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Critical analysis of two-dimensional classical XY model

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Critical analysis of two-dimensional classical XY model

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Abstract. We consider the two-dimensional classical XY model on a square lattice in the thermodynamic limit using tensor renormalization group and precisely determine the critical temperature corresponding to the Berezinskii–Kosterlitz–Thouless (BKT) phase transition to be 0.89290(5) which is an improvement compared to earlier studies using tensor network methods.

Keywords: classical phase transitions, numerical simulations, tensor network simulations

Contents

1. Introduction

The XY model, also known as planar rotor model is one of the most widely studied and the simplest two-dimensional spin model[1] with continuous symmetry because of the interesting features it possesses and the possibility of analytical treatment using some reasonable approximations. The model has $\mathsf{U}(1)$ or $\mathsf{O}(2)$ symmetry corresponding to the rotation on a two-dimensional plane. The spins on each lattice site interact via a nearest neighbour Hamiltonian. The model has numerous practical applications in studies related to superfluid helium, thin-films, superconductivity, liquid crystals, melting of two-dimensional crystals, and dielectric plasma transition from a dielectric phase (charges bound as neutral dipoles) to the conducting phase (free charges).

The seminal work by Berezinskii and subsequently followed by Kosterlitz and Thouless elaborated on the features of this model and provided an understanding of the infinite order phase transition without any order parameter. This phase transition does not accompany any symmetry breaking and from the point of view of the Ginzburg–Landau description of phase transitions, this is a very special case. The change in the functional form of the correlation functions across the critical temperature signals the phase transition. The correlation length obeys an exponential dependence above the phase transition unlike the familiar power-law and it is infinite below the critical temperature. Any determination of the critical temperature by probing the system close to the critical temperature (i.e. T_{BKT}) is a challenging numerical problem. For temperatures below this critical value, there is a line of fixed points down to zero temperature. This is a special property that it shares for example with supersymmetric $\mathcal{N} = 4$ Yang–Mills in four dimensions. The XY model at zero temperature in the absence of an external field has all spins aligned in a particular direction corresponding to a ferromagnetic phase and shows long-range order while at high temperatures it is in a symmetric paramagnetic phase in which all the directions on the plane are equivalent for all spins.

For many years, it was common folklore that two-dimensional nearest-neighbour spin systems cannot have phase transitions but the possibility of a finite temperature phase transition inferred by extrapolation from the high-temperature expansion was pointed out by Stanley and Kaplan in [3]. This led to interesting developments eventually culminating in a series of works [4–6] after which many groups continued studying this model in great detail. Even though the two-dimensional XY model can be understood to a great extent through analytical arguments based on mean-field theory, renormalization group methods, and by maps to other models in the same universality class (such as Coulomb gas, SOS (solid-on-solid) model), the exact determination of the critical temperature on some fixed lattice remains much a numerical problem. The study of the critical behaviour of the two-dimensional XY model has now been pursued for over four decades using high-temperature expansions (HTE), Monte-Carlo (MC) numerical approach, Hamiltonian strong coupling expansion and most recently using efficient ten-

[1] The history of this model is not well established but it appears that it was first discussed by Nambu in 1950 [1] and was named XY for the first time by Lieb *et al* [2].

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sor network (TN) algorithms. However, there is no general agreement on the critical temperature corresponding to the BKT transition and the available results differ from one other by several error bars.

In the majority of these explorations, MC approach (single-flip metropolis) was applied. However, this computational approach is prone to critical slowing down around the critical temperature and makes it highly inefficient. Several improved algorithms such as cluster algorithms[2] where a group of spins is updated at once were then formulated and was then used with parallel computations to locate the phase transition on large systems close to the thermodynamic limit. Though until a few decades ago, the most preferred tool to study lower-dimensional ($d \leqslant 2$) statistical systems were large-scale MC simulations, this is now giving way to TN techniques with two such studies already existing in the literature [7, 8] for the model we consider in this work. The reason of this paradigm shift is clear—in the last decade many efficient real-space TN algorithms have been developed which have enabled studies of the critical and off-critical statistical systems in the thermodynamic limit by carefully exploiting the interesting region of the otherwise huge Hilbert Space. In the TN description, the physical properties of the system is encoded in the local tensors and by performing the coarse-graining sufficiently many times, we can understand the global properties in a more intuitive way. TN have also been used to study spin-foam models in quantum gravity in various dimensions. They are also starting to play a crucial role in studying real-time path integrals which are otherwise impossible to study using MC because of highly oscillatory form of integrals for which the importance sampling method fails. The TN have also been useful in understanding some aspects of holography and understanding the connections between the many-body systems and gravity. For a review on TN and its various applications, see [9]. It is now also becoming evident that these methods can also be used to study gauge theories and some works along this direction are [10–14] [3].

In this paper, we take a step in this direction by applying a real-space coarse-graining algorithm and systematically determining the critical temperature for the topological transition in the XY model. By keeping a bigger fraction of the local space than achieved before, we have considerably improved on the earlier works. This resulted in our numerical estimate as being the most precise achieved to date using any TN approach. It also agrees with the most precise available MC result [15]. We introduce a small external magnetic field that breaks the $\mathsf{O}(2)$ symmetry to determine the critical temperatures at small field strengths by looking at the response of the network to the field by computing the magnetization and susceptibility. We now briefly outline the structure of the paper. In section 2, we discuss the phase transition and lack of ordering in two dimensions and explain the tensor construction of the model before discussing the observables we study. In section 3, we present the results for the free energy, magnetization, and determine the critical temperature from the peak of the susceptibility. We put down some numerical details in the appendix A for the convenience of the reader.

[2] For example, these include the Swendsen–Wang, Wolff, and embedded cluster algorithms.

[3] It is impossible to list the extended literature along these lines and we apologize in advance for all omissions.

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2. Phase transition, tensor construction, and observables

In two dimensions, a no-go theorem due to Mermin–Wagner–Hohenberg–Coleman (MWHC) states that it is not possible to have an ordered phase (long-range order)[4] which implies that there is no possibility of a phase transition from a disordered to an ordered phase accompanied by spontaneous symmetry breaking at any finite temperature. In high energy theory language, this is usually expressed as—there are no Goldstone bosons in two dimensions. The absence (or destruction) of long-range order is due to the strong low-energy fluctuations. Since there is no long-range order, there is no true order parameter. However, there does exist a well-known phase transition where in the absence of an order parameter, the task of classification of the phases depends on the behaviour of the correlation function. In the low-temperature phase of the XY model, there is a quasi-long-range order (QLRO) phase and we have:

$$\langle \mathbf{S}(\mathbf{r}) \cdot \mathbf{S}(0) \rangle \sim \mathrm{e}^{-\eta \ln r} = \frac{1}{r^{\eta}}, \tag{1}$$

while in the high-temperature disordered phase, we have:

$$\langle \mathbf{S}(\mathbf{r}) \cdot \mathbf{S}(0) \rangle \sim \mathrm{e}^{-r/\xi}, \tag{2}$$

where $\mathbf{S}(\mathbf{r})$ is a planar spin of magnitude one on site $\mathbf{r} = (x, y)$ of a square lattice, ξ is the correlation length and the exponent $\eta = T/(2\pi J)$ [5] is proportional to the temperature and is equal to its maximum value of $1/4$ at T_{BKT}. This power-law behaviour is not just at critical point but for all temperatures less than T_{BKT}. The QLRO is destroyed by unbinding of the vortex and anti-vortex pair at some critical temperature T_{BKT}, which is now well-known as the Berezinskii–Kosterlitz–Thouless (BKT) transition. This transition has a topological character associated with the proliferation of vortices. The BKT transition is a very special case of bypassing the MWHC theorem which rests on the fact that for temperatures $T < T_{\mathrm{BKT}}$, the algebraic ('power-law') decay of correlations functions means that there is *no* long range order *but* only QLRO where topological excitations/defects (vortex and anti-vortex with opposite topological charges) are bound together. At $T > T_{\mathrm{BKT}}$, defects unbind and starts to grow rapidly and results in exponential decay (also referred to as 'screening') given by:

$$\xi = \begin{cases} \sim \exp\left[\dfrac{-\mathrm{C}}{\sqrt{\tau}}\right], & T > T_{\mathrm{BKT}} \\ \infty, & T < T_{\mathrm{BKT}} \end{cases}, \tag{3}$$

where $\tau = (T - T_{\mathrm{BKT}})/T_{\mathrm{BKT}}$ and C is a positive constant. We now consider a square lattice with a spin on each lattice site $\mathbf{S}_i$. The Hamiltonian of the XY model is given

[4] We mean the absence of long-range order in the sense explained by Polyakov in [16]. If one considers a large but finite system and fixes the value of $\vec{S}$ at the boundary to be 1, the average value of $\langle \vec{S} \rangle$ inside the system vanishes as system size goes to infinity. This is equivalent to the fact that the angular deviation between spins increases with r i.e. $\langle (\theta(r) - \theta(0))^2 \rangle \sim \log(r)$.

[5] The was first noted down by Peierls and Landau in 1935 and 1937 respectively.

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by:

$$\mathcal{H} = -J\sum_{\langle ij\rangle}\cos(\theta_i - \theta_j) - h\sum_i \cos\ \theta_i, \tag{4}$$

where $\langle ij\rangle$ denotes the summation over the nearest neighbouring sites i and j, θ_i is the spin angle at site i, and we have set the modulus $|\mathbf{S}_i| = 1$ with J being the exchange coupling between the nearest neighbour spins, and h the applied external magnetic field. We will set $J = 1$ in what follows while the Boltzmann's constant, k_{B}, has already been set to 1. The Hamiltonian (4) with $h = 0$ has global $\mathsf{U}(1)$ symmetry: $\theta_i \to \theta_i + c$ which amounts to changing the angle by same amount at each lattice site and also has periodicity i.e. $\theta_i \to \theta_i + 2\pi n_i$. We can write the partition function of the model as:

$$Z = \frac{1}{2\pi}\int \prod_i \mathrm{d}\theta_i\ \exp\left(\beta\sum_{\langle ij\rangle}\cos(\theta_i - \theta_j) + \beta h\sum_i \cos\ \theta_i\right), \tag{5}$$

where $\beta = 1/T$ is the reciprocal of temperature and angles vary continuously in the interval $[0, 2\pi)$.[6] In order to construct the tensor representation, we decompose the Boltzmann factor (for $h = 0$) in a basis (also known as Jacobi–Anger expansion) as follows:

$$\exp\left(\beta\ \cos(\theta_i - \theta_j)\right) = I_0(\beta) + \sum_{\nu=-\infty,\neq 0}^{\infty} I_\nu(\beta)\mathrm{e}^{\mathrm{i}\nu(\theta_i-\theta_j)}, \tag{6}$$

where $I_\nu(\beta)$ is the modified Bessel function of the first kind. The partition function can then be written as [17]:

$$Z = \int \prod_i \mathrm{d}\theta_i \prod_{\nu_{ij},\mu_i} I_{\nu_{ij}}(\beta) I_{\mu_i}(\beta h)\mathrm{e}^{\mathrm{i}\nu_{ij}(\theta_i-\theta_j)+\mathrm{i}\mu_i\theta_i}. \tag{7}$$

By performing integration over the physical angular degrees of freedom θ_i, we proceed to define a tensor (dual) as:

$$\mathtt{T}_{\mathtt{ijkl}} = \mathtt{T}_{\mathtt{i,j,k,l}} = \sqrt{I_i(\beta)I_j(\beta)I_k(\beta)I_l(\beta)}\ \overbrace{I_{i+k-j-l}(\beta h)}^{\text{for } h=0,\text{ this enforces } \delta_{j+l}^{i+k}}, \tag{8}$$

where indices (i, j, k, l) denote the four legs of the tensor[7] and run from $-\infty, \cdots, \infty$. The size of each leg, which is infinite in principle from the expansion formula in (6) is truncated down to run only in range $[\lceil -\chi/2\rceil, \cdots, \lfloor\chi/2\rfloor]$, where we refer to χ as bond dimension. The reason this truncation is reasonable is that the series expansion coefficient $I_\nu(\beta)$ decreases quickly with increasing ν for all β considered in this work. Thus, we can truncate the series and approximate $\mathtt{T}_{\mathtt{ijkl}}$ by a tensor with finite bond dimension with relatively high precision. However, the errors due to this truncation can

[6] The model where this interval is split in Q-intervals is known as the Q-state Potts model which for $Q \to \infty$ is the XY model.
[7] We always use the order: left, right, up, down to denote a rank-four tensor in this work.

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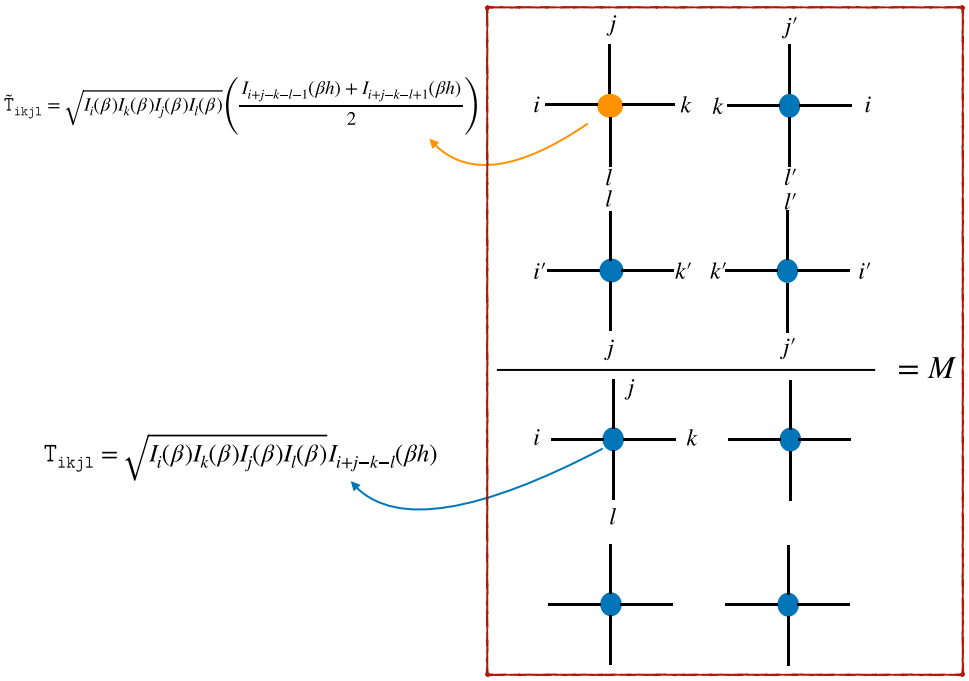

Figure 1. The 'observable' (sometimes also called 'impure') tensor shown in orange is inserted in place of one of the usual (blue) tensors. We then evaluate magnetization by dividing the contraction of the network in the numerator and the denominator. The contraction is over the same index label and the ordering and label of indices in the denominator is the same as in the numerator.

depend strongly on the temperature and the external field h as we will see later. This leads to a finite-dimensional tensor representation for the partition function:

$$Z = \mathbf{t}\ \mathbf{Tr}\left(\prod \mathtt{T}_{\mathtt{ijkl}}\right), \tag{9}$$

where $\mathbf{t}\ \mathbf{Tr}$ denotes the tensor trace and product is over all sites. It is well-known that in absence of magnetic field, the magnetization i.e. $M = \langle \vec{S}_i^x \rangle = \cos(\theta(\mathbf{r}))$ is zero in $d = 2$ for all non-zero temperatures. The average magnetization in presence of external field is evaluated as:

$$M = \frac{-\partial F}{\partial h} = \frac{1}{\beta}\frac{\partial\ \ln\ Z}{\partial h} = \mathbf{t}\ \mathbf{Tr}\left(\sqrt{I_i(\beta)I_j(\beta)I_k(\beta)I_l(\beta)}\,\frac{I_{i+k-j-l-1}(\beta h) + I_{i+k-j-l+1}(\beta h)}{2}\right). \tag{10}$$

Since the system has translational invariance, the average magnetization is the same for all spins. In principle, one can evaluate the magnetization by taking the numerical derivative of the logarithm of the partition function with respect to external field as in (10), but, this method is prone to errors and is not suited for determining the critical temperature. We evaluate the magnetization by inserting an additional

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tensor in the TN as described in detail in figure 1. The response function of the system when the external field is turned on is given by magnetic susceptibility defined as:

$$\mathbb{S} = \left.\frac{\partial M}{\partial h}\right|_T. \tag{11}$$

3. Results and conclusion

We use higher-order tensor renormalization group (HOTRG) [18] using periodic boundary conditions to study this model. This real-space coarse-graining scheme has been very useful in studying quantum and classical statistical systems in various dimensions [19, 20]. Instead of coarse-graining along a constant time-slice and then constructing the transfer matrix, we have used simultaneous coarse-graining along `x` and `y` direction. We then use the singular value decomposition (SVD) to truncate the tensor back to the original size while introducing a small error in the description of the system. This truncation becomes severe with decreasing h. We first calculate the free energy (using 12) and show the its variation with temperature for different external magnetic field h in figure 2. Unlike in the Monte Carlo simulations, the free energy (or density) is the simplest quantity to measure in the TN formulation. We checked that the free energy at $T = 1.0$ is the same up to an error of 10^{-4} whether $(N_x N_y, \chi)$ is $(2^{60}, 47)$ or $(2^{16}, 25)$.[8] One important feature of the phase transition in this system is that all derivatives of the free energy are zero as $T \to T_{\text{critical}}$ and there is no way of locating the transition by looking at any of its derivatives since there are no discontinuities at the critical temperature. This makes this system an exception to the usual Landau–Ginzburg paradigm. They belong to the class of topological phase transitions that are not characterized by a Landau order parameter. Our determination of the critical temperature was done by looking at $\mathbb{S}$ for different h and then taking the $\lim_{h\to 0}$ of the critical temperature using an ansatz (see appendix A). In an external magnetic field h, the magnetization behaves like $M \sim h^{\frac{1}{\delta}}$ at the critical temperature and the critical exponent describing the response to the field i.e. δ is given by $\delta = (d + 2 - \eta)/(d - 2 + \eta) = 15$. We evaluate the magnetization for various h in the thermodynamic limit (lattice of size $2^{50} \times 2^{50}$) and show a small subset of those measurements in figure 3. In order to determine the critical temperature, we find out the temperature corresponding to the peak of susceptibility for different field strengths as shown in figure 4. We then extrapolate our numerical data and find $T_{\text{critical}} = 0.89290(5)$ in the limit of vanishing field shown in figure 5. In order to precisely determine the critical temperature, it was essential to go to very small values of the external field which in turn was strongly dependent on the choice of χ. We initially started with $\chi = 41$ and found that it was not possible to explore less than $h \approx 10^{-7}$ while accurately determining the peak of susceptibility. We believe it was fortuitous that this bond dimension (χ) was sufficient to determine the critical temperature reasonably well and critical exponent to a within few percent of

[8] $N_x N_y$ denotes the number of sites along the `x` and `y` direction respectively. One of these is about 200 times faster than the other even without worrying about the memory.

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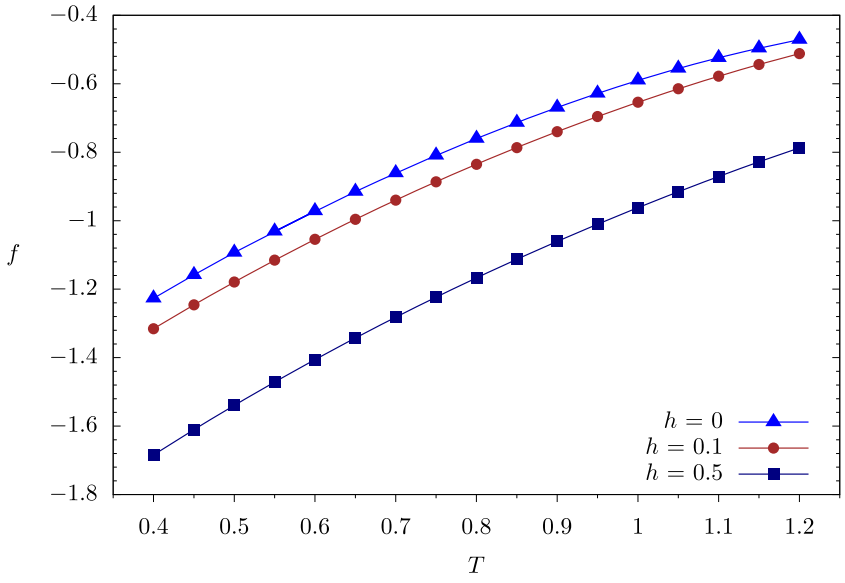

Figure 2. Free energy against temperature for different values of magnetic field. The system size is $2^8 \times 2^8$ and $\chi = 25$.

accuracy in [7]. For instance, even with $\chi = 53$, we could not precisely determine the critical exponent, δ, but certainly been able to reduce few orders of magnitude of error on the previous estimate of T_{critical}. As compared to earlier work, we kept almost double the number of states at each coarse-graining step because of using a slightly improved version of HOTRG and memory available. These extra states were crucial to explore much smaller magnetic fields down to $h = 10^{-15}$ compared to approximately $h = 10^{-7}$ in [7]. For instance, in [7], the critical temperature for $h = 1.5 \times 10^{-7}$ was found to be $T = 0.9172$ while we found $T = 0.9215(3)$. This is a clear sign that increasing χ on basically similar lattice size still helps the precision as one probes lower temperature and goes to zero field limit.

We now briefly mention some earlier works locating the critical temperature for this model (see table 1 for the list). Very recently, using uniform MPS and a well-defined method of extracting correlation length for discrete system as given in [27], this model was studied in [8] and $T_{\text{critical}} = 0.8930(1)$ was found. This was an improvement over the old work using TN which found $T_{\text{critical}} = 0.8921(19)$ [7]. This model was also studied in [15] using 256 GPUs on a 65 536$(= 2^{16}) \times 65\,536$ lattice using Monte Carlo. Some earlier studies differ significantly from our estimate and we guess that it might be because the lattice is too small. It was shown in [8] that already around $T = 0.95$, the correlation length can be more than a thousand sites. We note that among all these, the numerical study using Monte Carlo on the largest lattice is indeed also the most precise estimate to date which we have been able to match using TN in this work. Though the procedure in this paper is similar in spirit to the one in [7], we have been able to refine the results in that paper by going to a large bond dimension. For instance, for $h \sim 1.5 \times 10^{-4}$, the peak appears at $T = 0.98$ in the earlier work while we found that the

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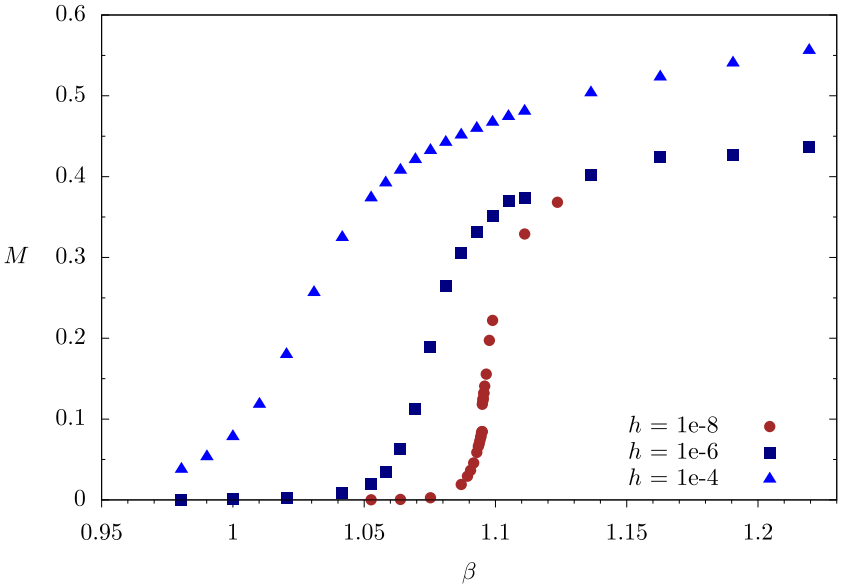

Figure 3. The dependence of magnetization on inverse temperature for different h.

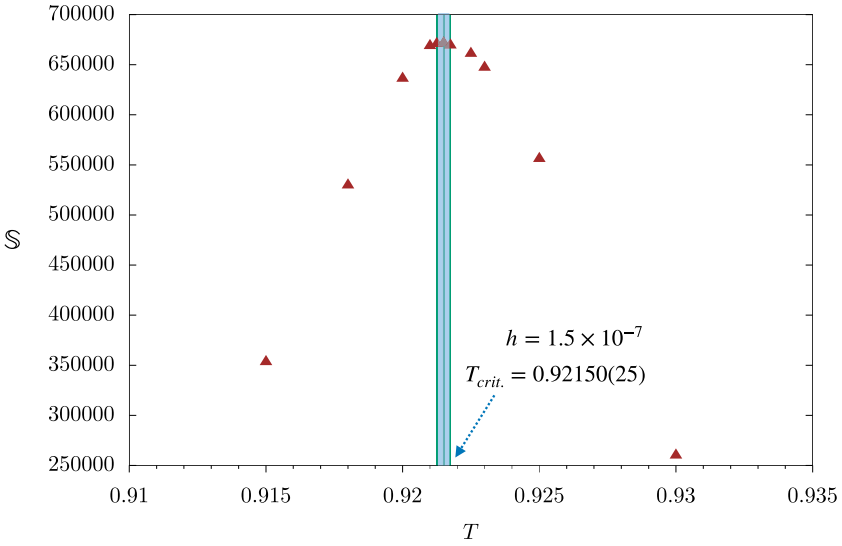

Figure 4. A representative example of the determination of the critical temperature for a given magnetic field. The vertical shaded band denotes the error in the estimate of the critical temperature.

peak is at $T = 0.9810(5)$. A more prominent difference is observed for $h \sim 1.5 \times 10^{-7}$, where earlier study found $T = 0.9172$ while we deduced $T = 0.9215(3)$.

In this work, the estimate of the critical temperature is the most precise that has yet been achieved using any TN approach and are level with precision from Monte Carlo methods. In the preliminary stages, we also implemented the tensor network renormalization (TNR) [28] algorithm which removes the short-range entanglement by

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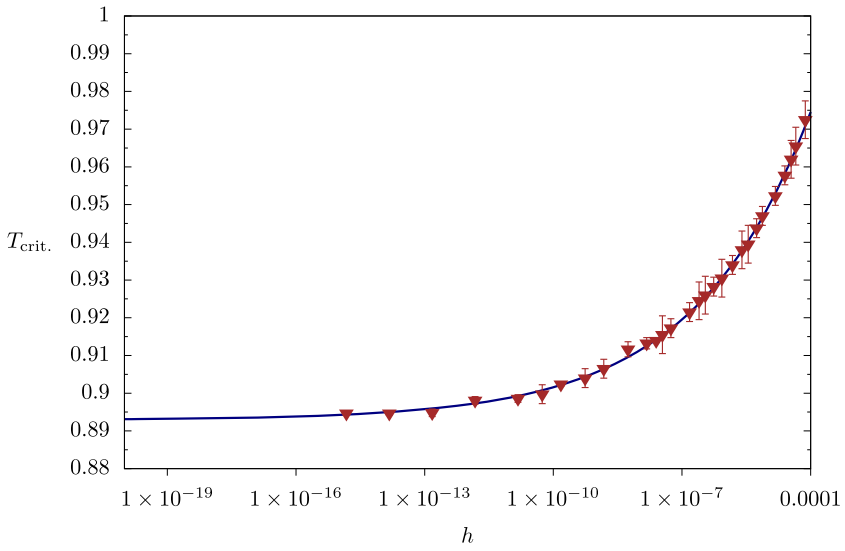

Figure 5. The dependence of critical temperature on external magnetic field h. We fit the data to the ansatz and obtain $\lim_{h\to 0} T_{\text{crit.}} =$ `0.89290(5)`. The errors have been scaled by a factor of 10 for visibility on the plot and determined as in figure 4. The data is for square lattice of size $2^{50} \times 2^{50}$ with $\chi_{\text{max.}} = 53$.

Table 1. The estimate of the temperature for the BKT transition in classical XY model with different methods. The three most recent estimates have all been done using real-space renormalization with TN.

Method	Year	System size	T_{critical}	
Monte Carlo [21]	1992	$2^9 \times 2^9$	`0.89400(500)`	
HTE [22]	1993	—	`0.89440(250)`	
Monte Carlo [23]	1995	$2^8 \times 2^8$	`0.89213(10)`	
Monte Carlo [24]	2005	$2^{11} \times 2^{11}$	`0.89294(8)`	
HTE [25]	2011	—	`0.89286(8)`	
Monte Carlo [15]	2012	$2^{16} \times 2^{16}$	`0.89289(5)`	
Monte Carlo [26]	2013	$2^9 \times 2^9$	`0.89350(10)`	
Higher-order TRG [7]	2013	$2^{40} \times 2^{40}$	`0.89210(190)`	TN
Uniform MPS [8]	2019	—	`0.89300(10)`	
Higher-order TRG [this work]	2020	$2^{50} \times 2^{50}$	`0.89290(5)`	

using disentanglers and makes the study at and near criticality more efficient compared to the other standard numerical RG approaches. We found that while the results for free energy and magnetization obtained using TNR are consistent with HOTRG, the complexity and the scaling of the TNR code was less encouraging. However, we believe that a systematic large-scale study of this model using efficient disentangling algorithms might be able to further improve on the errors we have reported

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here and extract the critical exponents precisely but it would be challenging. In the future, it will be interesting to explore phase transitions in *frustated* XY model and other spin models such as J-Q model exhibiting continuous symmetry using these methods.

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Appendix A. Numerical details

In this appendix, we elaborate on some numerical details and steps to determine the critical temperature. We normalize the tensor $\mathtt{T}_\nu$ at each coarse-graining step (denoted by ν) by the maximum element of the tensor having a total of χ^4 elements which can be implemented in Python using NumPy library as $\mathtt{norm}_\nu = \mathtt{numpy.max}(\mathtt{T}_\nu)$. We can then calculate the free energy density (f) from these normalization factors, see for instance [29]:

$$f = -\frac{1}{\beta}\left(\sum_{\nu=0}^{N}\frac{\log(\mathtt{norm}_\nu)}{4^\nu} + \frac{\log(Z_N)}{4^N}\right) = -\frac{1}{\beta 4^N}\left(\sum_{\nu=0}^{N}\log(\mathtt{norm}_\nu)4^{N-\nu} + \log\ Z_N\right), \tag{12}$$

where $Z_N = \mathbf{t}\,\mathbf{Tr}(\mathtt{T}_\mathtt{N})$ is calculated from the tensor contraction after the last step of CG and 4^N is the lattice volume and N is the number of times we do coarse-graining along $\mathtt{x}+\mathtt{y}$ direction. To compute expectation values, one needs to insert the appropriate 'observable' tensor in the network. By inserting $\tilde{\mathtt{T}}$, which is just the derivative of $\mathtt{T}$ with respect to h, we evaluated the magnetization for a range of magnetic fields at various temperatures. The tensor, $\tilde{\mathtt{T}}_\nu$, is normalized by $\mathtt{norm}_\nu$ as well and is calculated as $M = \frac{\mathrm{tTr}(\tilde{\mathtt{T}}_\nu)}{\mathrm{tTr}(\mathtt{T}_\nu)}$ at each step. The diagram representing this contraction is shown in figure 1. Though the free energy density converges rather quickly, we really need to work in the thermodynamic limit with as large χ as possible to precisely evaluate magnetization. In order to compute the magnetization for $\mathtt{10}^{-15} \leqslant h < \mathtt{10}^{-9}$, we used single-precision float ($\mathtt{np.float32}$) rather than the default double precision. This enabled us to go up to $\chi = \mathtt{53}$ compared to $\chi = \mathtt{47}$ for $h \geqslant \mathtt{10}^{-9}$. Once the magnetization M is computed for different h, we evaluate $\Delta M/\Delta h|_{T,h_{\mathrm{mid}}}$ and plot it against temperature and determine the critical temperature corresponding to the peak of the susceptibility. The data for

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the determination of critical temperature for various h can be found at [30]. We used Python's `curve_fit` which uses Levenberg–Marquardt algorithm and fit our data to the ansatz: $T_c = T_{c,h=0} + ah^b$, with a and b as two fitting parameters. The result of the fit is:

$$T_{c,h=0} = 0.89290(5), \mathtt{a} = 0.364(2), \text{and } \mathtt{b} = 0.162(1),$$

and is shown by the solid line in figure 5.

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