Analytical computation of the magnetization probability density function for the harmonic 2D XY model

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The probability density function (PDF) of some global average quantity plays a fundamental role in critical and highly correlated systems. For example, it has been used in the so-called hypothesis of universal fluctuations [1], which states that the PDF for critical systems -like the two dimensional XY model- as a function of the centered parameter of order divided by its standard deviation should be a universal function $F$ of a Gumbel type. This claim should hold independent of the size and temperature for the magnetic systems and Reynold number for turbulent experimental systems. Approximated Gumbel distributions appear in quite dissimilar physical systems, such as a confined turbulent flow or the roughness $1/f$ noise in a resistor [2].

There was some evidence against this hypothesis reported in [3]. In particular, in Ref. [4] for instance, an analytical expression for the PDF for the full 2D XY model was computed systematically by means of the loop expansion, and the validity of the "generalized universality" has been linked to renormalization group (RG) properties. The 2-loops analytical expression for the PDF shows an explicit temperature dependence. As a consequence, its skewness and kurtosis computed perturbatively up to two loops (first order in $T$) show an explicit temperature dependence. More recently [5], the third and fourth normalized moments of the PDF -the skewness and kurtosis respectively- were computed analytically in the two-dimensional harmonic XY model. Their explicit temperature dependence was explicitly demonstrated, which holds even in the thermodynamic limit. This result was an indirect analytical proof of the failure of the claim of universal fluctuations, allowing therefore to confirm the explicit temperature dependence of the PDF reported in [4].

In spite of this, further papers supporting the proposed "]generalized universality" were published [6], raising the question whether there is a underlying mechanism responsible for this approximated phenomenon.

In a recent paper [7] the shape of the different distributions appearing in several critical systems has been phenomenologically linked to scaling arguments and to the concept from Renormalization Group Theory of classification of scaling variables as irrelevant, marginal and relevant. Nevertheless, one should note at this point that the so-called "generalized universality" is not related to the concept of exact universality of RG, because it only holds approximately, as it was explicitly shown in ref. [4] by using the loop-or temperature- expansion in the context of the two-dimensional XY-model.

It is further stated in [7] that an explicit analytical computation of the PDF for the two dimensional XY model is still missing. This claim also motivates our present computation.

Now we will explain how to compute a general analytical expression for the PDF of the magnetization by using the spin wave or harmonic approximation of the 2D XY model. This expression is valid for arbitrary system size $L$ and temperature $T$. The 2D XY model consists of planar spins $\phi_x$ defined on a periodic two dimensional square lattice $\Lambda$ of $N = L^2$ lattice sites, which are coupled with nearest neighbors by cosine interactions. According to RG arguments [8], in the low temperature phase and sufficiently below the Berezinskii-Kosterlitz-Thouless critical temperature, the physics of this model is entirely described by its harmonic approximation, the 2D HXY model. Indeed, in [4] it has been explicitly shown -by means of the loop expansion- that the effect of the anharmonic corrections to the spin wave approximation on the PDF is merely a renormalization of the temperature. Nevertheless, and in spite of this fact, one should take into account the periodicity of the variables of the XY model for the boundary conditions, which leads to the contributions coming from winding configurations [9]. This contribution turns out to be numerically very small and therefore one expects to obtain with the present model a trustable numerical approximation of the...
2D XY model in the large volume limit and in the low temperature phase.

The Hamiltonian of the 2D HXY-model is up to a constant

\[ H(\phi) = \frac{1}{2} J \langle \phi, -\Delta \phi \rangle \]  

(1)

where \( \Delta \) is the Laplace operator on the lattice, \( J \) is the ferromagnetic constant and \( \langle \phi, \varphi \rangle = \sum \phi(x)^* \varphi(x) \) stands for the scalar product on the lattice. We use a system of units where Boltzmann’s constant is set equal to unity throughout the computations and identify \( T \) with the reduced temperature \( T/J \). Although this model has no phase transition, it is a critical model in the sense that it has an infinite correlation length. This Gaussian model has been analytically extensively studied, because it represents the starting point for perturbative expansions and due to the involvement of Gaussian integrals. Some useful physical quantities can be expressed in terms of the Fourier representation of the lattice propagator \( G \)

\[ G(x) = \frac{1}{N} \sum_{(K_L)^2 \neq 0} \exp(-iK \cdot x) \frac{1}{(K_L)^2} \]  

(2)

where \( K_L \) is the lattice momentum defined as usual as \( (K_L)_i = 2 \sin(K_i/2) \), with \( i = 1, 2 \) and \( K_i \) lies in the first Brillouin zone, \( K_i = (2\pi/L)n \) with \( n \in \mathbb{Z} \) and \(-\pi < K_i \leq \pi \). The sum runs over all possible values of \( K_i \) for which \((K_L)^2 \) does not vanish. This comes from the fact that the Goldstone mode, which is originated by the invariance of the original Hamiltonian under a global rotation of the spin variables, and which leads to the translation invariance on the lattice, must be removed from the calculation. As it was first shown in Ref. [4], the PDF can be defined as the Fourier transform of the partition function \( Z(q) \) of an auxiliary theory, which differs from the original theory by a dimension 0 perturbation with a very small imaginary coefficients \( iq/N \). This theory turns out to be asymptotically free in the infrared (this is the case of the 2D XY model), viz.

\[ P(M) = \int_{-\infty}^{\infty} dq \frac{dq}{2\pi} \exp\{iq(M - \langle M \rangle)\} Z(q) \]  

(3)

where

\[ Z(q) = \frac{e^{-i\langle M \rangle}}{Z_0} \int D\phi \exp\left\{ -\beta H(\phi) + \frac{iq}{N} \sum_{x \in \Lambda} \cos \phi_x \right\} \]  

(4)

with partition function \( Z_0 = \int D\phi \exp\{-\beta H(\phi)\} \). The mean \( \langle M \rangle \) and the higher order moments of the PDF are obtained as usual as the integrals \( \langle M^p \rangle = \int M^p P(M) dM \). In particular, the mean square fluctuation is defined by \( \sigma^2 = \langle (M - \langle M \rangle)^2 \rangle \). The partition function \( Z(q) \) can be written as an integral over the normalized Gaussian measure \( d\mu_{TG}(\phi) \) of covariance \( TG \):

\[ Z(q) = \exp\{iq \langle M \rangle\} \int d\mu_{TG}(\phi) \exp\left\{ \frac{iq}{N} \sum_{x \in \Lambda} \cos \phi_x \right\} \]  

(5)

where \( G \) denotes the lattice propagator given by eqn. (2).

In terms of the PDF, the hypothesis of BHP universality stipulates that the PDF considered as a function of the reduced variable \( \mu = (M - \langle M \rangle)/\sigma \) is a universal function \( F \), and should be the same for a wide class of strongly correlated critical systems, independent of the system temperature \( T \) and volume \( N \), provided \( N \) is large enough:

\[ F(\mu) = \sigma P\left\{ \frac{(M - \langle M \rangle)}{\sigma} \right\} \]  

(6)

FIG. 1. In this figure we plot the approximate expression for \( Z(q) \) given by equation (15) for \( L = 16 \). \( Z(q) \) is also evaluated numerically from eqn.(10) for a lattice with \( L = 16 \) and \( T = 10 \). In order to compare both results and to obtain an analytical simple expression a Gaussian fit is performed obtaining \( \chi^2 = 1 \).

Moreover, this universal function should be non-Gaussian and has a functional dependence very close to the one corresponding to a Gumbel distribution for certain exponent \( a \), which is known in the context of extremum statistics [10]. We notice that up to the first factor, the partition function \( Z(q) \) defined by the integral (4) corresponds to the partition function of the Sine-Gordon theory with a small imaginary fugacity \( z = iq/N \). It is straightforward to see that \( Z(q) \) is the generating functional of the centered high order moments of \( P \), i.e.

\[ i^n \left[ \frac{d^n}{dq^n} Z(q) \right]_{q=0} = \langle (M - \langle M \rangle)^n \rangle \]  

(7)

Motivated by the method used to study the renormalization group flow in the Sine-Gordon model [11], we will use the Fourier representation of an exponential factor (which is also known from the high temperature -or cluster- expansion of the XY model [12]),

\[ \exp\{i\lambda \cos \phi\} = \sum_{m=-\infty}^{\infty} i^m J_m(\lambda) \exp\{i m \phi\} \]  

(8)
where $J_m(\lambda)$ are the Bessel function of integer order $m$, and the functional identity for the generating function of the Gaussian measure $d\mu_{TG}(\phi)$ \cite{13}:

$$
\int d\mu_{TG}(\phi) \exp(i \langle \phi, f \rangle) = \exp(-\frac{1}{2} \langle f, TGf \rangle),
$$

(9)
to compute analytically the integral of eqn. (5). The resulting expression for $Z(q)$, which is our main analytical result, reads

$$
Z(q) = e^{-iq(M)} \sum_{m_1, m_2, \ldots, m_N} \prod_{k=1}^{N} \left( i^{m_k} J_{m_k}(q/N) \langle M \rangle^{m_k^2} \right) \times \exp \left\{ -T \sum_{i<j} m_i m_j G(x_i - x_j) \right\}
$$

(10)

From this explicit expression for $Z(q)$ and using eqn. (7) one can compute explicitly the moments of the PDF, obtaining for instance

$$
\langle M \rangle = \exp \left\{ -\frac{T G(0)}{2} \right\}
$$

(11)

$$
\sigma = \langle M \rangle \left\{ \frac{1}{N} \sum_{z \in \Lambda} (\cosh[TG(z)] - 1) \right\}^{1/2}
$$

(12)

$$
\langle M^3 \rangle = \frac{\langle M \rangle^3}{2N^2} \sum_{x,y \in \Lambda} \left( e^{-TG(x)} \cosh \left\{ T [G(y) + G(x - y)] \right\} + e^{TG(x)} \cosh \left\{ T [G(y) - G(x - y)] \right\} \right).
$$

(13)

These expressions are exact and agree with previous results reported in \cite{4}. Higher centered moments of the PDF can be computed as well by using equations (11) and (12). The result perfectly agrees with their corresponding expressions reported for instance in Ref. \cite{5} (see eqns. (2.4) and (2.5)).

In order to obtain the analytical expression for the "universal distribution function $F^m$" one has to insert the expression for $Z(q)$ given by eqn. (10) into (3), which leads to the result

$$
F(\mu; T) = \int \frac{dQ}{2\pi} \exp(iQ\mu) Z(-Q/\sigma),
$$

(14)

where $\langle M \rangle$ and $\sigma$ are given by eqns. (11) and (12).

Now we want to study numerically the expression for the PDF deduced for the 2D HXY model as a function of the system temperature $T$ and volume $N$. From the equation (11) it follows that in the high temperature limit, the mean magnetization goes to zero. In this limit, the exponential factor of equation (10) vanishes for all values of $m_k \in Z$ except for $m_k = 0$. Therefore, in this limit equation (10) goes into

$$
Z(q)_{T \to \infty} = [J_0(q/N)]^N
$$

(15)

Moreover, for large volume the above expression for $Z(q)$ becomes Gaussian. This point can be shown analytically performing a Taylor expansion valid for small arguments of $J_0(q/N)$. Within this approximation, the mean square fluctuation of $Z(q)$ is given by $\sigma \approx \sqrt{2N}$. On the other side, $Z(q)$ can be also evaluated numerically by performing the sums appearing in eqn. (10) over the relevant configurations of $m_k$-values. Both curves are displayed in Fig.1 for a square lattice of lattice size $L = 16$ and $T = 10$. They fell onto the same curve with remarkable accuracy. Perfect agreement is found when a Gaussian distribution is fitted to $Z(q)$, with a value of $\chi^2 = 1$. Also the numerical value for $\sigma = 22.51$ agrees with the analytical expression for $\sigma$ in the high-T limit.

FIG. 2. This figure shows the inverse Fourier transform of $Z(q)$—or equivalently the PDF defined by eq. (14)—corresponding to the data appearing in figure 1.

The PDF itself can be computed both numerically and analytically in the high temperature limit. Indeed, using the approximated numerical values obtained already for $Z(q)$, we evaluate its Fourier transformation defined by the integral of Eqn. (3). One may use instead the accurate analytical Gaussian expression for $Z(q)$ found in this limit to perform analytically the integral of Eqn. (3). Both results are in perfect agreement as it is shown in figure 2 where a lattice of lattice size $L = 16$ and temperature $T = 10$ was used. The values obtained for the skewness and kurtosis, $s \approx 0$ and $c \approx 3$ respectively, perfectly agree, within only a few percent of error with their corresponding values reported in Ref. [5].

Finally, we can obtain the PDF itself in the low temperature regime using direct numerical integration. In figure 3 a numerical evaluation of the distribution for the
FIG. 3. This figure shows with a dashed line the numerical inverse fourier transform of $Z(q)$ given by eq. (14) for lattice size $L = 16$ and temperature $T = 0.7$. For comparison we plot (full line) the analytical expression reported in ref. [2], found for the roughness $1/f$ noise. The agreement between both curves is noteworthy.

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