitations in the problem. However, one can perhaps apply extremal statistics to the complex and correlated structures that appear in real space for critical systems and for correlated systems in general [22–24]. Indeed, in simulations of the 2D Ising model at a temperature T^* slightly below the critical temperature, PDFs were found to be very similar to those for the 2D XY model, when calculated for both the magnetization and the magnetization coming uniquely from the largest cluster of connected spins [10]. There are clearly many open questions here but the above analysis strongly suggests that an observation of extremal statistics is a consequence of the presence of composite and correlated objects, rather than being a directly observable phenomenon among the most fundamental microscopic excitations that make up these objects.

4. Influence of the microscopic measure on the global measure

One might also ask the question: is the global PDF dependent on the existence of a Gibbs measure, or effective Gibbs measure for the fundamental excitations that contribute to the global fluctuations? Within the present framework this question can be addressed directly by changing the form of the generating function [8], while keeping the same dispersion for the standard deviations, $\sigma_q = \sqrt{\langle m_q^2 \rangle - \langle m_q \rangle^2} = \frac{1}{\sqrt{2\beta J N \gamma_q}}$. In figure 8 we show the global distribution produced from an array of flat generators

$$\begin{aligned} p(m_q) &= 1/x_q & m_q \leq x_q \\ p(m_q) &= 0 & m_q > x_q \end{aligned} \tag{19}$$

with $x_q = \sqrt{12}\sigma_q$, which satisfies the above criterion. As can be seen, the resulting distribution is radically different from that for the Gibbs measure. It is perfectly symmetrical despite the dispersion in mode amplitudes. The curve is almost, but not quite, Gaussian. We have not made a detailed analysis of this point, but the deviation from Gaussian behaviour suggests that the central limit theorem is still violated even though the distribution is now symmetrical. From this exercise we conclude that the dispersion in normal modes is not the only criterion

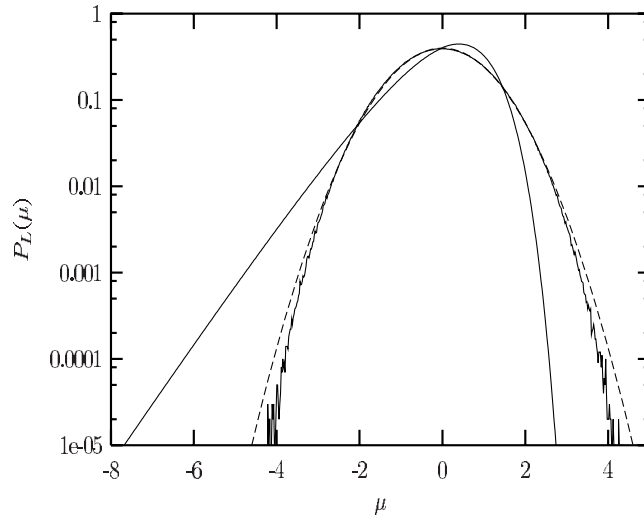


Figure 8. PDF calculated numerically from the flat generators, equation (19) (symmetric full line) compared with the PDF from equation (6) (asymmetric full line) and a Gaussian distribution (dashed line). All data are for $L = 100$.

for the asymmetric distribution we have observed. Our results suggest that in addition to this, we require microscopic generators that are themselves asymmetric. In fact, one can deduce this general result by considering Gaussian generators for m_q ; here, by definition $P_L(m)$ must be Gaussian, as the sum of any set of Gaussian variables must itself be a Gaussian variable and therefore symmetric.

One can see analytically how the global PDF varies from the original distribution to a Gaussian distribution by considering generators of the form

$$p_\alpha(m_q) = N_\alpha m_q^{\alpha-1} e^{-m_q/\langle m_q \rangle}. \quad (20)$$

Here $\alpha > 0$ in order to ensure the convergence of $p(m_q)$ and $N_\alpha = \frac{1}{\Gamma(\alpha)\langle m_q \rangle^\alpha}$ is a normalization constant. We again take $\langle m_q \rangle = 1/\beta J N \gamma_q$ so that $p_{\alpha=1/2}(m_q)$ accounts for the two-dimensional XY model with Gibbs measure.

We proceed as previously, defining m within a linear approximation only, for simplicity. We define

$$P(m) = \int p(m_{q_1}, \dots, m_{q_N}) \delta\left(m - \left(1 - \sum_{q \neq 0} m_q\right)\right) dm_{q_1} \cdots dm_{q_N} \quad (21)$$

and generate m_q using equation (20). The δ function imposing the constraints $m = 1 - \sum_q m_q$ can be rewritten as

$$\delta\left(m - \left(1 - \sum_{q \neq 0} m_q\right)\right) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{ik(m - (1 - \sum_{q \neq 0} m_q))}. \quad (22)$$

As modes are independent the conditional probability $p(m_{q_1}, \dots, m_{q_N})$ is just the product

$$p(m_{q_1}, \dots, m_{q_N}) = \prod_{q=1}^N p_\alpha(m_q) \quad (23)$$

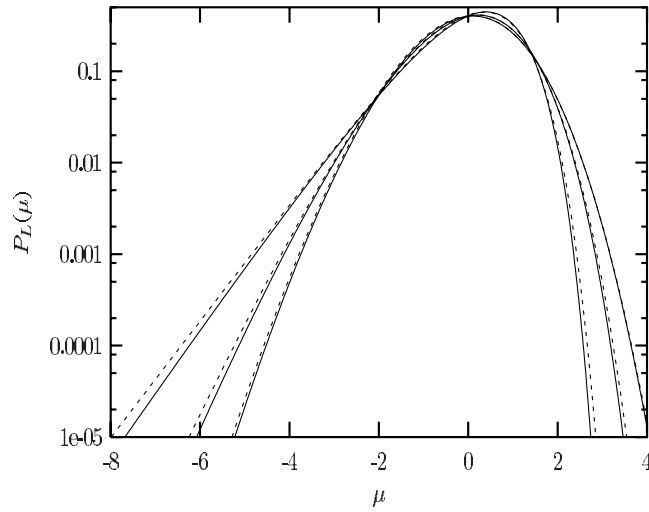


Figure 9. Influence of the microscopic distribution $p_\alpha(m_q)$ on $P_L(\mu)$, calculated result from equation (25) (full line), generalized Gumbel function fitting function (equation (15), dashed line). Data sets for decreasing skewness are for $\alpha = 1/2, 2, 5$.

so that

$$P(m) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{ikm} e^{-ik} \prod_{q=1}^N \int_0^{\infty} dm_q p_\alpha(m_q) e^{ikm_q}. \quad (24)$$

After some straightforward algebra, one can now express the PDF $P_L(\mu)$

$$P_L(\mu) = \int_{-\infty}^{\infty} \frac{dx}{2\pi} e^{ix\mu} \psi_\alpha(x) \quad (25)$$

where

$$\log(\psi_\alpha(x)) = \left(-ix \sqrt{\frac{\alpha}{g_2}} \text{Tr} \frac{G}{N} - \alpha \text{Tr} \log \left(1 - i \frac{x}{\sqrt{\alpha g_2}} \frac{G}{N} \right) \right) \quad (26)$$

which is just a generalization of (6) for arbitrary values of α , for which

$$\langle m \rangle = 1 - \alpha T \sum_q \frac{G(q)}{N} \quad \sigma = T \sqrt{\alpha g_2}. \quad (27)$$

As previously, the expression (25) can be transformed numerically for large but finite N . This procedure can again be tested by comparison with Monte Carlo simulation performed directly on the generators m_α . The results, which we do not show here, agree as well as they did in the initial problem. In figure 9 we show $P_L(\mu)$ for various α values calculated from equation (26). One can see that increasing α reduces the asymmetry of the global distribution, with it becoming Gaussian as α becomes large. This result can be interpreted physically by noting that the generator (20) is a χ^2 distribution for the variable m_q , which is the sum of $\nu = 2\alpha$ statistically independent positive definite variables. One can therefore think of the global PDF as being constructed from $\nu = 2\alpha$ replicas, or identical systems. As α increases, the number of contributions coming from each shell in the BZ, even those near $q = 0$, increases. The contribution from each shell will become Gaussian and $P_L(m)$ will therefore become Gaussian.

The analysis in terms of the Gumbel distribution can also be extended to include this variation in the form of the microscopic generators. Repeating the analysis of section 3 for the generating function ψ_α , we find

$$\frac{\Psi''(a)}{\Psi'(a)^{3/2}} = -2 \frac{g_3}{g_2^{3/2}} \frac{1}{\sqrt{\alpha}}. \quad (28)$$

The knowledge of a again allows one to evaluate the other constants b , s and w

$$b = \sqrt{\psi'(a)} \quad sb = \ln(a) - \psi(a) \quad w = \frac{a^\alpha b}{\Gamma(a)}$$

and numerically we find

- $\alpha = 2$:
 $a = 5.458\,02$, $b = 0.448\,35$, $s = 0.210\,54$, $w = 96.563$.
- $\alpha = 5$:
 $a = 13.0845$, $b = 0.2818$, $s = 0.1373$, $w = 194\,537.9$.

Data generated from equation (15) are included in figure 9 for comparison with the exact solution. The agreement is very good, indicating once again that the modified Gumbel function is a very useful working tool for data analysis. The small deviation between the Gumbel function and equation (25), observed along the exponential tail of the distribution for $\alpha = 1/2$, disappears as α increases.

For large values of α , one can expand (28) using Stirling expansions for the Γ function and its derivatives and find that

$$a \simeq 1 + \frac{\alpha g_2^3}{4g_3^2} \sim 1 + \frac{2\alpha}{\gamma^2}. \quad (29)$$

We actually find that this expression is quite accurate even outside the range of a values for which Stirling's formula is strictly valid.

This analysis is very similar to that recently made for the 2D XY model in the presence of a magnetic field [14]. In that case the field introduces a correlation length, ξ , which allows one to think of dividing the system into order $(L/\xi)^2$ statistically independent parts, just as we have proposed above for α different from $1/2$.

5. Conclusion

In this paper we have exploited the appealing property of the 2D XY model, that non-trivial behaviour of a correlated system appears despite the model being itself diagonalizable at low temperature. The magnetization can hence be described in terms of a sum over statistically independent variables. The PDF for order parameter fluctuations can, in consequence, be written as a convolution over χ^2 distributions for statistically independent variables, or particles of continuously varying amplitude. We have shown that, as one might expect for a critical system, it is the softest modes that influence the distribution most, with their diverging amplitude being directly responsible for the violation of the central limit theorem and the observed asymmetry for the PDF of this global quantity. However, we also explicitly show that the observed asymmetry is not a single or even a few-body phenomenon. Rather, a quantitative reconstruction of the PDF requires the sum over a number of modes that diverges in the thermodynamic limit. We have also analysed the 'extreme value' contribution from the largest mode from each configuration. The resulting distribution is consistent with the standard theory of extremal statistics and quantitatively different from the global PDF. Reconstructing

the PDF by summing successive shells leading out from the zone centre requires an arbitrary number of shells for arbitrary accuracy.

We show that the detailed form for the distribution depends on the precise form for the microscopic distributions for the individual modes. Hence we show that the form of the global PDF depends on a second criterion, the existence of a Gibbs measure, and that the nature of the violation of the central limit theorem depends on the form of microscopic distributions. This discovery is perhaps surprising given our empirical observation that a very similar distribution can be observed for complex systems driven far from equilibrium and in particular that for injected power fluctuations in a closed turbulent flow at constant Reynolds number [8]. This extra exigence suggests that, if an effective description of such non-equilibrium steady-state systems, in terms of statistically independent elements should exist, then the microscopic distributions should be similar to those appearing here, for the 2D XY model in thermal equilibrium.

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