

## Entanglement in a spin- $s$ antiferromagnetic Heisenberg chain

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The entanglement in a general Heisenberg antiferromagnetic chain of arbitrary spin- $s$  is investigated. The entanglement is witnessed by the thermal energy which equals the minimum energy of any separable state. There is a characteristic temperature below that an entangled thermal state exists. The characteristic temperature for thermal entanglement is increased with spin  $s$ . When the total number of lattice is increased, the characteristic temperature decreases and then approaches a constant. This effect shows that the thermal entanglement can be detected in a real solid state system of larger number of lattices for finite temperature. The comparison of negativity and entanglement witness is obtained from the separability of the unentangled states. It is found that the thermal energy provides a sufficient condition for the existence of the thermal entanglement in a spin- $s$  antiferromagnetic Heisenberg chain.

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### I. INTRODUCTION

The entanglement of quantum systems has been extensively implemented to realize quantum computation and secure communication. As an important resource in quantum information processing [1], it is necessary to qualify the entanglement. The entanglement of formation [2] and the relative entropy of entanglement [3,4] are basic measures for the bipartite systems. Using these measures, thermal entanglement [5–10] has been investigated in some solid state systems of Heisenberg spin-1/2 model. Anisotropy effect [6], non-nearest interaction [7], high dimensions [8], and multiple qubits [9] were considered. Meanwhile, the entanglement witness [11–17] for spin-1/2 systems was proposed. The existence of entanglement was observed in an experimental situation [18]. The thermal energy [13,14] and the magnetic susceptibility [18] were regarded as the entanglement witnesses for a macroscopic solid state system. The effect of the edges of lattices [13] was considered. The entanglement of the Bose-Hubbard model [14] has been witnessed by the energy. Besides a spin-1/2 model, a more universal quantum system focuses on a high spin- $s$  Heisenberg model [19–24]. In the integer spin systems such as CsNiCl<sub>3</sub> [20] and MnCl<sub>3</sub> (*bipy*) [24], there is the exciting phenomenon of Haldane gap [19–24]. Additionally, the efficiency of the quantum communication [25–28] was also enhanced by utilizing the entanglement between two qutrits (a three-dimensional quantum system). Due to many interesting features of high-spin quantum systems, the entanglement in a quantum Heisenberg system with arbitrary spin- $s$  needs to be studied. Recently, a computable measure of entanglement, i.e., the negativity [29], has been theoretically generalized to the high-spin systems using the separability principle [30,31]. Therefore one entanglement witness can be suggested to experimentally detect the entanglement in such high-spin quantum systems.

In this paper, the entanglement in a spin- $s$  antiferromagnetic Heisenberg chain is investigated. In Sec. II, one en-

tanglement witness for high-spin quantum systems is introduced. Thermal entanglement may be indicated by the characteristic temperature where the thermal energy equals to the minimum energy of all separable states. For bipartite lattices of spin- $s$ , the analytic expression of the minimum energy of the separable state is deduced. In Sec. III, it is demonstrated that the thermal energy provides a sufficient condition of the existence of the thermal entanglement for high-spin systems compared to the negativity.

### II. ENTANGLEMENT WITNESS FOR A SPIN- $S$ HEISENBERG CHAIN

For an isotropic spin- $s$  Heisenberg chain, the Hamiltonian  $H$  is given by

$$H = \sum_{i=1}^L J \vec{S}_i \cdot \vec{S}_{i+1}, \quad (1)$$

where  $\vec{S}_i = (S_i^x, S_i^y, S_i^z)$  and  $S_i^\alpha (\alpha = x, y, z)$  are the spin- $s$  operators for the  $i$ th spin, and  $J$  is the interaction coefficient. The spin operators  $S_i^x, S_i^y$  can be expressed by the lifting operator and the lowering one,  $S_i^+$  and  $S_i^-$ . In the Hilbert space of  $\{|m\rangle_i, m = -s, -s+1, \dots, s\}$ ,  $S_i^\pm |m\rangle_i = \sqrt{(s \pm m + 1)(s \mp m)} |m \pm 1\rangle_i$  and  $S_i^z |m\rangle_i = m |m\rangle_i$ . The periodic boundary condition of  $L+1 = 1$  is assumed. The cases of  $J > 0$  and  $J < 0$  correspond to the antiferromagnetic and ferromagnetic cases, respectively. In the following discussion, an antiferromagnetic chain is considered. The state at a thermal equilibrium temperature  $T$  is  $\rho(T) = e^{-H/kT}/Z$  where  $Z$  is the partition function. For the convenience, both Boltzmann constant  $k$  and Planck constant  $\hbar$  are assumed to be one. One entanglement witness for a spin- $s$  quantum system can be generalized to [13,14]

$$W = \langle H \rangle - E_{\min}, \quad (2)$$

where  $\langle H \rangle = \text{tr}(\rho H)$  is the thermal energy at the thermal state  $\rho$  and  $E_{\min}$  is the minimum energy that any separable state may be obtained. This minimum energy can always be achieved by a pure separable state  $|\psi\rangle_{\text{sep}}$ . When the value of  $W$  is nonnegative, the state  $\rho$  is the separable (unentangled)

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state. Only if  $W < 0$ , there is the thermal entanglement in the state of  $\rho$ . Because the ground energy  $E_0$  is always less than  $\langle H \rangle$ , there is a maximum gap for entanglement,  $G = |E_0 - E_{\min}|$ . In Eq. (2), the solution of the minimum energy  $E_{\min}$  for any separable state needs to be calculated. An isotropic spin- $s$  Heisenberg chain is an example of bipartite lattices. The Hamiltonian can be written by  $H = \sum_{i=1}^L H_i$  where  $H_i = J \vec{S}_i \cdot \vec{S}_{i+1}$ . If the minimum-energy separable state  $|\psi_i\rangle_{\text{sep}}$  for  $H_i$  is known, the total separable state for  $H$  can be expressed by  $|\psi\rangle_{\text{sep}} = \prod_{i=1}^L |\psi_i\rangle_{\text{sep}}$ . In the case of an isotropic antiferromagnetic chain, the state of  $|\psi_i\rangle_{\text{sep}}$  can be analyzed by the standard symmetry methods [32]. The minimum-energy separable state for  $H_i$  can be written as

$$|\psi_i\rangle_{\text{sep}} = \frac{1}{4^s} \sum_{m=0}^s \sqrt{C_m} (|s-m\rangle_i + |m-s\rangle_i) \otimes \sum_{m=0}^s (-1)^m \sqrt{C_m} \times (|s-m\rangle_{i+1} + |m-s\rangle_{i+1}), \quad 2s+1 \text{ is odd,}$$

$$|\psi_i\rangle_{\text{sep}} = \frac{1}{4^s} \sum_{m=0}^{s-1/2} \sqrt{C_m} (|s-m\rangle_i + |m-s\rangle_i) \otimes \sum_{m=0}^{s-1/2} (-1)^m \sqrt{C_m} \times (|s-m\rangle_{i+1} - |m-s\rangle_{i+1}), \quad 2s+1 \text{ is even.} \quad (3)$$

When  $2s+1$  is even, the coefficient satisfies  $C_{m+1} = 2s - m/m + 1 C_m$ . However, when  $2s+1$  is odd,  $C_{m+1} = 2s - m/m + 1 C_m$  for  $m < s-1$  and  $C_s = s+1/4s C_{s-1}$ . As an example, an antiferromagnetic Heisenberg chain with spin  $s = 1$  is investigated. Without losing generality, the parameters of the minimum-energy separable state  $|A\rangle|B\rangle$  can be assumed as

$$|j\rangle = a_j |1\rangle + b_j e^{i\phi_j^1} |0\rangle + c_j e^{i\phi_j^2} |-1\rangle, \quad j = A, B. \quad (4)$$

By means of the standard symmetry method,  $a_j = c_j$ ,  $\phi_j^2 = 0$  and  $\phi_A^1 - \phi_B^1 = \pi$ . To find the minimum energy, the energy can be calculated by

$$\langle A | \langle B | H | A \rangle | B \rangle = -16J a_j^2 b_j^2 \quad (2a_j^2 + b_j^2 = 1). \quad (5)$$

It is easily seen that the minimum energy for any separable state can be achieved by  $a_j = 1/2$ ,  $b_j = \sqrt{2}/2$ .

For the simplest case of  $L=2$ , the ground state energy can be expressed by  $E_0 = -2J(s^2 + s)$  while the minimum energy for any separable state is  $E_{\min} = -2Js^2$ . Therefore the maximum gap for entanglement  $G(s)$  is given by  $G(s) = 2Js$ . The bigger gap is obtained at the higher spin- $s$  system. That is, the entanglement is easily detected in a high-spin system. There is a characteristic temperature  $T_c$  for  $W=0$ . Since  $\langle H_i \rangle$  is increased with increasing value of the temperature [33], it is evident that  $W > 0$  when  $T > T_c$ . It is obvious that the thermal entanglement between two nearest neighboring spins exists only if  $T < T_c$ . In Fig. 1, the characteristic temperature  $T_c$  is plotted when the spin- $s$  is varied. It is found that  $T_c$  is almost linearly increased with  $s$ . The high spin quantum system can increase the temperature range for the existence of the thermal entanglement.

For an  $L$ -partite Heisenberg chain, the corresponding minimum energy is  $E_{\min} = -JLs^2$ . There is also a characteristic temperature  $T_c$  below which the entanglement exists be-

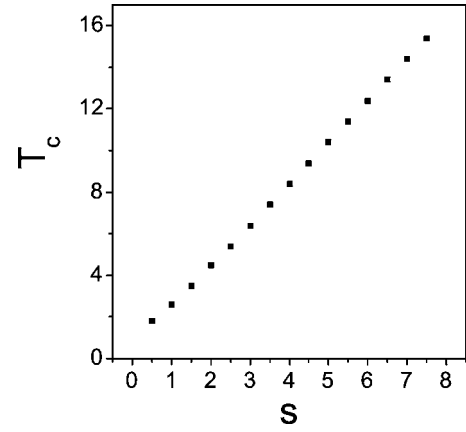


FIG. 1. The characteristic temperature  $T_c$  is plotted when the spin- $s$  is varied.

tween arbitrary two neighboring spins. The relation of  $T_c$  to the total number of lattices  $L$  is shown in Fig. 2 where the coupling is chosen to be  $J=1$ . The upper triangles represent the numerical results of  $T_c$  for spin  $s=1$  while the lower squares denote the values of  $T_c$  for spin  $s=1/2$ . It is seen that the characteristic temperatures  $T_c$  for both different spin- $s$  are monotonously decreased with  $L$  and then approaches a constant at a certain number of lattices. In the limit of  $L \rightarrow \infty$ , the constant value for  $s=1$  is approximately given by  $T_c = 1.05$  which is higher than that of  $T_c = 0.80$  for  $s=1/2$ . This is consistent with recent analyses [9,10,14]. For spin- $s = 1/2$ , the constant value of the characteristic temperature is  $T_{cc} = 0.8$  that is approximately 1/4 of the value in Ref. [14]. This is due to that the parameters chosen in our numerical calculations are about 1/4 of that in Ref. [14]. When the number of lattices  $L$  is very large, it is very interesting to note that the difference  $\Delta T_{cc}^s$  of the constant characteristic temperature  $T_{cc}$  between different spin- $s$  is a function of  $s$ . That is,  $\Delta T_{cc}^s = T_{cc}^{s+1/2} - T_{cc}^s \sim 0.4s$  for  $J=1$ . The fact that the characteristic temperature  $T_c$  approaches a constant can qualitatively explain the detection of the thermal entangle-

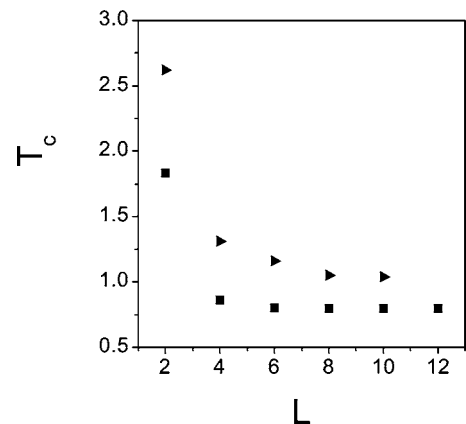


FIG. 2. The characteristic temperature  $T_c$  is plotted as a function of the total number of lattices  $L$ . The upper triangles are the results of  $T_c$  for  $s=1$ . The corresponding constant value is about  $T_c = 1.05$ . The lower squares represent the values of  $T_c$  for  $s=1/2$ , and the constant value of  $T_c$  is 0.80.

ment at finite temperature in a real solid state system of a larger number of lattices [18].

### III. RELATION OF ENTANGLEMENT WITNESS TO NEGATIVITY

Through the thermal energy, the entanglement of a Heisenberg chain can be witnessed. Based on the separability principle, the negativity  $N$  can be used to quantify the entanglement [29]. The negativity  $N$  is introduced by

$$N(\rho) = \left| \sum_i \mu_i \right|, \quad (6)$$

where  $\mu_i$  is the  $i$ th negative eigenvalue of  $\rho^T$  which is the partial transpose of the mixed state  $\rho$ . The measure corresponds to the absolute value of the sum of negative eigenvalues of  $\rho^T$ . For the separability of unentangled states, the partial transpose matrix  $\rho^T$  has nonnegative eigenvalues if it is unentangled. As an example of thermal states in an isotropic spin- $s$  antiferromagnetic chain, the relation of entanglement witness to negativity is investigated.

Considering a two-spin isotropic antiferromagnetic Heisenberg chain, any thermal state  $\rho$  is an SU(2)-invariant state [33]. In the case of  $s=1/2$ , the partial transpose matrix  $\rho^T$  has negative eigenvalues when the correlation function satisfies [33]

$$\langle \vec{S}_1 \cdot \vec{S}_2 \rangle < -\frac{1}{4}. \quad (7)$$

For a thermal state, Eq. (7) is also equivalent to  $\langle H \rangle < -J/2$  or  $W < 0$  where  $E_{\min} = -J/2$ . The negativity can also be expressed by

$$N(\rho) = -\frac{W}{J}. \quad (8)$$

It shows that the thermal entanglement exists for  $N > 0$  or  $W < 0$ . That is, both the entanglement witness and the negativity provides the same condition for thermal entanglement in the case of  $s=1/2$ . The temperature range for thermal entanglement is given by  $T < 2J/\ln 3$ . However, for a thermal state of  $s=1$ , the negative partial transpose needs

$$\langle (\vec{S}_1 \cdot \vec{S}_2)^2 \rangle > 2, \quad (9)$$

which is also expressed by  $\langle H^2 \rangle > 8J^2$ . Equation (9) determines a temperature range for the existence of the entanglement. That is, the entanglement exists when  $T < 2J/\ln 2.08$ . Compared with the entanglement witness of Eq. (2), the thermal energy satisfies

$$\langle H \rangle < -2J. \quad (10)$$

This temperature range of Eq. (10) is  $T < 6J/\ln 10$ . It shows that the area of thermal entanglement decided by the negativity is larger than that determined by the entanglement witness. The exact relation of negativity and entanglement witness can be expressed as

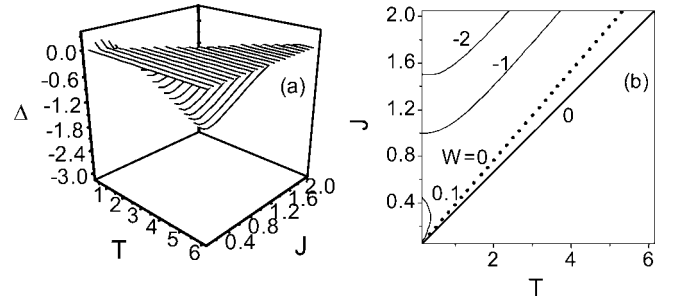


FIG. 3. (a) The difference  $\Delta = N - |W|$  of the negativity  $N$  and the witness  $W$  is plotted when the temperature and coupling are varied. (b) The corresponding contour map. The dotted line represents  $W = 0$ .

$$N(\rho) = \frac{1}{8J^2} [(W - 2J)^2 + V(H)] - 1, \quad (11)$$

where the variance  $V(H)$  is written by  $V(H) = \langle H^2 \rangle - \langle H \rangle^2$ . When the temperature  $T \geq T_c$ , the entanglement witness may be assumed to  $W = 0$ . The difference of  $\Delta = N - |W|$  is plotted in Fig. 3 when the temperature and coupling are varied. It shows that there is almost no differences for the weak coupling in Fig. 3(a). When the coupling  $J$  is increased, the difference becomes large. The contour map is shown in Fig. 3(b) where the dotted line represents  $W = 0$ . Since the temperature area of entanglement decided by negativity is larger than that by the witness, the difference  $\Delta = 0$  corresponds to the negativity  $N = 0$ . It is seen that the critical temperature of  $N$  is higher than that of  $W$ . It demonstrates that the entanglement witness  $W$  provides a more sufficient condition for thermal entanglement.

### IV. DISCUSSION

The entanglement in an isotropic spin- $s$  antiferromagnetic Heisenberg chain is investigated using the entanglement witness of thermal energy and the negativity. The analytic expression of the minimum-energy separable state is deduced. The entanglement witness determines a characteristic temperature  $T_c$  below which an entangled thermal state can be obtained. It is found that the characteristic temperature is almost linearly increased with the increasing number of spin- $s$ . For an  $L$ -partite spin chain,  $T_c$  decreases with increasing the number of lattices. However,  $T_c$  approaches a constant when the number of lattices is very large. This shows that the entanglement can be detected in a real solid state system of a large number of lattices even for finite temperature. It is also shown that the characteristic temperature is a linear function of the coupling. From the separability principle, the entanglement witness is different from the negativity in detecting thermal entanglement of high-spin quantum systems. The thermal energy provides a more sufficient condition for the existence of the entanglement.

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