Direct evidence of the discontinuous character of the Kosterlitz-Thouless jump

Petter Minnhagen
NORDITA, Blegdamsvej 17, DK 2100, Copenhagen, Denmark

Beom Jun Kim
Department of Molecular Science and Technology, Ajou University, Suwon 442-749, Korea
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It is numerically shown that the discontinuous character of the helicity modulus of the two-dimensional *XY* model at the Kosterlitz-Thouless (KT) transition can be directly related to a higher-order derivative of the free energy without presuming any *a priori* knowledge of the nature of the transition. It is also suggested that this higher-order derivative is of intrinsic interest in that it gives an additional characteristic of the KT transition which might be associated with a universal number akin to the universal value of the helicity modulus at the critical temperature.

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I. INTRODUCTION

The Kosterlitz-Thouless (KT) transition has attracted a steady interest since its discovery.[1,2] This is both because its unusual characteristic properties and its applicability to many systems with two-dimensional (2D) character, like, e.g., superfluid/superconducting films.[3] The critical properties are given by Kosterlitz's renormalization equations (KRE).[4] A key characteristic feature is the discontinuous universal superfluid jump to zero at the transition.[5] The generic model for the KT transition is the two-dimensional *XY* model and in this case the discontinuous jump is associated with the helicity modulus.[2,1] The 2D *XY* model has been the subject of very many computer simulations directed at verifying or disproving the various characteristics of the KT transition as given by KRE.[6,7] Although the general consensus is that the 2D *XY* model does indeed undergo a KT transition, there have also been claims from simulations that the predictions from KRE may not be entirely correct.[6,7] In particular, these earlier works have been focused on the question whether or not the divergence of the correlation length (when the transition is approached from above), is governed by an essential singularity, as predicted by KRE, or by a conventional power-law singularity. Some evidence for the latter possibility was found in Refs. 7 and 8. Alternatively, in Ref. 6 it was argued that the divergence is given by an essential singularity which is not entirely consistent with KRE. All this reflects the difficulty of verifying the precise nature of the transition through computer simulations.[9]

Similarly, it is difficult to directly verify from simulations that there is a discontinuous jump in the helicity modulus as predicted by KRE. The reason for this is illustrated in Fig. 1: Simulations can only be performed on a finite system, resulting in the helicity modulus as a continuous function without any singularity. As seen in Fig. 1 the drop at the transition gets steeper and steeper as the system size is increased. However, the size dependence is shown to be rather weak. Consequently, although numerical results like those presented in Fig. 1 for the helicity modulus are consistent with a discontinuous jump for an infinite system size, one cannot on this evidence alone, exclude the possibility that the helicity modulus remains continuous in the thermodynamic limit. The correctness of the discontinuous character of the jump has in practice only been verified from simulations in more indirect ways which make use of additional KRE predictions for the KT transition like, e.g., that the leading size dependence of the helicity modulus at the critical temperature is logarithmic.[10]

Thus one may ask if there exists a more direct way of inferring from simulations that there is a discontinuous jump, without resorting to more indirect methods which use additional KRE predictions. In this paper we show that such a more direct way does indeed exist.

Our approach is based on the calculation of a higher-order correlation function. This correlation function appears to give an additional and somewhat unexpected characteristic feature of the KT transition. We speculate that this feature

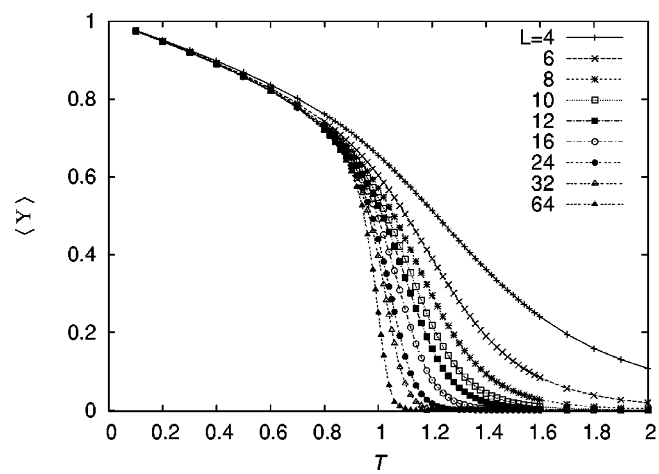

FIG. 1. Helicity modulus $\langle \Upsilon \rangle$ for the 2D *XY* model for lattice sizes $L=4$ to 64. The transition is signaled by a rapid decrease of the helicity modulus in the vicinity of $T=1$ as temperature is increased. This decrease becomes sharper with increasing L. The question is whether or not this rapid decrease develops into a discontinuous jump from a finite positive value to zero as predicted by the Kosterlitz-Thouless scenario. The data are consistent with such a scenario, but on the basis of this type of data alone one cannot rule out that the helicity modulus instead goes continuously to zero.

might be associated with a universal number akin to the universal value of the helicity modulus at the critical temperature.

II. MODEL

The 2D *XY* model on a square lattice of the size $L\times L$ is defined by the Hamiltonian

$$H=-J\sum_{\langle ij\rangle}\cos\left(\phi_{ij}\equiv\theta_i-\theta_j-\frac{1}{L}\mathbf{r}_{ij}\cdot\boldsymbol{\Delta}\right),\tag{1}$$

where J is the coupling strength (set to unity from now on), the sum is over nearest-neighbor pairs separated by the displacement $\mathbf{r}_{ij}=\hat{\mathbf{x}}$ or $\hat{\mathbf{y}}$ (we set the lattice spacing $a\equiv1$), and the phase angle θ_i ($0\leqslant\theta_i\leqslant2\pi$) at the lattice point i satisfies the periodicity $\theta_{i+L\hat{\mathbf{x}}}=\theta_{i+L\hat{\mathbf{y}}}=\theta_i$. For generality, we have also included an externally imposed global twist across the sample, $\boldsymbol{\Delta}=(\Delta_x,\Delta_y)$, defined by that the summation of the phase difference ϕ_{ij} along the x (y) direction equals Δ_x (Δ_y). The partition function Z is given by

$$Z=\prod_i\int\frac{d\theta_i}{2\pi}e^{-H/T}\tag{2}$$

and the free energy by $F(\boldsymbol{\Delta})=-T\ln Z$. The ground state corresponds to the configuration where all spins point in the same direction (i.e., all $\phi_{ij}=0$) which means that the minimum of the free energy corresponds to $\boldsymbol{\Delta}=0$. From the symmetry in the Hamiltonian, all odd-order derivatives such as $\partial F/\partial\Delta|_{\Delta=0}$ and $\partial^3F/\partial\Delta^3|_{\Delta=0}$ vanish. Accordingly, in the following we will from standard Monte Carlo (MC) simulations obtain the two first nonvanishing derivatives of the free energy with respect to $\boldsymbol{\Delta}$ at $\boldsymbol{\Delta}=0$, i.e., the second-order modulus, usually called the helicity modulus, $\langle\Upsilon\rangle\equiv\partial^2F/\partial\Delta^2|_{\Delta=0}$, and the fourth-order modulus $\langle\Upsilon_4\rangle\equiv\partial^4F/\partial\Delta^4|_{\Delta=0}$, where $\langle\cdots\rangle$ denotes the thermal average. The former (the helicity modulus) can be expressed as

$$\langle\Upsilon\rangle=\langle e\rangle-\frac{L^2}{T}\langle s^2\rangle,$$

where

$$e\equiv\frac{1}{L^2}\sum_{\langle ij\rangle_x}\cos(\theta_i-\theta_j),$$

$$s\equiv\frac{1}{L^2}\sum_{\langle ij\rangle_x}\sin(\theta_i-\theta_j),$$

and the sum is over all links in one direction. This means that $\langle e\rangle$ is the energy per link and $\langle s\rangle$ is the average current per link in one direction (here taken to be the x direction). Note that $\langle s\rangle=0$ by symmetry, in contrast to the current-current correlation $\langle s^2\rangle$ which measures the current fluctuation. The fourth-order modulus can be expressed as

$$\langle L^2\Upsilon_4\rangle=-4\langle\Upsilon\rangle+3\left[\langle e\rangle-\frac{L^2}{T}\langle(\Upsilon-\langle\Upsilon\rangle)^2\rangle\right]+\frac{2L^6}{T^3}\langle s^4\rangle.\tag{3}$$

In the following, we will measure these two correlation functions, $\langle\Upsilon\rangle$ and $\langle\Upsilon_4\rangle$, in standard MC simulations to demonstrate the existence of a discontinuous jump of the helicity modulus to zero at the phase transition.

III. STABILITY ARGUMENT

Since the global minimum of the free energy $F(\Delta)$ corresponds to zero twist, it follows that $F(0)\leqslant F(\Delta)$. To lowest orders in the Δ expansion we have

$$F(\Delta)=\langle\Upsilon\rangle\frac{\Delta^2}{2}+\langle\Upsilon_4\rangle\frac{\Delta^4}{4!}.$$

This means that $\langle\Upsilon\rangle\geqslant0$ since the lowest order nonvanishing derivative of the free energy will always dominate for small enough Δ. However, it also implies that the next order derivative $\langle\Upsilon_4\rangle$ likewise has to be $\geqslant0$ at any T where $\langle\Upsilon\rangle=0$ in the thermodynamic limit. Our argument is then the simple observation that $\langle\Upsilon\rangle$ cannot go continuously to zero at the transition temperature T_c if $\langle\Upsilon_4\rangle$ at the same time approaches a nonzero negative value at T_c. But, since $\langle\Upsilon\rangle$ is indeed zero in the high-temperature phase, this means that if $\langle\Upsilon_4\rangle$ approaches a negative value at T_c then the jump has to be discontinuous. The point is, as we will show below, that the conclusion that $\langle\Upsilon_4\rangle$ is nonzero and negative at T_c can be convincingly drawn from standard MC simulations.

IV. SIMULATION RESULTS

Our simulation of the helicity modulus for 2D model is shown in Fig. 1 up to sizes $L=64$. The conclusions which can safely be drawn by analyzing the finite-size dependence of $\langle\Upsilon\rangle$ is that it is finite in the low-temperature phase and is zero in the high-temperature phase. Since this is well established we will not discuss it further here. As mentioned in Sec. I, the difficult part from a simulation aspect is to determine *how* the helicity modulus approaches zero at T_c in the thermodynamic limit.

To this end we will use the stability argument given above and instead focus on the size dependence of the correlation function $\langle L^2\Upsilon_4\rangle$ (see Fig. 2). Figure 2(a) shows that $\langle L^2\Upsilon_4\rangle$ vanishes in the high-temperature phase and goes to a nonzero negative value in the low-temperature phase as the system size becomes larger. The interesting features is the divergent dip. This occurs in the region where the helicity modulus for finite L goes rapidly towards zero. Thus this singularity in $\langle L^2\Upsilon_4\rangle$ can safely be associated with T_c. The conclusion from Fig. 2(a) is that $\langle L^2\Upsilon_4\rangle$ diverges at T_c for $L\to\infty$, goes to zero above, and goes to a negative nonzero value below. This conclusion is further supported by the fact that the half width of the divergent dip decreases towards zero for $L\to\infty$ as illustrated in the inset of Fig. 2(a). The crucial point is now what this divergence in the correlation function $\langle L^2\Upsilon_4\rangle$ implies for $\langle\Upsilon_4\rangle$. This is shown in Fig. 2(b), which

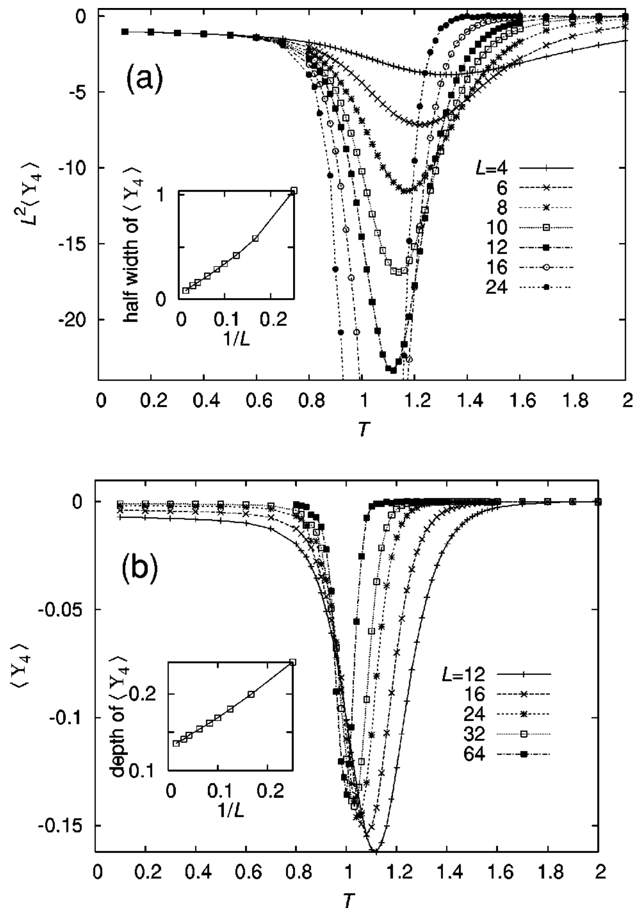

FIG. 2. (a) The correlation function $\langle L^2\Upsilon_4\rangle$. As seen this correlation function is always negative or zero. In the high-T phase it approaches zero from below. In the low-T phase it goes to finite negative values, as is apparent from the data points somewhat below $T=1$. The most interesting feature is the divergent dip in the vicinity of $T=1$. This divergence at T_c is the manifestation of the phase transition for this correlation function. The inset illustrates that the half width of the dip goes to zero for large L. (b) The fourth order modulus $\langle \Upsilon_4\rangle$ for lattices sizes $L=12$–64. As seen this modulus goes to zero both below and above T_c. However, the crucial point is that the depth of the dip remains finite, as is shown in the inset where the data are plotted against $1/L$. The linear extrapolation to $L=\infty$ gives $\langle \Upsilon_4\rangle \approx -0.130\pm 0.005$ at T_c.

gives the result for $L\geqslant 12$. The inset in Fig. 2(b) gives the depth of the dip as a function of size. As is apparent from the inset, the depth goes to a finite value in the thermodynamic limit. Linear extrapolation in $1/L$ to $L=\infty$ gives the value 0.130 ± 0.005. Thus we conclude that $\langle \Upsilon_4\rangle$ is indeed negative and nonzero precisely at T_c. Using the stability argument in Sec. III this means that the helicity modulus has to be positive and nonzero precisely at T_c. However, above T_c the helicity modulus is zero from which follows that the helicity modulus has to be discontinuous at T_c.

One may also note from Fig. 2(b) that the position of the minimum of the dip decreases towards lower T with increasing L. However, the approach towards the known value of T_c (≈ 0.89) is rather slow making a precise determination of T_c based on $\langle \Upsilon_4\rangle$ data less advantageous.

V. FINAL REMARKS

We have shown that the discontinuous character of the jump of the helicity modulus at the transition for the 2D *XY* model can be established from MC simulations of the fourth-order modulus given by Eq. (3). It seems very likely that the singularity found here for the fourth-order modulus in case of the 2D *XY* model is part of the general KT transition scenario. Thus we suggest that it sometimes may be advantageous to study the singularity of this 4th-order modulus in simulations, when trying to determine if a transition for a particular model is of KT type. It is also tempting to speculate that the finite value of $\langle \Upsilon_4\rangle \approx -0.130$ at T_c is associated with a universal number, akin to the universal value of the helicity modulus $\langle \Upsilon\rangle = 2T_c/\pi$.

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