Entanglement and quantum phase transition in quantum mixed spin chains

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The ground entanglement and thermal entanglement in quantum mixed spin chains consisting of two integer spins 1 and two half integer spins \(\frac{1}{2}\) arrayed as \(J_1 - 1 - 1\) in a unit cell with antiferromagnetic nearest-neighbor couplings \(J_1, J_2\) between the spins of equal (different) magnitudes, are investigated by adopting the log-negativity. The ground entanglement transition found here is closely related with the valence bond state transition, and the thermal entanglement near the critical point is calculated and shown that two distinct behaviors exist in the nearest neighbor same kind of spins and different kind of spins, respectively. The potential application of our results on the quantum information processing is also discussed.

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I. INTRODUCTION

Entanglement, one of the most striking features of quantum mechanics, has been recognized as an important resource for quantum information processing. Recently, the entanglement in the systems of condensed matter physics as well as the Heisenberg models has caused much attention. The Heisenberg models have gapless spectrum with algebraic decay of correlations at zero temperature and integer spin ones should be gapped with exponential decay of correlations. Recently, some authors have addressed whether the entanglement length is finite or infinite in the Heisenberg spin-1 chain and numerically the mixed quantum spin chains, such as the alternating quantum spin chain with \(S^1 = 1/2\) and \(S^2 = 1\) with antiferromagnetic nearest-neighbor exchange interaction or more complicated hypothetical 1D periodic structures of different spins with ferrimagnetic properties. The topology of spin arrangements in the ferrimagnetic chain plays an essential role on the variation of energy gap associated with Haldane conjecture and on the magnetism of ground states. The ground state of ferrimagnetic chain with two kinds of different spins is either a spin singlet or ferrimagnetic due to the setup of the bipartite lattices following Marshall theorem. By applying the Lieb-Schultz-Mattis theorem, one can find whether the ferrimagnetic chains have a gapless excitation though the theorem failed to predict the existence of a gapped excitation. In this Letter, we consider the ground state entanglement and thermal state entanglement in an interesting model which is called as quantum mixed spin 1/2-1/2-1-1 chain by making use of the quantum Monte Carlo method with a improved loop cluster algorithm. Over the past years, the quantum Monte Carlo method with a improved loop cluster algorithm has proven it to be a efficient numerical tool to deal with the complicated coupled spin chains. So it is very credible to numerically investigate the nonclassical properties such as the entanglement of the mixed spin chain by adopting this method.

For first time, we investigate the ground state entanglement of the mixed spin chain up to 128 sites by exploring the log-negativity as an entanglement measure. Two distinct behaviors of pairwise entanglement are found. We provide a evidence that the ground state entanglement between two 1/2 spins or between 1/2 spin and 1 spin are closely related to the so-called VBS phase transition. At the point of VBS phase transition, the ground state between two 1/2 spins can be transferred to two different kinds of spins i.e. the spin 1/2 and spin 1 or vice versa. Furthermore, the thermal state pairwise entan-
FIG. 1: Graphical representation of the Hamiltonian in Eq.(1), the black and white circles represent spins $\frac{1}{2}$ and 1, respectively.

...vanishes at a critical point $\alpha = J_2/J_1$.

This paper is organized as follows: In Sec.II, we briefly outline the basic content of the quantum mixed spin chain and investigate the ground state entanglement between two nearest-neighbor spins $\frac{1}{2}$ or between two nearest-neighbor spins $\frac{1}{2}$ and 1. In Sec.III, we investigate the thermal state entanglement between two nearest-neighbor spins $\frac{1}{2}$ or between two nearest-neighbor spins $\frac{1}{2}$ and 1. It is shown that the entanglement can be enhanced by improving the temperature. In Sec.IV, there are some conclusive remarks.

II. The ground state entanglement and the VBS phase transition of quantum mixed spin chain

Now we consider the quantum antiferromagnetic mixed spin $S^1 - S^1 - S^2 - S^2$ chain displayed by Fig.1, whose Hamiltonian can be given by

$$H = \sum_{n=1}^{N/4} \left( J_1 S_{4n-3}^1 \cdot S_{4n-2}^1 + J_2 S_{4n-2}^1 \cdot S_{4n-1}^1 \right) + J_1 S_{4n-1}^2 \cdot S_{4n}^2 + J_2 S_{4n}^2 \cdot S_{4n+1}^2. \tag{1}$$

Here, the periodic boundary condition is adopted. In the case with $S^1 = \frac{1}{2}$ and $S^2 = 1$, the model has been studied by quantum Monte Carlo (QMC) simulation \cite{38} and the nonlinear $\sigma$ model (NLSM) \cite{37,38}. The ground state of this model is nonmagnetic with gapped excitations. The gap varies as a function of the parameter $\alpha = J_2/J_1$, and vanishes at a critical point $\alpha_c$, which implies a quantum phase transition between two different VBS states. Since the VBS states of the mixed spin chains actually contain an ensemble of spin singlet state which can be regarded as the abundance quantum information resource, it is very desirable to study how the parameter $\alpha$ affects the entanglement of this model or what is the relation between the gapped excitation and the thermal entanglement.

We study both the ground state entanglement and the thermal state entanglement of this system. The state of a quantum system at thermal equilibrium can be described by the density operator $\rho = \frac{1}{Z} \exp(-\beta H)$, where $\beta = \frac{1}{k_B T}$ with $k_B$ the Boltzmann’s constant. $Z = \text{Tr} e^{-\beta H}$ is the partition function. The entanglement in the ground state or thermal state is called ground state entanglement or thermal entanglement, respectively. For antiferromagnetic mixed spin chains, the ground state is not degenerate. So the ground state can be directly expressed by the density operator $\rho = \frac{1}{Z} \exp(-\beta H)$ with $\beta \to \infty$. By utilizing the SU(2) invariance of this system, the reduced density matrix $\rho^{(1)}$ for two spins $\frac{1}{2}$ or $\rho^{(1,2)}$ for one spin $\frac{1}{2}$ and one spin 1 can be obtained as follows \cite{15}:

$$\rho^{(1)} = g^{(1,1)} |0,0 \rangle \langle 0,0 | + \frac{1}{3} g^{(1,1)} \sum_{i=-1}^{1} |i,i \rangle \langle i,i|, \tag{2}$$

and

$$\rho^{(1,2)} = \frac{1}{2} \sum_{i=-1/2}^{1/2} |\frac{1}{2},i \rangle \langle \frac{1}{2},i| + \frac{1}{4} g^{(1,2)} \sum_{i=-3/2}^{3/2} \sum_{j=3/2}^{3/2} \frac{3}{2} \langle j/2, i \rangle |j/2, i \rangle. \tag{3}$$

where $|J_1, J_2\rangle$ denotes the state of total spin $J$ and $z$ component $J_z$, and $g^{(1,1)}$ and $g^{(1,2)}$ are the function of temperature. For characterizing the ground state pairwise entanglement and the thermal state pairwise entanglement, we adopt the log-negativity as the entanglement measure, which has been proven to be an operational good entanglement measure. The log-negativity $N(\rho_r)$ for the two particle reduced density operator $\rho_r$ is defined as \cite{39}:

$$N(\rho_r) = \log_2 ||\rho_r^T||, \tag{4}$$

where $\rho_r^T$ is the partial transpose of $\rho_r$ and $||\rho_r^T||$ denotes the trace norm of $\rho_r^T$, which is the sum of the singular values of $\rho_r^T$. For the isotropic mixed spin chains with SU(2) symmetry, the log-negativity between any two spins can be proven to be directly related with the two-particle correlation function. Therefore, we can directly calculate the log-negativity by slightly changing the program for the QMC. In Fig.2, we numerically calculate the log-negativity $N^{(1,1)}$ of the reduced density operator of two nearest-neighbor spin $\frac{1}{2}$ in a unit cell of the ground state and the log-negativity $N^{(1,2)}$ of two nearest-neighbor different spin $\frac{1}{2}$ and 1. It is shown that $N^{(1,1)}$ decreases from 1 to zero as the parameter $\alpha$ increases from 0 to 1. At the point of VBS phase transition labelled by $\alpha_c \simeq 0.768$, the entanglement experience a sharply descent. While the entanglement between two nearest-neighbor different spins $\frac{1}{2}$ and 1 characterized by log-negativity $N^{(1,2)}$ is zero for small values of $\alpha$, and near the critical point it increases with $\alpha$ and experience a sharply ascent at the critical point. Unfortunately, we find that the ground state entanglement only exists between two spins in the same unit cell. In the numerical calculation of the log-negativity of the ground state, we have set $\beta = 200$ and $N = 128$. We conjecture that the descent or ascent of log-negativity near the critical point can be more sharp if the value of $\beta$ is chosen very very large, though this can consume more and more computation time. From Fig.2, one
can imagine that the quantum mixed spin chain in zero temperature can be utilized as a very good entanglement switch by controlling the parameter $\alpha$. Recently, Pachos and Plenio have shown that some kinds of atomic lattice can be used to simulate the Hamiltonian of various controllable Heisenberg spin chain \([22]\). It can motivate us to realize the quantum mixed spin chain in the system of atomic lattice. Then we easily obtain the quantum mixed spin chain with controllable parameter $\alpha$. The details of suggestion is discussed elsewhere.

III. The thermal state entanglement of quantum mixed spin chain

In what follows, we turn to consider the thermal entanglement of the mixed spin chain. In Fig.3, we calculate the log-negativity $N^{(1,1)}$ characterizing the entanglement of two nearest-neighbor as the function of $k_B T$. It is shown that, if the parameter $\alpha$ is smaller than the critical point $\alpha_c$, the entanglement decreases with the temperature and vanishes when the temperature goes beyond a threshold value. However, in the cases with $\alpha > \alpha_c$, the entanglement firstly increases with temperature and achieves a local maximal value, then decreases with temperature and eventually vanishes. We can also find that in the cases with low temperature, the entanglement between two nearest-neighbor spin $\downarrow$ significantly decreases with $\alpha$. It is natural to conjecture that the thermal state entanglement is closely related with fact whether this system has the gapped excitation.

In Fig.4, we plotted the log-negativity $N^{(1,2)}$ as the function of $k_B T$ for three different values of $\alpha$ near the critical point. Being distinct from the entanglement of two spin $\downarrow$, if the parameter $\alpha$ is larger than the critical point, the entanglement between two nearest-neighbor different spin $\downarrow$ and $1$ decreases with the temperature and vanishes when the temperature goes beyond another threshold value which is about half of the threshold value concerning the two spin $\downarrow$. In the case with $\alpha < \alpha_c$, the entanglement of spin $1/2$ and spin $1$ firstly increases with the temperature, and achieves a local maximal value and then decreases with temperature. From Fig.4, we can also find that the thermal entanglement increases with $\alpha$, which is consistent with the ground state entanglement.

For more deeply understanding the relation between thermal entanglement and the gapped excitation, the analysis of the entanglement of the excited state of the quantum mixed spin chain is necessary. In what follows, we briefly present a simple numerical method to calculate the log-negativity of the first excited state. In fact, the reduced density matrix of two spins in the first excited state can be obtained by the following procedure.

$$\rho = \frac{1}{Z} e^{-\beta H} \approx \frac{1}{Z} (e^{-\beta E_g} |g\rangle\langle g| + e^{-\beta E_1} |e_1\rangle\langle e_1|)$$

If the temperature is very very low. Then the reduced density matrix of any two spins can also be expressed as the weight sum of the reduced density matrices of the ground state and the first excited state. By iterating this procedure, we can obtain the log-negativity of two spins in any excited state. The details of this work will be presented elsewhere.

V. CONCLUSION

In this paper, we investigate the ground state entanglement of the mixed spin chain up to 128 sites by exploring the log-negativity as an entanglement measure. Two distinct behaviors of pairwise entanglement are found. We provide a evidence that the ground state entanglement between two 1/2 spins or between 1/2 spin and 1 spin are closely related to the so-called VBS phase transition. At the point of VBS phase transition, the ground
state between two 1/2 spins can be transferred to two different kinds of spins i.e. the spin 1/2 and spin 1 or vice versa. Furthermore, the thermal state pairwise entanglement is also studied and whether the thermal entanglement can be improved by increasing the temperature or not is also addressed, which strongly depends on the parameter $\alpha = J_2/J_1$. It is shown that $N^{(1,1)}$ decreases from 1 to zero as the parameter $\alpha$ increases from 0 to 1. At the point of VBS phase transition labelled by $\alpha_c \approx 0.768$, the entanglement experience a sharply descent. While the entanglement between two nearest-neighbor different spins $\frac{1}{2}$ and 1 characterized by log-negativity $N^{(1,2)}$ is zero for small values of $\alpha$, and near the critical point it increases with $\alpha$ and experience a sharply ascent at the critical point. Unfortunately, we find that the ground state entanglement only exists between two spins in the same unit cell. In the numerical calculation of the log-negativity of the ground state, we have set $\beta = 200$ and $N = 128$. if the parameter $\alpha$ is smaller than the critical point $\alpha_c$, the entanglement decreases with the temperature and vanishes when the temperature goes beyond a threshold value. However, in the cases with $\alpha > \alpha_c$, the entanglement firstly increases with temperature and achieves a local maximal value, then decreases with temperature and eventually vanishes. We can also find that in the cases with low temperature, the entanglement between two nearest-neighbor spin $\frac{1}{2}$ significantly decreases with $\alpha$. Being distinct from the entanglement of two spin $\frac{1}{2}$, if the parameter $\alpha$ is larger than the critical point, the entanglement between two nearest-neighbor different spin $\frac{1}{2}$ and 1 decreases with the temperature and vanishes when the temperature goes beyond another threshold value which is about half of the threshold value concerning the two spin $\frac{1}{2}$. In the case with $\alpha < \alpha_c$, the entanglement of spin 1/2 and spin 1 firstly increases with the temperature, and achieves a local maximal value and then decreases with temperature. It is natural to conjecture that the thermal state entanglement is closely related with fact whether this system has the gapped excitation.

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