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The two-dimensional XY model at the transition temperature: a high-precision Monte Carlo study

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Abstract

We study the classical XY (plane rotator) model at the Kosterlitz–Thouless phase transition. We simulate the model using the single-cluster algorithm on square lattices of a linear size up to $L = 2048$. We derive the finite-size behaviour of the second moment correlation length over the lattice size ξ_{2nd}/L at the transition temperature. This new prediction and the analogous one for the helicity modulus Υ are confronted with our Monte Carlo data. This way $\beta_{KT} = 1.1199$ is confirmed as inverse transition temperature. Finally, we address the puzzle of logarithmic corrections of the magnetic susceptibility χ at the transition temperature.

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1. Introduction

We study the classical XY model on the square lattice. It is characterized by the action

$$S = -\beta \sum_{x,\mu} \vec{s}_x \vec{s}_{x+\hat{\mu}}, \tag{1}$$

where $\vec{s}_x$ is a unit vector with two real components, $x = (x_1, x_2)$ labels the sites on the square lattice, where $x_1 \in \{1, 2, \ldots, L_1\}$ and $x_2 \in \{1, 2, \ldots, L_2\}$,[1] μ gives the direction on the lattice and $\hat{\mu}$ is a unit vector in the μ-direction. We consider periodic boundary conditions in both directions. The coupling constant has been set to $J = 1$ and β is the inverse temperature. In our notation, the Boltzmann factor is given by $\exp(-S)$. Sometimes, in the literature, the present model is also called the 'plane rotator model', while the name XY model is used for a model with three spin components.

Kosterlitz and Thouless [1] have argued that the XY model undergoes a phase transition of infinite order. The low-temperature phase is characterized by a vanishing-order parameter and

[1] In our simulations, we use $L_1 = L_2 = L$ throughout.

an infinite correlation length ξ, associated with a line of Gaussian fixed points. At a sufficiently high temperature, pairs of vortices unbind and start to disorder the system resulting in a finite correlation length ξ. In the neighbourhood of the transition temperature T_{KT}, it behaves as

$$\xi \simeq a \exp(bt^{-1/2}), \tag{2}$$

where $t = (T - T_{\mathrm{KT}})/T_{\mathrm{KT}}$ is the reduced temperature, and a and b are non-universal constants. In subsequent work (e.g. [2, 3]), the results of Kosterlitz and Thouless had been confirmed and the arguments had been put on a more rigorous basis.

This rather good theoretical understanding of the Kosterlitz–Thouless (KT) phase transition is contrasted by the fact that the verification of the theoretical predictions in Monte Carlo simulations had often been inconclusive or even in contradiction. Only starting from the early 1990s, Monte Carlo simulations allowed one to favour clearly the KT behaviour (2) over a power law $\xi \propto t^{-\nu}$, which is characteristic for a second-order phase transition. A typical example for such a work is [4], where the XY model with the Villain action [5] was studied on lattices of a size up to 1200^2.

The difficulties in Monte Carlo simulations might be explained by logarithmic corrections that are predicted to be present in the neighbourhood of the transition.

In the present paper, we would like to address two puzzling results presented in the literature that are related to this problem:

- The two most precise results [6, 7] for the transition temperature T_{KT} of the XY model differ by about eight times the quoted errors.
- The magnetic susceptibility is predicted to scale as $\chi \propto L^{2-\eta}(\ln L)^{-2r}$ with $\eta = 1/4$ and $r = -1/16$ at the transition temperature[2]. However, the authors of [10, 11] find in their Monte Carlo simulations $r = -0.023(10)$[3] and $r = -0.0270(10)$, respectively.

In [7, 13], the authors have shown that XY models with different actions share the universality class of the BCSOS model. This had been achieved by matching the renormalization group (RG) flow of the BCSOS model at the critical point with that of the exact duals [14] of the XY models using a particular Monte Carlo renormalization group method. As a result of this matching, the estimate $\beta_{\mathrm{KT}} = 1.1199(1) = 1/0.892\,94(8)$ for the XY model (1) has been obtained[4]. The BCSOS model is equivalent with the six-vertex model [15]. The exact result for the correlation length of the six-vertex model [16–18] shows the behaviour of equation (2) predicted by the KT theory. The main advantage of the matching approach is that the logarithmic corrections and, in particular, also subleading logarithmic corrections are the same in the XY model and the BCSOS model[5].

In a more standard approach, Olsson [6] and Schultka and Manousakis [19] have studied the finite-size behaviour of the helicity modulus arriving at the estimates $1/\beta_{\mathrm{KT}} = 0.892\,13(10)$ and $1/\beta_{\mathrm{KT}} = 0.892\,20(13)$, respectively. These authors studied lattice sizes up to $L = 256$ and $L = 400$, respectively. While in their approach leading logarithmic corrections are taken properly into account, subleading logarithmic corrections are missed. This might explain the mismatch of the results for the transition temperature. Here, we shall resolve this discrepancy by brute force: we study the helicity modulus (and, in addition, the second moment correlation length) on lattices up to $L = 2048$.

[2] Note that the analogous result $\chi \propto \xi^{2-\eta}(\ln \xi)^{-2r}$ for the thermodynamic limit in the high-temperature phase does not hold. In [8, 9], it was argued and numerically verified that instead $\chi \propto \xi^{2-\eta}(1 + c/(\ln \xi + u)^2 + \cdots)$ is correct.

[3] The authors confirmed their numerical result for r by a study of Lee–Yang zeros [12].

[4] In the case of the Villain action, the matching method gives $\beta_{\mathrm{V,KT}} = 0.7515(2)$, while the authors of [4] had found $\beta_{\mathrm{V,KT}} = 0.752(5)$ fitting their data for the correlation length with the ansatz (2) and a similar fit for the magnetic susceptibility.

[5] A brief discussion of this fact will be given in section 3.

Having an accurate estimate of T_{KT} and numerical results for large lattice sizes at hand, we then study the scaling of the magnetic susceptibility. Here, it turns out that the puzzling result for the value of the exponent r can be resolved by taking into account subleading corrections.

A major purpose of the present paper is to check the reliability of standard methods to determine the temperature of the transition and to verify its KT nature. This aims mainly at more complicated models, e.g. quantum models or thin films of three-dimensional systems with non-trivial boundary conditions, where the duality transformation is not possible, and hence the method of [7, 13] cannot be applied.

The outline of the paper is the following. In the next section, we give the definitions of the observables that are studied in this paper: the helicity modulus, the second moment correlation length and the magnetic susceptibility. Next, we summarize some results from the literature on duality and the RG flow at the KT transition. We re-derive the finite-size behaviour of the helicity modulus at the transition temperature. Along the same lines, we then derive a new result for the dimensionless ratio $\xi_{2\mathrm{nd}}/L$. This is followed by Monte Carlo simulations using the single-cluster algorithm for lattices of a linear size up to $L = 2048$ for $\beta = 1.1199$ and $\beta = 1.120\,91$. Fitting the data for $\beta = 1.1199$, we find the behaviour of the helicity modulus and $\xi_{2\mathrm{nd}}/L$ predicted by the theory for the transition temperature, while for $\beta = 1.120\,91$ there is clear mismatch. Finally, we analyse the data of the magnetic susceptibility at $\beta = 1.1199$.

2. The observables

In this section we shall summarize the definitions of the observables that we have measured in our simulations. The total magnetization is defined by

$$\vec{M} = \sum_x \vec{s}_x. \tag{3}$$

The magnetic susceptibility is then given as

$$\chi = \frac{1}{L^2}\vec{M}^2. \tag{4}$$

2.1. The second moment correlation length $\xi_{2\mathrm{nd}}$

The second moment correlation length on a lattice of the size L^2 is defined by

$$\xi_{2\mathrm{nd}} = \frac{1}{2\sin(\pi/L)}\left(\frac{\chi}{F} - 1\right)^{1/2}, \tag{5}$$

where χ is the magnetic susceptibility as defined above and

$$F = \frac{1}{L^2}\sum_{x,y}\langle\vec{s}_x\vec{s}_y\rangle\cos(2\pi(y_1 - x_1)/L). \tag{6}$$

Note that the results obtained in this paper only hold for the definition of $\xi_{2\mathrm{nd}}$ given in this subsection.

2.2. The helicity modulus Υ

The helicity modulus Υ gives the reaction of the system under a torsion [20]. To define the helicity modulus we consider a system where rotated boundary conditions in one direction are introduced: for pairs x, y of nearest-neighbour sites on the lattice with $x_1 = L_1$, $y_1 = 1$ and $x_2 = y_2$, the term $\vec{s}_x\vec{s}_y$ is replaced by

$$\vec{s}_x \cdot R_\alpha\vec{s}_y = s_x^{(1)}\big(\cos(\alpha)s_x^{(1)} + \sin(\alpha)s_x^{(2)}\big) + s_x^{(2)}\big(\cos(\alpha)s_x^{(2)} - \sin(\alpha)s_x^{(1)}\big). \tag{7}$$

The helicity modulus is then defined by the second derivative of the free energy with respect to α at $\alpha = 0$

$$\Upsilon = -\frac{L_1}{L_2} \left. \frac{\partial^2 \ln Z(\alpha)}{\partial \alpha^2} \right|_{\alpha=0} . \tag{8}$$

Note that we have skipped a factor 1/T in our definition of the helicity modulus to obtain a dimensionless quantity. It is easy to write the helicity modulus as an observable of the system at $\alpha = 0$ [21]. For $L_1 = L_2 = L$, we get

$$\Upsilon = \frac{\beta}{L^2} \langle \vec{s}_x \vec{s}_{x+\hat{1}} \rangle - \frac{\beta^2}{L^2} \left\langle \left(s_x^{(1)} s_{x+\hat{1}}^{(2)} - s_x^{(2)} s_{x+\hat{1}}^{(1)} \right)^2 \right\rangle . \tag{9}$$

3. KT theory

In this section we summarize results from the literature that are relevant for our numerical study and also derive a novel result for the finite-size behaviour of the second moment correlation length at the transition temperature.

XY models can be exactly mapped by a so-called duality transformation [14] into solid-on-solid (SOS) models. For example, the XY model with the action (1) becomes

$$Z_{XY}^{\mathrm{SOS}} = \sum_{\{h\}} \prod_{x,\mu} I_{|h_x - h_{x+\hat{\mu}}|}(\beta), \tag{10}$$

where I_n are the modified Bessel functions and h_x are integer. The XY model with Villain action [5] takes a simpler form under duality:

$$Z_{\mathrm{V}}^{\mathrm{SOS}} = \sum_{\{h\}} \exp\left(-\frac{1}{2\beta} \sum_{x,\mu} (h_x - h_{x+\hat{\mu}})^2 \right), \tag{11}$$

where h_x are integer again. This model is also called the discrete Gaussian (DG) model. In the context of finite-size scaling, one should pay attention to the fact that the boundary conditions transform non-trivially under duality. For example, periodic boundary conditions in the XY model require that in the SOS model one sums over all integer shifts h_1 and h_2 at the boundaries in the 1- and 2-direction, respectively.

It turned out to be most convenient to study the Kosterlitz–Thouless phase transition using generalizations of SOS models (see, e.g., [2, 3]).

3.1. The sine-Gordon model

The sine-Gordon model is defined by the action

$$S_{\mathrm{SG}} = \frac{1}{2\beta} \sum_{x,\mu} (\phi_x - \phi_{x+\hat{\mu}})^2 - z \sum_x \cos(2\pi \phi_x), \tag{12}$$

where the variables ϕ_x are real numbers. For positive values of z, the periodic potential favours ϕ_x close to the integers. In particular, in the limit $z \to \infty$, we recover the DG–SOS model. In the limit $z = 0$, we get the Gaussian model (or in the language of high-energy physics, a free field theory). The sine-Gordon model (using cut-off schemes different from the lattice) can be used to derive the RG flow associated with the KT phase transition. For $\beta > 2/\pi$ the coupling z is irrelevant, while for $\beta < 2/\pi$ it becomes relevant. To discuss the RG flow, it is convenient to define

$$x = \pi\beta - 2. \tag{13}$$

The flow equations are derived in the neighbourhood of $(x, z) = (0, 0)$. To leading order, they are given by

$$\frac{\partial z}{\partial t} = -xz + \cdots, \tag{14}$$

$$\frac{\partial x}{\partial t} = -\text{const}\, z^2 + \cdots, \tag{15}$$

where $t = \ln l$ is the logarithm of the length scale l at which the coupling is taken. Note that we consider a fixed lattice spacing and a running length scale l, while e.g. in [3] the cut-off scale is varied. This explains the opposite sign in the flow equations compared with e.g. [3]. The 'const' in the above equation depends on the particular type of cut-off that is used. Corrections of $O(z^3)$ have been computed in [3] and confirmed in [22]. Here, we are mainly interested in the finite-size behaviour at the transition temperature. Therefore, the trajectory at the transition temperature is of particular interest. It is characterized by the fact that it ends in $(x, z) = (0, 0)$. To leading order, it is given by

$$x = \text{const}^{1/2} z. \tag{16}$$

It follows that the RG flow on the critical trajectory is given by

$$\frac{\partial x}{\partial t} = -x^2, \tag{17}$$

i.e. on the critical trajectory

$$x = \frac{1}{\ln l + C}, \tag{18}$$

where C is an integration constant that depends on the initial value x_i of x at $l = 1$. Taking into account the next to leading order result of [3], the flow on the critical trajectory becomes

$$\frac{\partial x}{\partial t} = -x^2 - \frac{1}{2}x^3 \cdots. \tag{19}$$

Implicitly, the solution is given by [3]

$$\ln l = \frac{1}{x} - \frac{1}{x_i} - \frac{1}{2}\ln\frac{1/x + 1/2}{1/x_i + 1/2}, \tag{20}$$

where now the initial value x_i of x takes the role of the integration constant. The authors of [3] give an approximate solution of this equation that is valid for $x_i \gg x$. This leads to corrections to equation (18) that are proportional to $\ln|\ln L|/|\ln L|^2$. However, in our numerical simulations, we are rather in a situation where x_i and x differ only by a small factor. Therefore, we make no attempt to fit our data taking explicitly into account the last term of equation (20).

An important result of [3] is that corrections proportional to $\ln|\ln L|/|\ln L|^2$ arise from the RG flow in the (x, z)-plane and are not caused by some additional marginal operators, which might have different amplitudes in different models. Therefore, the two-parameter matching of [7, 13] is sufficient to take properly into account the corrections proportional to $\ln|\ln L|/|\ln L|^2$ (and beyond).

3.2. *Finite-size scaling of dimensionless quantities*

Here, we compute the values of the helicity modulus Υ and the ratio ξ_{2nd}/L at T_{KT} in the limit $L \to \infty$ and leading $1/\ln L$ corrections to it. Since for both quantities the coefficient of the order z is vanishing, this can be achieved by computing both quantities at $z = 0$ (i.e. for the Gaussian model) and plugging in the value of β given by equation (18).

3.2.1. The helicity modulus. The helicity modulus can be easily expressed in terms of the SOS model dual to the XY model:

$$\Upsilon = \frac{L_2}{L_1}\langle h_1^2\rangle_{\mathrm{SOS}}, \tag{21}$$

where h_1 is the shift at the boundary in the 1-direction. In this form, we can compute the helicity modulus in the sine-Gordon model. To this end, we have to compute the free energy as a function of the boundary shifts h_1, h_2:

$$F(h_1, h_2) = -\ln(Z(h_1, h_2)/Z(0, 0)), \tag{22}$$

where $Z(h_1, h_2)$ is the partition function of the system with a shift by h_1 and h_2 at the boundaries in the 1- and 2-direction, respectively. From the SG action (12), we directly read off that $F(h_1, h_2)$ is an even function of z. Hence, the leading z-dependent contribution is $O(z^2)$. Hence, for our purpose, the purely Gaussian result $z = 0$ is sufficient. For the action (12) at $z = 0$, we get

$$\begin{aligned} Z(h_1, h_2) &= \int \mathrm{D}[\phi]\exp\left(-\frac{1}{2\beta}\sum_{x,\mu}(\phi_x - \phi_{x+\hat{\mu}} - d_\mu)^2\right) \\ &= \int \mathrm{D}[\phi]\exp\left(-\frac{1}{2\beta}\left[L_1L_2\left(d_1^2 + d_2^2\right) + \sum_{x,\mu}(\phi_x - \phi_{x+\hat{\mu}})^2\right]\right) \\ &= \exp\left(-\frac{1}{2\beta}L_1L_2\left(d_1^2 + d_2^2\right)\right) Z(0, 0) \\ &= \exp\left(-\frac{1}{2\beta}\left[\frac{L_2}{L_1}h_1^2 + \frac{L_1}{L_2}h_2^2\right]\right) Z(0, 0), \end{aligned} \tag{23}$$

where we have defined $d_\mu = h_\mu/L_\mu$. Note that we have distributed the boundary shift along the lattice by a reparametrization of the field:

$$\phi_x = \tilde{\phi}_x + x_1 d_1 + x_2 d_2, \tag{24}$$

where $\tilde{\phi}_x$ is the original field. It follows that

$$\Upsilon = \frac{L_2}{L_1}\frac{\sum_{h_1}\exp\left(-\frac{1}{2\beta}\frac{L_2}{L_1}h_1^2\right)h_1^2}{\sum_{h_1}\exp\left(-\frac{1}{2\beta}\frac{L_2}{L_1}h_1^2\right)}. \tag{25}$$

Alternatively, we might evaluate the helicity modulus in the spin-wave limit of the XY model on the original lattice. This is justified by the duality transformation presented in [2] in appendix D. Here, we are only interested in the Gaussian limit of the model. Under duality, the β of the Gaussian model transforms as $\tilde{\beta} = 1/\beta$. Secondly, we have to take into account that even though vortices are not present in the limit $z = 0$, the periodicity of the XY model has to be taken into account for the boundary conditions. Hence, the proper spin-wave (SW) description of the XY model on a finite lattice with periodic boundary conditions is

$$Z_{\mathrm{SW}} = \sum_{n_1,n_2} W(n_1, n_2) Z(0, 0), \tag{26}$$

where n_1 and n_2 count the windings of the XY field along the 1- and 2-direction, respectively. In the Gaussian model, they are given by shifts by $2\pi n_1$ and $2\pi n_2$ at the boundaries. The corresponding weights are

$$W(n_1, n_2) = \exp\left(-\frac{(2\pi)^2}{2\tilde{\beta}}\left[\frac{L_2}{L_1}n_1^2 + \frac{L_1}{L_2}n_2^2\right]\right). \tag{27}$$

Here, we can easily introduce a rotation by the angle α at the boundary:

$$Z_{\mathrm{SW},\alpha} = \sum_{n_1,n_2} \exp\left(-\frac{(2\pi)^2}{2\tilde{\beta}}\left[\frac{L_2}{L_1}[n_1+\alpha/(2\pi)]^2 + \frac{L_1}{L_2}n_2^2\right]\right) Z(0,0). \tag{28}$$

Plugging this result into definition (8) of the helicity modulus, we get

$$\Upsilon = \frac{1}{\tilde{\beta}} - \frac{L_2}{L_1}\frac{\sum_{n_1}\exp\left(-\frac{(2\pi n_1)^2}{2\tilde{\beta}}\frac{L_2}{L_1}\right)\left[\frac{2\pi n_1}{\tilde{\beta}}\frac{L_2}{L_1}\right]^2}{\sum_{n_1}\exp\left(-\frac{(2\pi n_1)^2}{2\tilde{\beta}}\frac{L_2}{L_1}\right)}. \tag{29}$$

In the literature, often only $\Upsilon = 1/\tilde{\beta} = \beta$ is quoted and the (tiny) correction due to winding fields is ignored. We have checked numerically that the results of equations (25) and (29) indeed coincide. Here, we are interested in the case of an L^2 lattice in the neighbourhood of $\beta = 2/\pi$. One gets

$$\Upsilon_{L^2,z=0} = 0.636\,508\,178\,19\ldots + 1.001\,852\,182\ldots(\beta - 2/\pi) + \cdots. \tag{30}$$

Plugging in the result (18) and identifying the lattice size L with the scale at which the coupling is taken, we get

$$\Upsilon_{L^2,\mathrm{transition}} = 0.636\,508\,178\,19\ldots + \frac{0.318\,899\,454\ldots}{\ln L + C} + \cdots. \tag{31}$$

Contributions of $O(z^2)$ that we have ignored here are proportional to $1/(\ln L + C)^2$ at the transition.

3.2.2. The second moment correlation length. In this section we derive a result for the dimensionless ratio $\xi_{2\mathrm{nd}}/L$ analogous to equation (31) for the helicity modulus. To this end, we have to compute the XY two-point correlation function as a series in z. For the limit $L \to \infty$, the result can be found in the literature. It is important to note that similar to the helicity modulus, $O(z)$ contributions to the correlation function vanish, i.e. here also the Gaussian result is sufficient for our purpose. The non-trivial task is to take properly into account the effects of periodic boundary conditions on the finite lattice. The starting point of our calculation is the spin-wave model (26). Following definition (24), a difference of variables $\tilde{\phi}_x$ and $\tilde{\phi}_y$ of the system with shifted boundary conditions can be rewritten in terms of the system without shift:

$$\tilde{\phi}_x - \tilde{\phi}_y = \phi_x - \phi_y + p_1 n_1(x_1 - y_1) + p_2 n_2(x_2 - y_2), \tag{32}$$

with $p_i = 2\pi/L_i$. Using this results, the spin–spin product can be written as

$$\begin{aligned}\vec{s}_x\vec{s}_y &= \Re\exp(\mathrm{i}[\tilde{\phi}_x - \tilde{\phi}_y]) \\ &= \Re\exp(\mathrm{i}[\phi_x - \phi_y])\exp(\mathrm{i}[p_1 n_1(x_1 - y_1) + p_2 n_2(x_2 - y_2)]),\end{aligned} \tag{33}$$

where we have interpreted $\tilde{\phi}_x$ as the angle of the spin $\vec{s}_x$.

The expectation value in the spin-wave limit becomes

$$\langle\vec{s}_x\vec{s}_y\rangle_{\mathrm{SW}} = \frac{\sum_{n_1,n_2} W(n_1,n_2)\langle\exp(\mathrm{i}[\phi_x - \phi_y])\rangle_{0,0}\cos(p_1 n_1(x_1 - y_1) + p_2 n_2(x_2 - y_2))}{\sum_{n_1,n_2} W(n_1,n_2)}, \tag{34}$$

where $\langle\cdot\rangle_{0,0}$ denotes the expectation value in a system with vanishing boundary shift. Configurations with a winding (i.e. with a shift in $\tilde{\phi}$) give only minor contributions, e.g. $W(1,0) = 3.487\ldots \times 10^{-6}$ for an L^2 lattice at $\beta = 2/\pi$.

We have computed $\langle\exp(\mathrm{i}[\phi_x - \phi_y])\rangle_{0,0}$ numerically using the lattice propagator. To this end, we have used lattices up to $L = 2048$. For details of this calculation, see the appendix.

The results for $\langle s_x s_y \rangle$ were plugged into definition (5) of the second moment correlation length. Extrapolating the finite lattice results to $L \to \infty$ gives

$$\xi_{2nd}/L = 0.750\,6912\ldots + 0.667\,37\ldots(\beta - 2/\pi) + \cdots. \tag{35}$$

Inserting $\frac{1}{\ln L+C} = \pi(\beta - 2/\pi)$ for the critical trajectory, we obtain

$$\xi_{2nd}/L = 0.750\,6912\ldots + \frac{0.212\,430\ldots}{\ln L + C} + \cdots. \tag{36}$$

Note that a similar result for the exponential correlation length on a lattice with strip geometry, i.e. an $L \times \infty$ lattice, can be found in the literature [23]:

$$\xi_{exp}/L = 2\beta. \tag{37}$$

Inserting $\frac{1}{\ln L+C} = \pi(\beta - 2/\pi)$ into (37) gives

$$\xi_{exp}/L = \frac{4}{\pi} + \frac{2}{\pi}\frac{1}{\ln L + C} + \cdots \tag{38}$$

at the KT transition. This prediction had been compared with Monte Carlo results in [24] for lattice sizes up to $L = 64$.

It is interesting to note that the limit

$$\lim_{\xi_{exp,\infty} \to \infty} \xi_{exp}/L|_{z=L/\xi_{exp,\infty}}, \tag{39}$$

where $\xi_{exp,\infty}$ is the exponential correlation length in the infinite volume limit in the high-temperature phase, is exactly known for any $z = L/\xi_{exp,\infty}$ [25]. Note that this limit corresponds to the RG trajectory that flows out of the point $(x, z) = (0, 0)$, while the present study is concerned with the trajectory that flows into $(x, z) = (0, 0)$.

4. Monte Carlo simulations

We have simulated the XY model at $\beta = 1.1199$, which is the estimate of [7] for the inverse transition temperature, and $\beta = 1.120\,91$, which is the estimate of Olsson [6] and consistent within error bars with the result of Schultka and Manousakis [19]. For both values of β, we have simulated square lattices up to a linear lattice size of $L = 2048$. The simulations were performed with the single-cluster algorithm [26]. A measurement was performed after ten single-cluster updates. In units of these measurements, the integrated autocorrelation time of the magnetic susceptibility is less than 1 for all our simulations.

For each lattice size and β-value, we have performed 5 000 000 measurements, except for $L = 2048$ where only 2 500 000 measurements were performed. We have used our own implementation of the G05CAF random number generator of the NAG library. For each run, we have discarded at least 10 000 measurements for equilibration. Note that this is more than what is usually considered as safe. On a PC with an Athlon XP 2000+CPU, the simulation of the $L = 2048$ lattice at one value of β took about 76 days.

In table 1, we have summarized our results for the helicity modulus Υ, the second moment correlation length over the lattice size ξ_{2nd}/L and the magnetic susceptibility χ at $\beta = 1.1199$. In table 2, we give analogous results at $\beta = 1.120\,91$.

First, we fitted the helicity modulus Υ with the ansatz

$$\Upsilon = 0.636\,508\,178\,19 + \text{const}/(\ln L + C), \tag{40}$$

where 'const' and C are the free parameters of the fit. Note that $O((\ln L)^2)$ corrections that are due to e.g. the $O(z^2)$ contribution to Υ are effectively taken into account by the fit parameter

Table 1. Monte Carlo results for the helicity modulus Υ, the second moment correlation length over the lattice size ξ_{2nd}/L and the magnetic susceptibility χ for two-dimensional XY model on a square lattice of linear size L at $\beta = 1.1199$.

L	Υ	ξ_{2nd}/L	χ
16	0.725 36(7)	0.798 01(17)	133.011(9)
32	0.708 83(7)	0.792 03(18)	452.114(31)
64	0.697 85(7)	0.786 91(18)	1 536.58(11)
128	0.690 01(7)	0.783 08(18)	5 220.99(36)
256	0.684 00(7)	0.779 77(19)	17 729.9(1.2)
512	0.679 26(6)	0.777 45(18)	60 185.8(4.0)
1024	0.675 44(7)	0.775 32(19)	204 160.(15.)
2048	0.672 46(10)	0.773 00(28)	692 146.(74.)

Table 2. Same as table 1 but for $\beta = 1.120\,91$.

L	Υ	ξ_{2nd}/L	χ
16	0.726 95(7)	0.798 92(18)	133.174(10)
32	0.710 59(7)	0.792 87(18)	452.856(31)
64	0.699 82(7)	0.788 78(18)	1540.31(11)
128	0.692 25(7)	0.784 62(18)	5235.34(36)
256	0.686 29(7)	0.781 57(19)	17 794.7(1.2)
512	0.681 86(7)	0.779 51(19)	60 436.6(4.3)
1024	0.678 26(7)	0.777 33(20)	205 185.(15.)
2048	0.675 28(10)	0.775 47(28)	696 308.(75.)

Table 3. Fits of the helicity modulus at $\beta = 1.1199$ with the ansatz (40). Data with $L = L_{min}$ up to $L = 2048$ have been included into the fit.

L_{min}	const	C	χ^2/d.o.f.
64	0.2957(11)	0.668(21)	3.53
128	0.2988(17)	0.740(37)	2.67
256	0.3033(29)	0.847(67)	2.10
512	0.3097(52)	1.01(13)	1.77
1024	0.326(14)	1.43(37)	–

C. Also corrections [3] proportional to $\ln|\ln L|/(\ln L)^2$ contribute to the value of C, since $\ln|\ln L|$ varies little for the values of L that enter into the fits.

The results of the fits for $\beta = 1.1199$ are summarized in table 3 and for $\beta = 1.120\,91$ in table 4. For $\beta = 1.1199$, the χ^2/d.o.f. stays rather large even up to $L_{min} = 512$. Also the value of C is increasing steadily with increasing L_{min}. However, this is not too surprising, since corrections that are not taken into account in our ansatz decrease slowly with increasing L. However, the results for 'const' approach the theoretical prediction $0.318\,899\,454\ldots$ as L_{min} increases. For $L_{min} = 64$ and 128, the χ^2/d.o.f. for $\beta = 1.120\,91$ is much larger than for $\beta = 1.1199$. However, for $L_{min} = 256$, it becomes about $\simeq 1$ for $\beta = 1.120\,91$. This should however be seen as a coincidence, since the value of 'const' is increasing with L_{min} and already for $L_{min} = 64$ the value of 'const' is larger than the value predicted by the theory.

We conclude that our fit results are consistent with $\beta = 1.1199$ being the inverse transition temperature, while $\beta = 1.120\,91$ is clearly ruled out. One should note however that fits with

Table 4. Fits of the helicity modulus at $\beta = 1.120\,91$ with the ansatz (40). Data with $L = L_{\min}$ up to $L = 2048$ have been included into the fit.

$L_{\min}$	const	C	χ^2/d.o.f.
64	0.3382(13)	1.201(14)	16.56
128	0.3473(21)	1.399(42)	9.87
256	0.3616(36)	1.724(79)	1.03
512	0.3688(68)	1.90(16)	0.30
1024	0.377(16)	2.09(40)	–

Table 5. Fits of the second moment correlation length of the lattice size ξ_{2nd}/L at $\beta = 1.1199$ with the ansatz (41). Data with $L = L_{\min}$ up to $L = 2048$ have been included into the fit.

$L_{\min}$	const	C	χ^2/d.o.f.
64	0.2095(39)	1.62(12)	0.77
128	0.2090(58)	1.61(20)	1.02
256	0.2112(97)	1.69(36)	1.49

Table 6. Fits of the second moment correlation length over the lattice size ξ_{2nd}/L at $\beta = 1.120\,91$ with the ansatz (41). Data with $L = L_{\min}$ up to $L = 2048$ have been included into the fit.

$L_{\min}$	const	C	χ^2/d.o.f.
64	0.2451(48)	2.32(15)	1.94
128	0.2588(79)	2.79(26)	0.55
256	0.265(13)	3.01(46)	0.63

ansätze such as equation (40) are problematic, since corrections that are not included die out only very slowly as the lattice size is increased.

Next, we fitted the results for the second moment correlation length with an ansatz similar to that used for the helicity modulus

$$\xi_{2nd}/L = 0.750\,6912\ldots + \text{const}/(\ln L + C). \tag{41}$$

The results of these fits are summarized in table 5 for $\beta = 1.1199$ and in table 6 for $\beta = 1.120\,91$. In contrast to the helicity modulus, we get a small χ^2/d.o.f. already for $L_{\min} = 64$. This might be partially due to the fact that the relative statistical accuracy of ξ_{2nd}/L is less than that of the helicity modulus Υ. The result for 'const' at $\beta = 1.1199$ is quite stable as $L_{\min}$ is varied, and furthermore it is consistent with the theoretical prediction const $= 0.212\,430\ldots$ derived in this work. On the other hand, the fit results of 'const' at $\beta = 1.120\,91$ are clearly larger than the theoretical prediction, and furthermore the value of 'const' is even increasing as $L_{\min}$ is increased. These results are consistent with the analysis of the helicity modulus: while our results are consistent with $\beta = 1.1199$ being the inverse transition temperature, $\beta = 1.120\,91$ is clearly ruled out.

4.1. The magnetic susceptibility

The magnetic susceptibility at the transition temperature is predicted to behave as

$$\chi = \text{const}\, L^{2-\eta}(\ln L)^{-2r}\cdots, \tag{42}$$

Table 7. Fits of the magnetic susceptibility at $\beta = 1.1199$ with the ansatz (42). Data with $L = L_{\min}$ up to $L = 2048$ have been included into the fit.

$L_{\min}$	const	$-2r$	χ^2/d.o.f.
32	0.9611(2)	0.0699(1)	382.5
64	0.9539(3)	0.0741(2)	119.2
128	0.9485(4)	0.0772(2)	35.7
256	0.9439(6)	0.0798(3)	5.2
512	0.9412(11)	0.0812(6)	1.5

Table 8. Fits of the magnetic susceptibility at $\beta = 1.1199$ with the ansatz (44), fixing the exponent to the value $-2r = 1/8$. Data with $L = L_{\min}$ up to $L = 2048$ have been included into the fit.

$L_{\min}$	const	C	χ^2/d.o.f.
8	0.8121(1)	4.423(9)	307.2
16	0.8146(1)	4.187(11)	115.0
32	0.8170(2)	3.953(14)	32.5
64	0.8187(2)	3.786(20)	6.6
128	0.8197(3)	3.690(28)	1.5
256	0.8204(5)	3.625(43)	0.4

with $r = -1/16$ and 'const' depends on the particular model. This result can be obtained e.g. by the integration of

$$\langle s_x s_y \rangle \propto R^{-1/4} (\ln R)^{1/8} \tag{43}$$

given in [3] for the correlation function, where $R = |x - y|$. Leading corrections to equation (42) are due to the integration constant in equation (18):

$$\chi = \text{const}\, L^{2-\eta} (\ln L + C)^{-2r} \cdots. \tag{44}$$

In [10], Kenna and Irving simulated the same model as studied in this work on lattices up to $L = 256$. Using the ansatz (42), leaving r as a free parameter, they find $r = -0.023(10)$, which is about half of the value predicted by the theory. Later, Janke [11] repeated this analysis for the XY model with the Villain action and lattices up to $L = 512$. He finds, also fitting with the ansatz (42), $r = -0.0270(10)$, which is consistent with the result of Kenna and Irving.

Here, we shall check whether the value of r changes as larger lattice sizes are included into the fit. To this end, we only discuss the data for $\beta = 1.1199$. In table 7, we give results for fits with the ansatz (42), where we have taken $-2r$ as a free parameter. The χ^2/d.o.f. is very large up to $L_{\min} = 256$. For $L_{\min} = 32$, our results for $-2r$ are slightly larger than that of [10, 11]. As we increase $L_{\min}$, $-2r$ also increases. However, even for $L_{\min} = 512$, the result for $-2r$ is by more than 70 standard deviations smaller than the value predicted by the KT theory.

Next, we checked whether this apparent discrepancy can be resolved by adding the leading correction predicted by the theory as a free parameter to the fit. In table 8, we give our results for fits with the ansatz (44), where we have fixed $-2r = 1/8$. We see that already for $L_{\min} = 128$ an acceptable χ^2/d.o.f. is reached.

Finally, we performed fits with the ansatz (44), where now also $-2r$ is used as a free parameter. The results are summarized in table 9. The χ^2/d.o.f. becomes acceptable for $L_{\min}$ starting from $L_{\min} = 128$. Now the fit results for $-2r$ for $L_{\min} = 128$ and 256 are consistent within the statistical errors with the theoretical prediction.

Table 9. Fits of the magnetic susceptibility at $\beta = 1.1199$ with the ansatz (44). Data with $L = L_{\mathrm{min}}$ up to $L = 2048$ have been included into the fit.

L_{min}	const	C	$-2r$	$\chi^2/\mathrm{d.o.f.}$
32	0.685(15)	7.73(45)	0.177(6)	4.92
64	0.747(19)	5.83(55)	0.152(7)	1.97
128	0.789(26)	4.58(76)	0.136(10)	1.49
256	0.857(38)	2.5(1.1)	0.112(14)	0.01

We conclude that the apparent discrepancy with the KT theory that was observed in [10, 11] can be resolved by adding a correction term, which is predicted by the KT theory, to equation (42).

5. Summary and conclusions

We have studied the finite-size behaviour of various quantities at the Kosterlitz–Thouless transition of the two-dimensional XY model. For the helicity modulus Υ, the value at the Kosterlitz–Thouless transition in the $L \to \infty$ limit and the leading logarithmic corrections to it are exactly known. Here, we have derived the analogous result (36) for the second moment correlation length over the lattice size $\xi_{2\mathrm{nd}}/L$:

$$\xi_{2\mathrm{nd}}/L = 0.750\,6912\ldots + \frac{0.212\,430\ldots}{\ln L + C} + \cdots.$$

We have performed Monte Carlo simulations of the 2D XY model at $\beta = 1.1199$ and $\beta = 1.120\,91$, which are the estimates of the transition temperature of [7, 6], respectively. Using the single-cluster algorithm, we simulated lattices of a size up to 2048^2, which is by a factor of 5^2 larger than the lattices that had been studied in [6]. Analysing our data for the helicity modulus Υ and the ratio $\xi_{2\mathrm{nd}}/L$, we confirm $\beta = 1.1199$ as the transition temperature, while $\beta = 1.120\,91$ is clearly ruled out.

Fitting Monte Carlo data with the ansätze (40) and (41) is certainly a reasonable method to locate the transition temperature and to verify the Kosterlitz–Thouless nature of the transition. However, one should note that the large values of $\chi^2/\mathrm{d.o.f.}$ of our fits and the running of the fit parameter C with the smallest lattice size L_{min} that is included into the fits, indicate that subleading corrections that are not taken into account in the ansätze (40) and (41) are still large for the lattice sizes that we have studied. Since these corrections decay only logarithmically with the lattice size, it is difficult to estimate the systematic errors that are due to these corrections.

Finally, we studied the finite-size scaling of the magnetic susceptibility. At the transition, it should behave like $\chi \propto L^{2-\eta} \ln L^{-2r}$ with $\eta = 1/4$ and $r = -1/16$. However, fitting numerical data, the authors of [10, 11] found $r = -0.023(10)$ and $r = -0.0270(10)$, respectively. Including larger lattices into the fits, our result for r moves towards the predicted value. Extending the ansatz to $\chi \propto L^{2-\eta}(\ln L + C)^{-2r}$, where C is an additional free parameter consistent with the theory, the apparent contradiction is completely resolved: for a minimal lattice size $L_{\mathrm{min}} = 256$ that is included into the fit, we get $r = -0.056(7)$.

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Appendix. The correlation function at $z = 0$

Here, we compute the spin–spin correlation function for $z = 0$, i.e. for the spin-wave approximation, for finite lattices with periodic boundary conditions.

To this end, let us first summarize a few basic formulae on multi-dimensional Gaussian integrals as they can be found in textbooks on field theory.

Our starting point is the generating functional

$$\frac{1}{Z}\int D[\phi]\exp\left(-\frac{1}{2\beta}(\phi, A\phi) + \mathrm{i}k\phi\right) = \exp\left(-\frac{\beta}{2}(k, A^{-1}k)\right), \tag{A.1}$$

where

$$\frac{1}{2\beta}(\phi, A\phi) = \frac{1}{2\beta}\sum_{x,y} A_{xy}\phi_x\phi_y = \frac{1}{2\beta}\sum_{x,\mu}\left[(\phi_x - \phi_{x+\hat{\mu}})^2 + m^2\phi_x^2\right] \tag{A.2}$$

is the action of the Gaussian model on a square lattice and the partition function is given by

$$Z = \int D[\phi]\exp\left(-\frac{1}{2\beta}(\phi, A\phi)\right), \tag{A.3}$$

with

$$\int D[\phi] = \prod_x \int \mathrm{d}\phi_x. \tag{A.4}$$

For a square lattice with periodic boundary conditions, A^{-1} can be easily obtained using a Fourier transformation:

$$(A^{-1})_{xy} = \frac{1}{L^2}\sum_p \frac{\mathrm{e}^{\mathrm{i}p(x-y)}}{\hat{p}^2 + m^2}, \qquad \hat{p}^2 = 4 - 2\cos p_1 - 2\cos p_2, \tag{A.5}$$

where $p_i, i = 1, 2,$ are summed over the values $\{0, \ldots, L-1\}\cdot(2\pi/L)$. Here, we are interested in the massless limit $m \to 0$. Note that for $\sum_x k_x = 0$, the contributions to $(k, A^{-1}k)$ from $(p_1, p_2) = (0, 0)$ exactly cancel, while for $\sum_x k_x \neq 0$, in the limit $m \to 0$, the right-hand side of equation (A.1) vanishes due to the divergent zero-momentum contributions to $(k, A^{-1}k)$. Hence, we get

$$\lim_{m\to 0}\frac{1}{Z}\int D[\phi]\exp\left(-\frac{1}{2\beta}(\phi, A\phi) + \mathrm{i}k\phi\right) = \begin{cases}\exp\left[-\frac{1}{2}\beta(k, Ck)\right], & \text{if } \sum_x k_x = 0,\\ 0, & \text{otherwise,}\end{cases} \tag{A.6}$$

with

$$C_{xy} = \frac{1}{L^2}\sum_{p\neq 0}\frac{\mathrm{e}^{\mathrm{i}p(x-y)} - 1}{\hat{p}^2}. \tag{A.7}$$

Note that adding a constant to C_{xy} does not change the result. Here, we have chosen this constant such that $C_{xx} = 0$.

Now we are in a position to compute the two-point correlation function (34) required for the computation of the second moment correlation length (5):

$$\langle \exp(\mathrm{i}2\pi[\phi_x - \phi_y])\rangle_{00} = \exp[-4\pi^2\beta C_{xy}]. \tag{A.8}$$

Due to translational invariance, it is sufficient to compute $g(x) = C_{(0,0),x}$, for all lattice sites x. Employing the reflection symmetry of the lattice with respect to various axes, the number of sites can be further reduced by a constant factor. Still, the direct implementation of equation (A.7) would result in a computational effort $\propto V^2$ for the calculation of $\xi_{2\mathrm{nd}}$, where V is the number of lattice points. A more efficient method is discussed below.

First, we compute $g(x)$ with $x = (x_1, 0)$ for $x_1 > 0$:

$$g(x_1, 0) = \frac{1}{L^2} \sum_{p_1 \neq 0} Q(p_1)[\mathrm{e}^{\mathrm{i}p_1 x_1} - 1], \tag{A.9}$$

with

$$Q(p_1) = \sum_{p_2} \frac{1}{\hat{p}^2}, \tag{A.10}$$

i.e. these $g(x)$ can be computed with an effort proportional to V.

Next, we note that $g(x)$ satisfies Poisson's equation (see, e.g., [27] and references therein):

$$\begin{aligned} 4g(x) &- g(x-(1,0)) - g(x+(1,0)) - g(x-(0,1)) - g(x+(0,1)) \\ &= \frac{1}{L^2}\sum_{p\neq 0} \frac{\mathrm{e}^{\mathrm{i}px}(4 - \mathrm{e}^{\mathrm{i}p_1} - \mathrm{e}^{-\mathrm{i}p_1} - \mathrm{e}^{\mathrm{i}p_2} - \mathrm{e}^{-\mathrm{i}p_2})}{\hat{p}^2} = \frac{1}{L^2}\sum_{p\neq 0}\frac{\mathrm{e}^{\mathrm{i}px}\hat{p}^2}{\hat{p}^2} \\ &= \frac{1}{L^2}\sum_{p\neq 0}\mathrm{e}^{\mathrm{i}px} = \begin{cases} 1 - L^{-2}, & \text{if} \quad x = (0,0), \\ -L^{-2}, & \text{otherwise.} \end{cases} \end{aligned} \tag{A.11}$$

In principle, the remaining $g(x)$ can now be computed recursively using equation (A.11). First, one has to note that $g(x_1, 1) = g(x_1, -1)$, where we identify $L-1$ with -1, for symmetry reasons. Therefore,

$$g(x_1, 1) = \tfrac{1}{2}[4g(x_1, 0) - g(x_1 - 1, 0) - g(x_1 + 1, 0) + L^{-2}]. \tag{A.12}$$

Then, for $x_2 > 1$, one gets

$$g(x_1, x_2) = 4g(x_1, x_2 - 1) - g(x_1 - 1, x_2 - 1) - g(x_1 + 1, x_2 - 1) - g(x_1, x_2 - 2) + L^{-2}. \tag{A.13}$$

Unfortunately, rounding errors rapidly accumulate, and the recursion is useless, at least when using double-precision floating point numbers, for the lattice sizes we are aiming at.

Instead, we have used an iterative solver to solve equation (A.11). We imposed $g(x_1, 0) = g(0, x_1)$ obtained from equation (A.9) as Dirichlet boundary conditions. As a solver we have used a successive overrelaxation (SOR) algorithm. With the optimal overrelaxation parameter, the computational effort is proportional to L^3. We controlled the numerical accuracy of the solution by computing $g(x)$ from equation (A.7) for a few distances x. Since we could extract sufficiently accurate results for the limit $L \to \infty$ from lattice sizes up to $L = 2048$, we did not implement more advanced solvers such as e.g. multigrid solvers.

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