The tensor renormalization group study of the general spin-S Blume-Capel model

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We focus on the special parameter point $D = 2J$ of the general spin-S Blume-Capel model on the square lattice. The phase transition behaviors with the temperature variation are discussed by the newly developed tensor renormalization group method. For the case of the integer spin-S, the system will undergo $S$ first-order phase transitions with the successive spontaneous breaking of the magnetization $M = S, S - 1, \ldots$. For the half-integer spin-S, there are similar $S - 1/2$ first order phase transition with $M = S, S - 1, \ldots 1/2$ stepwise structure, in addition, there is a continuous phase transition due to the spin-flip $Z_2$ symmetry breaking. For the first order phase transitions, the location of the critical temperature is the same, independent of the value of the spin-S. It is a different picture compared to the previous results $T_c = 0$.

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The Blume-Capel model$^1$ and the extended Blume-Energy-Griffiths model$^2$ have attracted the general interests in the several decades. The Monte-Carlo algorithm$^{3,4}$, finite-size scaling$^5$ and mean-field approximation$^6$ demonstrate the rich phase diagrams of this model. The richness originates, not only from the spin-flip $Z_2$ symmetry breaking, but also from the density fluctuations with $S + 1$ (for integer $S$) or $S + 1/2$ (for half-integer $S$) optional values$^7$ for $S^2$. Furthermore, It is a characterization for the experimental 3He-4He mixtures$^8$ and metamagnets$^9$, which inspired the vector version of this model$^{10,11}$.

The Hamiltonian of the Blume-Capel model$^1$ with general spin-S is

$$H = -J \sum_{<i,j>} S_i S_j + D \sum_{i} S_i^2,$$

(1)

where the spin variable $S$ takes $2S + 1$ values: $\{ -S, -S + 1, \ldots, S - 1, S \}$. $J$ is the coupling constant and $D$ is the strength of the single-ion anisotropy. The sum of the first term runs over all the nearest neighbors. When $D = 0$, this model is reduced to the classical Ising model. When $D$ goes to the positive infinity, the energy favorable state is the one with the full classical Ising model. For the integer spin cases, the component is $S = 0$. For the half-integer cases, the component is $S = \pm 1/2$.

If we look at the Hamiltonian of any bond linking two sites $i, j$, then we have

$$H_{ij} = -JS_i S_j + D(S_i^2 + S_j^2)/q.$$

(2)

Here, $q$ is the coordination number depending on the lattice structure. This formula can be rewritten as

$$H_{i,j} = J(S_i - S_j)^2/2 + (D/q - J/2)(S_i^2 + S_j^2),$$

(3)

from which, it leads to the following conclusions for the ferromagnetic coupling($J > 0$): when $D > qJ/2$, the configuration of the ground state is $S_i = S_j = 0$,

$S_i = S_j = 1/2(-1/2)$ (depending on the spontaneous breaking), respectively for the integer and half-integer spin-S cases; when $D < qJ/2$, the configuration of the ground state is $S_i = S_j = \max(S)$ for any spin-S cases. As a result, we have a special situation, i.e., $D = qJ/2$, where the ground state is $S_i = S_j$ with $(2S + 1)$-fold degeneracy.

Without loss of the generality, we focus on the square lattice hereafter. Then, $q = 4$ and $D = 2J$ is the special parameter. The phase boundaries of the square lattice$^{11,12}$ end at $(T/J, D/J) = (0, 2)$, i.e., for $D = 2J$, the critical temperature is $T_c = 0$ for the general spin cases.

Motivated by the special parameter point and the thought how the phase boundary approaches the ending point, we calculate the temperature dependence behaviors of this model in the case of $D = 2J$ by the recently developed tensor renormalization group algorithm$^{13}$. For a classical lattice model with the local interactions, the partition function can be represented as the tensor product$^{14}$.

$$Z = \text{Tr} \prod_{i} T_{l,r,u,d},$$

(4)

where $i$ runs over all the lattice sites and $\text{Tr}$ is to sum over all bond indices. The local tensor $T$ is defined at each lattice site as shown in Fig. 1 and the indices $l, r, u, d$ mean the left, right, up and down directions respectively. Here, the initial tensor $T$ is a order-4 tensor due to the four indices. The initial dimension $d_0 = (2S + 1)$ of each order is the degree of freedom for the spin. The detailed information about the construction of the tensor can be found in Ref. 14.

To contract the tensor network, i.e., trace over all sites, we will face the exponential increasing problem of the dimension of each order of the tensor. After $n$-th contraction along the horizontal and vertical directions, the dimension varies by $d_n = d_{n-1}^2 - 1$. The contraction process will make the dimension go beyond the calculability. In
2007, Levin and Nave proposed a cutoff scheme for $d_n$ by the singular value decomposition (SVD), to get a good approximation for the partition function calculation, by which the thermodynamic properties of the system can be obtained consequently.

Recently, we proposed an coarse graining tensor network renormalization group (RG) based on the high order singular value decomposition (HOSVD), which provides an accurate but low computational cost technique for studying two- or three-dimensional (3D) lattice models. The following results are all from the newly developed RG scheme. Hereafter, the coupling constant $J$ is used as the energy unit, and $K_B$ is set as 1.

**I. THE CASE OF $S = 1$**

In the case of $S = 1$, there are three optional values: ±1, 0 for each spin variable. It is the case catching the most attention. On one side, there exists the tricritical point enriching the phase diagram. On the other side, it is affordable computational cost for the different numerical methods.

In the limit of infinite $D$, the energy favorable state is $N(S = 0) = 1$, which means that all sites are occupied by $S = 0$. We can name $S = 0$ as the vacancy or hole, the state full of holes is just the hole condensed phase, whose quantum correspondence is the one-dimensional $S = 1$ quantum model with single-ion anisotropy of our previous paper. The hole condensed states also emerge in the other general integer spin-$S$ cases.

As is shown in Fig. 2, the system undergoes the first order phase transitions accompanying the emergence of the hole condensed phase as the temperature varies. The magnetization jumps from 1 to 0, whose location is consistent with the kink of the occupation number of the holes $N(S = 0)$. The critical point reads $T_c = 0.123$. For the terrace of the magnetization $M = 0$, the starting point is the condensation of the holes, which determines the first order phase transition behaviors other than Ising-like continuous phase transitions from the ferromagnetic to paramagnetic phase. With the temperature increasing, the components $N(S = 1, -1)$ come back to the system again with the equal-weight occupation, which means that the system remains in the paramagnetic state of $M = 0$. In the limit of the high temperature, the occupation numbers of the three different components $S = 1, 0, -1$ all go to 1/3.

**II. THE CASE OF $S = 2$**

Here, there are five optional values: 0, ±1, ±2 for the spin variable. Compared to the case of $S = 1$, there is one more optional pair $S = ±2$, which renders one more jump of the magnetization from $M = 2$ to $M = 1$. The system undergoes the first order phase transitions twice with the temperature increasing.

The first platform $M = 2$ corresponds to the full occupation of $N(S = 2) = 1$ after the spontaneous breaking of the pair $S = ±2$. The second platform $M = 1$ emerges with the disappearance of $N(S = 2, -2)$ and full occupation of $N(S = 1) = 1$ after the spontaneous breaking of the pair $S = ±1$. The second jump of the magnetization comes with the hole condensed phase $N(S = 0) = 0$. With the temperature further increasing, the occupation of the hole drops down continuously. The pairs $S = ±1$ and $S = ±2$ come back to the system successively. $N(S = 0) + N(S = 1, -1) ≃ 1$ keeps until the considerable temperature. Accompanying the successive disappearance of $S = ±2$ and $S = ±1$, the two critical points are located at $T_{c1} = 0.123$ and $T_{c2} = 0.365$ respectively.
For $S = 3/2$, there are four optional values: $\pm 3/2, \pm 1/2$ for each spin variable. Similar to the case of $S = 1$, the system exhibits the spontaneous breaking which start from the magnetization $M = 3/2$. The first jump of the magnetization from $M = 3/2$ to $M = 1/2$ results from the competition of the occupation of two pairs between $S = \pm 3/2$ and $S = \pm 1/2$. The spontaneous breaking brings us the full occupation change from $N(S = 3/2)$ to $N(S = 1/2)$. The discontinuity of the physical quantities mean the first order phase transition.

When the temperature increases further, the Ising-like continuous phase transition shows up due to spin-flip $Z_2$ symmetry breaking. The results support the physical picture of the separated first order and second order phase transition line in Ref. [4]. By the behaviors of the magnetization, the two critical points are located at $T_{c1} = 0.123$ and $T_{c2} = 0.649$ respectively. The location of $T_{c2}$ is close to the data shown in Fig. 2 in Ref. [4].

IV. THE CASE OF $S = 5/2$

There are six optional values: $\pm 1/2, \pm 3/2, \pm 5/2$ for each spin variable.

When the temperature increases slowly for the zero point, the system spontaneously breaks into the state $M = 5/2$, with the full occupation $N(S = 5/2) = 1$. With the temperature further rising, the system enters into the state $M = 3/2$ with the full occupation $N(S = 3/2) = 1$, then becomes the state $M = 1/2$ with the full occupation $N(S = 1/2) = 1$. The stepwise breaking is clearly shown in the profile of the occupation number $N(S = 3/2, -3/2)$. At the first terrace $M = 5/2$, the degrees of freedom $S = (3/2, -3/2), (1/2, -1/2)$ are gone. On the way to increase the temperature, the first jump of the magnetization $M$ and the occupation number $N$ demonstrates the disappearance of $N(S = 5/2, -5/2)$ and full occupation of $N(S = 3/2, -3/2)$. The spontaneously breaking of the spin pair $S = (3/2, -3/2)$ brings $N(S = 3/2) = 1$. Then the second jump of $M$ and $N$ represents the ensuing replacement of $N = (S = 3/2, -3/2)$ by $N = (S = 1/2, -1/2)$. The spontaneously breaking of the spin pair $S = (1/2, -1/2)$ brings $N(S = 1/2) = 1$.

However, with the temperature further increasing, $M$ drops to 0 continuously, accompanying the continuous phase transition, and the system enters into the paramagnetic phase. Here, the occupation number $N(S = 3/2, -3/2)$ increases continuously from 0. A further calculation shows that $N(S = 1/2) = N(S = -1/2), N(S = 3/2) = N(S = -3/2)$ in the paramagnetic phase, where $N(S = 1/2, -1/2) + N(S = 3/2, -3/2) \simeq 1$ keeps until the considerable temperature until the equal-weight dis-
tribution of all the degree of freedom in the high temperature limit. The three critical points read \( T_{c_1} = 0.123, T_{c_2} = 0.366, T_{c_3} = 0.685 \).

Reviewing the data about the critical points, we find that the critical temperature for the first phase transition of first order is fixed at \( T_{c_1} = 0.123 \) for the above four cases \( S = 1, 3/2, 2, 5/2 \), and the second one of first order is \( T_{c_2} = 0.365 \) for \( S = 2 \) and \( T_{c_2} = 0.366 \) for \( S = 5/2 \) respectively. The location of the first order phase transition is independent of the value of the spin-S. It is yield at first sight, why does it happen?

Let us turn to the principle about the minimal free energy, \( F = U - TS \). The phase transition lies in the competition between the internal energy and the entropy. The density fluctuations of the optional values bring the change of the internal energy at the interface of the two different clusters composed of single spin value. It changes the possible configurations of the occupation simultaneously, which is exactly the entropy. The first order phase transition occurs with the replacement of the optional spin values related to the successive spontaneous breaking, which is irrelevant for the value of spin value \( S \). The interval of \( S \) is always 1 no matter that it is the integer or half-integer case, which induces the same internal energy difference. The balance of the free energy is the same for the different spin-S cases. For these low temperature transition points, the relative Boltzmann weight \( e^{-\beta \Delta E} \) due to the variation of the spin value is quite small. As a consequence, we can’t see the appreciable thermal fluctuations.

As was pointed out in Ref. [17], a symmetry breaking phase with \( n \) degenerate states is represented by fix-point tensors, which is a direct sum of \( n \) dimension-one trivial tensor. \( X_1 \) is a visualized parameter of the fix-point tensor with the following definition,

\[
X_1 = \frac{\left( \sum_{\mu\nu} T_{\mu\nu} u_{\mu} u_{\nu} \right)^2}{\sum_{\mu\nu} T_{\mu\nu} u_{\mu} u_{\mu}},
\]

and its graphical demonstration was referred to Fig. (13) in Ref. [17].

For the integer case of \( S = 2 \), the visualization \( X_1 \) bears the step-wise structure: 5, 3, 1. The 5-fold degeneracy associated to \( T^{Z_2} \bigoplus T^{Z_2} \bigoplus T^{TRI} \) is represented by the first platform valued 5. \( T^{Z_2} \) corresponds to the spin flip of the pair \((s, -s)\) and \( T^{TRI} \) comes from the degree of freedom \( S = 0 \). With the temperature increasing, the system undergoes two phase transitions. The first jump of \( X_1 \) from 5 to 3 and \( T^{Z_2} \) originating from \( S = \pm 2 \) is gone, where \( \mathcal{N}(S = 1) = 0 \). The platform of \( X_1 = 3 \) corresponds to \( T^{Z_2} \bigoplus T^{TRI} \) referring to \( S = 0, 1, -1 \). The platform of \( X_1 = 1 \) is the consequent vanishing of \( T^{Z_2} \) from another pair \( S = \pm 1 \), where \( \mathcal{N}(S = 0) = 1 \).

For the half-integer case of \( S = 5/2 \), the visualization \( X_1 \) bears the step-wise structure: 6, 4, 2, 1. The 6-fold degeneracy comes from the three pairs \( \pm 5/2, \pm 3/2, \pm 1/2 \), corresponding to \( T^{Z_2} \bigoplus T^{Z_2} \bigoplus T^{Z_2} \). The first two jumps of \( X_1 \) represent the two first order phase transitions, which are similar to the case of \( S = 2 \) accompanying with the successive vanishing of the occupation pairs. The difference lies in the last jump of \( X_1 \) from 2 to 1, which is the continuous phase transition with \( Z_2 \) spin-flip symmetry breaking. The gap of \( X_1 \) is 2 for all the first order phase transitions and 1 for the last continuous phase transition respectively.

We can come to the general conclusion that the visualization parameter \( X_1 \) bears the step-wise structure: \( 2S + 1, 2S - 1, ..., 3, 1 \) for the integer spin \( S \), \( 2S + 1, 2S - 1, ..., 2 \) for the half-integer spin \( S \). It is tricky to locate the position of the critical point by the step of \( X_1 \) because of the subtlety of \( X_1 \) due to the cutoff in the contraction process, however, the integer platform of \( X_1 \) associated to the degeneracy of the system is intrinsic, which comes from the deep insight that the fix-point of the tensor representation corresponds to the fix point of RG flow associated to the phase transition. It does open...
the new window to observe the phase transition. The improvement and exploration about the visualization like $X_1$ from the tensor itself is still on the way.

In summary, we discuss the phase transitions of the Blume-capel model on the square lattice using the recently developed tensor network renormalization group scheme. We focus on the special situation with the high degeneracy, $D = 2J$, where the bond Hamiltonian is the form of the square sum. The calculation shows, for the first order phase transition, the different phase boundary ending points successively locate at $T_{cn}(n=1,2,...)$ on the vertical line $D = 2J$. Here, $\max(n) = S$ for integer spin-$S$ and $\max(n) = S - 1/2$ for half-integer spin-$S$. Unlike the results that the ending points always touch at $(T/J, D/J) = (0, 2)$ from the mean-field approximation and finite-size scaling method. We fix the first two critical points $T_{c1} = 0.123, T_{c2} = 0.36(5)$ of the first order phase transitions for the general spin-$S$ cases. Through the magnetization and the occupation number of different optional spin values, the first order phase transition behaviors are clarified, accompanying the successive disappearance of the optional spin pairs. The visualization parameter $X_1$ associated to the degenerate states provides the further evidence for the phase transition process. Compared to the integer spin-$S$ cases, there is one more Ising-like continuous phase transition with spin-flip $Z_2$ symmetry breaking for half-integer spin $S$-cases.

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