Hybrid Berezinskii-Kosterlitz-Thouless and Ising topological phase transition in the generalized two-dimensional XY model using tensor networks

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In tensor network representation, the partition function of a generalized two-dimensional XY spin model with topological integer and half-integer vortex excitations is mapped to a tensor product of one-dimensional quantum transfer operator, whose eigen-equation can be solved by an algorithm of variational uniform matrix product states. Using the singularities of the entanglement entropy, we accurately determine the complete phase diagram of this model. Both the integer vortex-antivortex binding and half-integer vortex-antivortex binding phases are separated from the disordered phase by the usual Berezinskii-Kosterlitz-Thouless (BKT) transitions, while a continuous topological phase transition exists between two different vortex binding phases, exhibiting a logarithmic divergence of the specific heat and exponential divergence of the spin correlation length. A new hybrid BKT and Ising universality class of topological phase transition is thus established. We further prove that three phase transition lines meet at a multi-critical point, from which a deconfinement crossover line extends into the disordered phase.

Introduction. - It is well-known that topological vortices/defects govern the critical behavior and produce rich physics in two dimensional (2D) systems. One prominent example is the Berezinskii-Kosterlitz-Thouless (BKT) phase transition\cite{1,2}, which is associated with the binding of integer vortices and antivortices in pairs with quasi-long-range order. Such a transition cannot be characterized by spontaneous symmetry breaking with local order parameter and constitutes the first example of topological phase transitions beyond the Landau paradigm. A prototype model exhibiting these fascinating features is given by the 2D classical XY spin model, which can be realized in superfluid helium films\cite{3,6} and 2D superconductor films/arrays\cite{4,6}. When an extra spin-nematic interaction with $\pi$ period is introduced, the generalized XY model contains both integer vortices and half-integer vortices along with their associated topological strings\cite{7,8}. Although great efforts have been devoted to establish a complete phase diagram\cite{9,11}, there are still some standing puzzles: what is the nature of the phase transition between the integer vortex binding and half-integer vortex binding phases\cite{8,10}, how does this transition line merge into two BKT transition lines\cite{11} and is there a deconfinement transition in the disordered phase\cite{12}? However, the accurate determination of the transition lines and the possible multi-critical point remain a great challenge.

Recently, tensor network method has become a powerful theoretical tool to characterize correlated quantum many-body phases in the thermodynamic limit\cite{13,14}. Since the partition function of a 2D classical statistical model can be represented as a tensor product of 1D quantum transfer operator\cite{15}, the eigen-equation of this transfer operator can be solved by the variational uniform matrix product state (VUMPS) algorithm\cite{16,18}, and all thermodynamic properties are thus accurately obtained. In this scheme, the critical temperature of the BKT transition in the usual 2D XY model is estimated with high precision and the exponential divergence of the spin correlation length is confirmed\cite{19}. Therefore, it becomes possible to apply the tensor network approach to resolve those puzzles about the generalized XY spin model, shedding new light on the nature of the topological phase transition between two different vortex binding phases.

In this paper, we carry out such tensor network calculations for the generalized 2D XY spin model, and accurately determine the topological phase transitions using the singularities in the entanglement entropy associated to the 1D quantum transfer operator. The complete phase diagram of the generalized XY model is thus obtained. In particular, we show that a continuous phase transition occurs between two different vortex binding phases, where the logarithmic divergence of the specific heat of the 2D Ising transition and the exponential divergence of the spin correlation length of the BKT transition display simultaneously, establishing a new hybrid BKT and Ising universality class. From the analysis of the entanglement spectrum, a deconfinement crossover line is found in the disordered phase, separating the region with dominant integer vortex excitations from the dominant half-integer vortex region.

Model and Method. - The generalized XY spin model on a 2D square lattice is given by

\begin{equation}
H = -J \sum_{\langle ij \rangle} \left[ \Delta \cos (\theta_i - \theta_j) + (1 - \Delta) \cos (2\theta_i - 2\theta_j) \right],
\end{equation}

where $\theta_i \in [0, 2\pi]$ denotes the spin orientation at the lattice site $i$ and the summation runs over all nearest-neighbour sites. $\Delta = 1$ corresponds to the usual XY spin model with integer vortex excitations, while $\Delta = 0$
The partition function is written as

$$Z = \prod_i \int \frac{d\theta_i}{2\pi} \prod_{\langle i,j \rangle} e^{\beta[\Delta \cos(\theta_i - \theta_j) + (1 - \Delta) \cos 2(\theta_i - \theta_j)]},$$

(2)

where the temperature $T$ is in the unit $J/k_B$. To find its tensor network representation, we take a duality transformation, which changes the phase variables into number indices on the links. Such a transformation is obtained by the character expansion for the Boltzmann factor $e^{x \cos \theta} = \sum_{n=-\infty}^{\infty} I_n(x) e^{i n \theta}$, where $I_n(x)$ are the modified Bessel functions of the first kind. Then the partition function is written as

$$Z = \prod_s \int \frac{d\theta_s}{2\pi} \prod_{l \in \mathcal{L}} \sum_{n_1} a_n(\beta, \Delta) e^{i n (\theta_s - \theta_j)} = \prod_s \int \frac{d\theta_s}{2\pi} \prod_{l \in \mathcal{L}} a_n(\beta, \Delta) e^{i n (\theta_s - \theta_j)},$$

(3)

where $a_n(\beta, \Delta) = \sum_{m=-\infty}^{\infty} I_{n-2m}(\beta \Delta) I_m(\beta(1 - \Delta))$, $l$ runs over all the links and $s$ labels all the lattice sites. By integrating out the physical degrees of freedom $\theta$, the partition function is represented as a tensor network

$$Z = t \text{Tr} \prod_s O_{n_1,n_2}^{n_3,n_4}(s),$$

(4)

where $t \text{Tr}$ denotes the tensor contraction and each local tensor is given by $O_{n_1,n_2}^{n_3,n_4} = \left( \prod_{i=1}^4 a_n(\beta, \Delta) \right)^{1/2} \delta_{n_1+n_2}^{n_3+n_4}$.

The partition function is shown in Fig. 1(a). Actually the continuous symmetry of the model has been encoded in the tensor-network representation: $O_{n_1,n_2}^{n_3,n_4} \neq 0$ only if $n_1 + n_2 - n_3 - n_4 = 0$, i.e., the conservation law of $U(1)$ charges. Since the expansion coefficients decrease exponentially with increasing $n$, an appropriate truncation can be performed on the virtual legs of the tensor $O$ without loss of accuracy.

The fundamental object in the tensor-network partition function is the row-to-row quantum transfer operator,

$$T(\beta, \Delta) = \sum_{s,p,q,...} \text{Tr} \left( \cdots O_{n_1}^{s}(s) O_{n_2}^{p}(p) O_{n_3}^{q}(q) \cdots \right),$$

(5)

where $s, p, q, \ldots$ refer to the lattice sites in a row. This operator plays the same role as the matrix product operator (MPO) for quantum spin chains[15]. Then the partition function is determined by the dominant eigenvalues of $T(\beta, \Delta)$. For a translational invariant MPO, the leading eigenvector as the fixed-point of $T(\beta, \Delta)$ can be represented by a uniform matrix product states (uMPS) [16]

$$|\Psi(A)\rangle = \sum_{\cdots \delta_{\beta \theta \cdots}} \text{Tr} \left( \cdots A_n^{n_1} A_{n_2}^{p} A_{n_3}^{q} \cdots \right),$$

(6)

where $A_n^{n_1}$ is a three-leg tensor with bond dimension $D$, controlling the accuracy of this approximation. Since the transfer operator $T(\beta, \Delta)$ is hermitian, the eigenvalue as shown in Fig. 1 (b)

$$\text{max}_A \langle \Psi(A)|T(\beta, \Delta)|\Psi(A)\rangle / \langle \Psi(A)|\Psi(A)\rangle,$$

can be transformed as an optimization problem

$$\text{max}_A \langle \Psi(A)|T(\beta, \Delta)|\Psi(A)\rangle / \langle \Psi(A)|\Psi(A)\rangle,$$

(7)

for the local tensor $A$. To solve this optimization problem, we apply the VUMPS algorithm[16–18], which provides an efficient variational scheme to approximate the largest eigenvector $|\Psi(A)\rangle$. Then various physical quantities can be estimated from the fixed-point uMPS.

For the entanglement entropy, we perform a bipartition on $|\Psi(A)\rangle$ via Schmidt decomposition

$$|\Psi(A)\rangle = \sum_{\alpha,\beta=1}^D s_\alpha \delta_{\alpha,\beta} |\Psi_{\alpha}^{\infty,n}\rangle |\Psi_{\beta}^{\infty}\rangle.$$
where $s_\alpha$ are the singular values. The entanglement entropy $S_E$ is given by

$$S_E = -\sum_{\alpha=1}^{D} s_\alpha^2 \ln s_\alpha^2$$

in the same way as the quantum entanglement measure for a many-body quantum state [20]. Moreover, the entanglement spectrum [21] can be defined by $\varepsilon_n = -\log s_\alpha^2$ to yield more information on the fixed-point uMPS. The evaluations of a local observable $m(\theta_i)$ can be represented as,

$$\langle m(\theta_i) \rangle = \frac{1}{Z} \prod_j \int \frac{d\theta_j}{2\pi} e^{-\beta E(\{\theta_j\})} m(\theta_i),$$

where $E(\{\theta_j\})$ is the energy under a given configuration $\{\theta_j\}$. Compared to the partition function (2), the $m(\theta_i)$ on the right hand side of Eq.(9) simply changes the $O_{n_1,n_2}^{n_3,n_4}(i)$ tensor into an impurity local tensor

$$M_{n_1,n_2}^{n_3,n_4} = \left( \prod_{i=1}^{4} a_{n_i}(\beta, \Delta) \right)^{1/2} \int \frac{d\theta}{2\pi} e^{i\theta(n_1+n_2-n_3-n_4)} m(\theta).$$

Using the uMPS fixed-point, the contraction of the tensor network of $\langle m(\theta) \rangle$ is reduced to a trace of an infinite sequence of channel operators

$$\langle m(\theta) \rangle = \text{Tr} (\cdots T_O T_O T_M T_O T_O \cdots),$$

where the channel operator is defined by

$$T_X = \sum_{i,j} \tilde{A}^i \otimes X^{i,j} \otimes A^j.$$  

In the same fashion, the contraction of channel operators is determined by the leading eigenvectors ($F_L$) and ($F_R$) of $T_O$ as shown in Fig. 1 (c) and (d). Thus the expectation value of a local observable can be obtained by contraction of the leading eigenvectors $\langle F_L |$ and $| F_R \rangle$ with $T_M$

$$\langle m(\theta) \rangle = \langle F_L | T_M | F_R \rangle,$$

as shown in Fig. 1 (e). Moreover, the correlation functions between two local observables $m(\theta_i)$ and $m(\theta_j)$ defined by $G(r) = \langle m(\theta_i)m(\theta_j) \rangle$ can also be represented as a contraction of a tensor network with two local impurity tensors $M_i$ and $M_j$. As displayed in Fig. 1 (f), with the help of fixed-points of the channel operator, we can easily derive

$$G(r) = \langle F_L | T_{M_1} T_{O} T_{O} \cdots T_{O} T_{M_j} | F_R \rangle.$$  

Numerical results. -In the tensor network framework, the entanglement entropy of the fixed-point uMPS for the 1D quantum transfer operator exhibits singularities, which can be used to accurately determine all possible phase transitions. Firstly, we estimate the critical temperature of the BKT transition for the usual XY model at $\Delta = 1$ as $T_{\text{BKT}} \approx 0.8933$, sufficiently close to the result from high-temperature expansion with high precision [22, 23]. Then we calculate the entanglement entropy for a general value of $0 < \Delta < 1$. In Fig. 2(a) and (b), the entanglement entropy $S_E$ develops two sharp peaks at $T_{c,1} \approx 0.44$ and $T_{c,2} \approx 0.77$ for a small value $\Delta = 0.2$, and one sharp peak at $T_c \approx 0.91$ for a large value $\Delta = 0.8$. The peak positions are almost unchanged with the bond dimensions $D = 90, 100, 110$. So we can accurately locate the phase boundaries, and the complete phase diagram is thus derived as displayed in Fig. 2(c). We find two BKT phase transition lines $AC$ and $BC$ corresponding to the integer vortex-antivortex binding and the half-integer vortex-antivortex binding transitions, respectively. More importantly, there is another topological phase transition line between the integer vortex-antivortex binding phase and the half-integer vortex-antivortex binding phase, and three phase transition lines merge at a multi-critical point $C$ ($\Delta \approx 0.330, T \approx 0.705$).

Moreover, the entanglement spectrum of the fixed-
point uMPS for the 1D quantum transfer operator exhibits some intriguing features. In Fig. 3 (d), the five lowest entanglement levels are displayed for a given temperature $T = 0.85$, where varying $\Delta$ goes through all three phases. Exactly at the two critical BKT transitions $\Delta_{c,1} \simeq 0.10$ and $\Delta_{c,2} \simeq 0.58$, the first and second excited entanglement levels become degenerate when entering the disordered phase. Inside the disordered phase, we find an unusual feature that the two-fold degenerate excited levels have a further crossing to form a four-fold degenerate point at $\Delta^* \simeq 0.43$. With a careful numerical analysis, we find that this four-fold degenerate point just starts from the multi-critical point $C$ and extends into the disordered phase. In the phase diagram Fig. 3 (c), these highly degenerate points are plotted in a dotted line, which approaches $\Delta = 0.5$ asymptotically as increasing the temperature. According to the discussion in a dual height model[12], this special line should correspond to the deconfinement crossover line separating the region with dominant integer vortex excitations $(0.5 < \Delta < 1)$ from the half-integer vortex dominant region $(0 < \Delta < 0.5)$. Therefore, the unique advantages of tensor network approach have been demonstrated in dealing with complex systems with topological excitations.

To further understand the topological phase transition between the integer vortex-antivortex binding phase and the half-integer vortex-antivortex binding phase, we calculate the specific heat, which can be represented in the tensor-network language based on two nearest neighbor impurity tensors. Using the contraction in (13), the internal energy per site can be calculated as

$$u = -\Delta(\cos(\theta_i - \theta_{i+1})) - (1 - \Delta)(\cos(2\theta_i - 2\theta_{i+1})),$$

and the specific heat per site is given by $C_V = \partial u / \partial T$. For $\Delta = 0.2$, all three phases can be reached as varying the temperature, while for $\Delta = 0.8$ there are only two phases. As shown in Fig. 3 (c), the specific heat shows a bump around two BKT type transitions but a logarithmic divergence at the transition between the half-integer vortex-antivortex binding phase and the integer vortex-antivortex binding phase. Such a logarithmic specific heat is usually regarded as a characteristic feature of the 2D Ising transition[7][12]. However, this phase transition accompanies with vanishing topological strings associated to the half-integer vortices without any symmetry breaking, indicating the topological nature of this transition different from the ordinary 2D Ising transition.

Actually the nature of this phase transition between two different vortex binding phases can also be revealed by studying the following correlation functions

$$G_1(r) = \langle \cos(\theta_i - \theta_{i+r}) \rangle, \quad G_2(r) = \langle \cos(2\theta_i - 2\theta_{i+r}) \rangle,$$

which describe the correlations of the spins and nematic spins, respectively. Within the tensor network framework, these two correlation functions can be calculated readily using local impurity tensors of $e^{\pm i\delta_1}$ and $e^{\pm i\delta_2}$. It has been known that $G_1(r)$ decays algebraically only in the integer vortex-antivortex binding phase, while $G_2(r)$ exhibits algebraic decay both in the half-integer vortex-antivortex binding and integer vortex-antivortex binding phases[5][6]. When $G_1(r)$ and $G_2(r)$ decay exponentially, two different correlation lengths $\xi_1$ and $\xi_2$ are defined by

$$G_1(r) \sim \exp(-r/\xi_1), \quad G_2(r) \sim \exp(-r/\xi_2). \quad (14)$$

In particular, $G_1(r)$ decays exponentially in the half-integer vortex-antivortex binding phase, so we can study the critical behavior of the correlation length $\xi_1$ when approaching the phase transition. In Fig. 3 (a), we show the correlation length $\xi_1$ as a function of temperature for $\Delta = 0.2$ with a sharp divergence at the critical point $T_c \simeq 0.44$ between two low-temperature phases, as well as $\Delta = 0.8$ with a sharp divergence at the BKT transition point $T_c \approx 0.91$. Similarly, the correlation length $\xi_2$ for $\Delta = 0.2$ as displayed in Fig. 3 (b) has a divergence at the half-BKT transition point $T_c \approx 0.77$. When approaching the critical points from the high-temperature side, all correlation lengths are found to be well fitted by an exponentially divergent form

$$\xi(T) \propto \exp\left(\frac{b}{\sqrt{T - T_c^+}}\right), \quad T \rightarrow T_c^+ \quad (15)$$

where $b$ is a non-universal positive constant. This distinct behavior of the spin correlation length is a characteristic and unique property of the BKT transition[23], strongly demonstrating that the transition from the half-integer vortex-antivortex binding phase to the integer vortex-
antivortex binding phase is a hybrid BKT and Ising transition, i.e., a new universality class of topological phase transition.

Furthermore, we can extract the central charges for those critical field theories by numerically fitting the entanglement entropy with the correlation lengths obtained at different bond dimensions.

\[ S_E \propto \frac{c}{6} \ln \xi_D. \]  \hfill (16)

In Fig. 3 (c), the numerical fitting clearly shows the central charges equal to \( c = 1 \) for all three transitions, precisely the value for the BKT-type transition. In Fig. 3 (d), we also fit the correlation lengths close to the multi-critical point \( C \), and the corresponding central charge is determined as \( c = 5/2 \). To understand these central charge values, we propose that there is another correlation length for the non-local string operator for the Ising-BKT transition, whose critical behavior follows the same form as that for the 2D Ising transition. So there exists two different characteristic correlation lengths for this Ising-BKT transition and the critical field theory with \( Z_2 \times U(1) \) symmetry should be described by the conformal field theory with the central charge \( c = 1 + 1/2 \), where a supersymmetry emerges. And this Ising-BKT transition line merges with the BKT transition line \( ACB \) at the multi-critical point \( C \), giving rise to the central charge \( c = 1 + 3/2 \).

**Conclusion and Outlook.** We have employed the tensor network method to solve the generalized two-dimensional classical XY spin model with topological integer and half-integer vortex excitations as well as the string excitations. Using the singularities of entanglement entropy, we have accurately determined the phase diagram of this model. In particular, a new hybrid BKT and Ising phase transition has been established between the integer vortex-antivortex binding phase and the half-integer vortex-antivortex binding phase. In recent years, a large amount of investigations have focused on a gas of attractive bosons, which can form two distinct superfluid phases: an atomic superfluid of bosons and a molecular superfluid of boson pairs. The former corresponds to the integer vortex-antivortex binding phase and the latter is the half-integer vortex-antivortex binding phase. The established hybrid topological phase transition may be experimentally realized in these physical systems.

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