Entanglement of the Heisenberg chain with the next-nearest-neighbor interaction

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The features of the concurrences between the nearest-neighbors and that of the next-nearest-neighbors for the one-dimensional Heisenberg model with next-nearest-neighbor coupling J are studied as functions of temperature and J. The two concurrences exhibit a different dependence on J at the ground state, which could be interpreted from the point of view of the correlation functions. The threshold temperature at which the concurrence is zero and the temperature effect on the two concurrences for systems up to 12 sites are studied numerically.

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I. INTRODUCTION

Much attention has been paid to the entanglement in spin systems [1–7] and indistinguishable particle systems [8] because it plays an important role in quantum physics [9,10]. Entanglement is not only a useful concept in quantum teleportation, but also relevant to quantum phase transitions [11,12] in condensed matter physics. Typical models include the Ising model in a transverse field [11] and the anisotropic Heisenberg model [7]. However, as far as we are aware, most discussions of the spin chains merely focused on the model with nearest-neighbor spin coupling. The entanglement of formation between two spins mostly vanishes unless the two sites under consideration are at most next-nearest neighbors [11]. It is therefore worthwhile to investigate the problem by taking account of next-nearest-neighbor coupling [13]. This is not merely a purely scholastic consideration, for there exist some quasi-one-dimensional compounds, such as $CuGeO_3$ [14] and NaV_2O_5 [15], that manifest such interactions. For the particular interests in the field of condensed matter physics, those systems have been well studied by the exact diagonalization method [17,18] and density matrix renormalization group (DMRG) approach [19–21]. All those works enriched our understanding of the ground-state properties, such as gap formation, dimerization, etc.; however, the relationship between next-nearest-neighbor coupling and entanglement, which is known as a pure quantum correlation and a resource in quantum communication, has not been investigated yet.

In this paper, we study the pairwise entanglement between the nearest-neighbor sites and that of the next-nearest-neighbor sites in a Heisenberg chain with next-nearest-neighbor coupling both at finite temperatures and at the ground state. The two quantities are characterized by the entanglement of formation, the concurrence [16]. In the next section we introduce the model and show how to calculate the entanglement of formation on the basis of the ground-state energy at $T=0$ and the partition function at finite T. In Sec. III, we study the properties of entanglement at the ground state and discuss some special cases. Our results show that the coupling between next-nearest-neighbor sites does not enhance the entanglement between nearest-neighbor sites, regardless of whether it is a ferromagnetic or antiferromagnetic coupling. In Sec. IV, we study the concurrence at finite temperatures. The dependence of threshold temperature on the next-nearest-neighbor coupling constant J is obtained explicitly. The summary and discussion are given in Sec. V.

II. MODEL AND ITS GENERAL FORMULATION

We consider a one-dimensional Heisenberg chain with next-nearest-neighbor coupling,

$$H(J) = \sum_{j=1}^{L} [\sigma_j \, \sigma_{j+1} + J\sigma_j\sigma_{j+2}], \tag{1}$$

where σ_j denote Pauli matrices for the spin at the jth site, L denotes the total number of sites, and the dimensionless parameter J refers to the ratio between the next-nearest-neighbor coupling and the nearest-neighbor coupling. This model is invariant under translation once the periodic boundary condition $\sigma_1=\sigma_{L+1}$ is imposed. Additionally, it is invariant under a global SU(2) rotation, which implies total spin conservation. Thus the reduced density matrix for the subspace of any two sites takes the form

$$\rho_{jl} = \begin{pmatrix} u^+ & 0 & 0 & 0 \\ 0 & w_1 & z & 0 \\ 0 & z^* & w_2 & 0 \\ 0 & 0 & 0 & u^- \end{pmatrix}, \tag{2}$$

which is expressed in the conventional bases $|00\rangle$, $|01\rangle$, $|10\rangle$, $|11\rangle$. The entities of the reduced density matrix (2) can be calculated from the correlation functions $G^{\alpha\beta}=\langle\sigma^\alpha\sigma^\beta\rangle$, namely,

$$u^+ = u^- = \frac{1}{4}(1+G^{zz}),$$

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$$z = \frac{1}{4}(G^{xx} + G^{yy} + iG^{xy} - iG^{yx}). \tag{3}$$

Consequently, the concurrence for arbitrary two sites [1] is evaluated as

$$C = 2\max[0, |z| - \sqrt{u^+u^-}] = \frac{1}{2}\max[0, 2|G^{zz}| - G^{zz} - 1], \tag{4}$$

The correlation function between next-nearest-neighbor sites at finite temperatures is given by

$$G_2^{zz}(T) = -\frac{T}{3Z}\frac{\partial Z}{\partial J}, \tag{5}$$

where Z is the partition function. The correlation function at zero temperature can be calculated according to the Hellman-Feynman theorem

$$G_2^{zz}|_{T=0} = \frac{1}{3}\frac{dE_0(J)}{dJ}, \tag{6}$$

where $E_0(J)$ denotes the ground-state energy. The correlation function for neighboring sites is evaluated as

$$G_1^{zz} = \frac{E}{3L} - JG_2^{zz}, \tag{7}$$

where $E = \langle H \rangle$ is the internal energy of the system. Clearly, the key point here is to study the two-site correlation function for the next-nearest neighbors. Although the concurrence defines a measurement of pure quantum correlation, it still depends on the correlation functions, which are applicable to both quantum and classical systems. The entanglement, however, only distills the quantum part from the system.

III. GROUND-STATE CONCURRENCE

As is well known, there are no exact results of the Hamiltonian (1) for general J except for some special values. When $J=0$, the Bethe-ansatz method was successfully applied to solve the ground state and excited states [22,23], from which the correlation function G_1^{zz} is easily obtained as $E/3L$. In terms of the internal energy, the thermal concurrence is evaluated to be 0.386 at the ground state. When $J=1/2$, the ground state is a uniformly weighted superposition of the two nearest-neighbor valence bond states [13] :

$$|\psi_1\rangle = [1,2][3,4]\cdots[L-1,L],$$

$$|\psi_2\rangle = [L,1][2,3]\cdots[L-2,L-1], \tag{8}$$

where

$$[i,j] = \frac{1}{\sqrt{2}}(|0\rangle_i|1\rangle_j - |1\rangle_i|0\rangle_j). \tag{9}$$

Then the ground-state concurrence can be simply written as

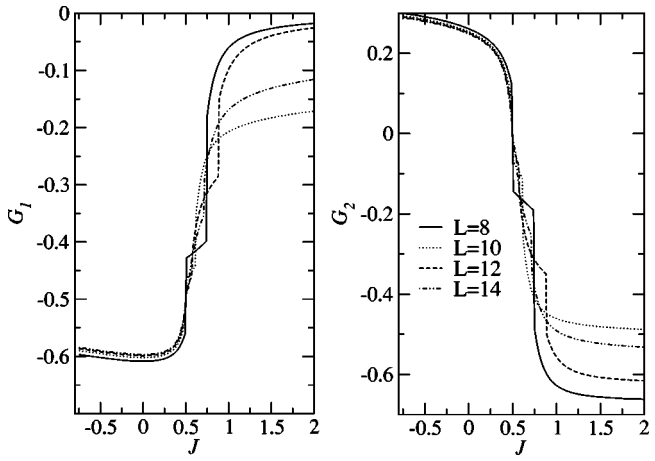

FIG. 1. The ground-state correlation function G_1 (left) and G_2 (right) versus J for various lattices. The singularity at $J=1/2$ arises from the level crossing (degeneracy).

$$C = \left(\frac{1}{2} + \frac{(-1)^{L/2}}{2^{L/2}}\right)\left(2 + \frac{(-1)^{L/2}}{2^{L/2-2}}\right)^{-1}, \tag{10}$$

for $L>2$, which tends to $1/4$ in the thermodynamic limit.

In general, one can numerically solve the eigenvalue problem of the Hamiltonian for a finite-size system. It is known that the ground state of the system for $J<0$ is an antiferromagnetic state [24], while for $J>0$ many numerical results indicate that the ground state is antiferromagnetic for a finite chain [25]. Thus we only need to consider the invariant subspace spanned by those states with an equal number of down spins and up spins—i.e., $S^z_{\text{total}}=0$. This subspace should include the eigenstates with the lowest eigenvalue of the system due to the global SU(2) symmetry. The ground-state energy can be obtained by diagonalizing the Hamiltonian in this subspace.

The correlation function of the nearest-neighbor sites G_1 and that of the next-nearest-neighbor sites G_2 are plotted in Fig. 1. The corresponding concurrences C_1 and C_2 are plotted in Fig. 2. The curves in those two figures show that G_1 reaches a minimum at $J=0$, which implies that the next-nearest-neighbor coupling J does not enhance the antiferromagnetic correlation between the nearest-neighbor sites. This may be regarded as evidence to support the argument that the presence of interactions with a third party generally suppresses the entanglement between the original biparties. This fact brings about a maximum value of the concurrence C_1 at $J=0$. Moreover, in the region with antiferromagnetic frustrated coupling $J>0$, the concurrence C_1 is significantly affected by the magnitude of J. Particularly, in the neighborhood of $J=1/2$, the antiferromagnetic correlation of G_1 is dramatically broken by the frustration effect. The C_1 is suppressed down to zero rapidly beyond a threshold value of J which is about 0.6 for $L=12$. In contrast, the correlation function G_2 and the concurrence C_2 behave in a completely different way. From the Hamiltonian, we can easily conclude that the frustration interaction $J>0$ supports the formation of an antiferromagnetic correlation G_2 and that C_2 is an increasing function of J, as shown in Fig. 2. Moreover, we can also

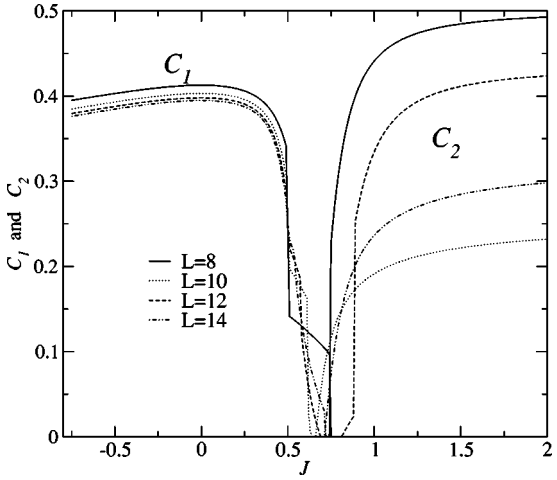

FIG. 2. The ground concurrence C_1 and C_2 versus J for various lattices. Their singularities around $J=1/2$ are caused by the level crossing (or degeneracy).

see from those figures that the concurrence as well as the correlation functions is not smoothly continuous for all values of J. We interpret this phenomenon as a consequence of the ground-state level crossing at $J=1/2$.

IV. THERMAL CONCURRENCE AND THRESHOLD TEMPERATURE

Since the density matrix at a finite temperature is a summation of Boltzmann weights over all states and becomes a diagonal matrix with equal entities when $T\to\infty$, G^{zz} goes to zero, causing the entanglement to vanish at this limit. The concurrence ought to be a descendent function of temperature. This implies that the thermal fluctuation at a finite temperature tends to suppress the pairwise entanglement. Therefore a threshold temperature T_{th} at which the concurrence vanishes is expected to exist. In the following we determine the dependence of the threshold temperature on the coupling constant J.

To observe its finite-size effect, we calculate the threshold temperature for systems with $L=4,5,\ldots,12$ numerically. The threshold temperature for the concurrence of nearest-neighbor sites is plotted in Fig. 3. Apparently, it converges rapidly as L increases. This is due to the fact that the concurrence studied here is only related to the nearest-neighbor correlation function, so even a system as small as $L=10$ can describe the physical properties of the thermodynamic system well. The system with up to $L=12$ sites is sufficient to specify the threshold temperature for the infinite system. We also observe that the system with an even (or odd) number of sites manifests different features. If $J<0$, the threshold temperature of the system with an even number of sites is larger than that with an odd number of sites just like in the traditional isotropic Heisenberg model [26]. This is because a ferromagnetic coupling J does not frustrate the tendency of singlet formation between nearest neighbors. If $J>0$, however, the situation becomes different due to the frustration. From the left panel Fig. 3, we see that the line of $L=5$ crosses with the other lines around $J=0.125$, so does $L=4$.

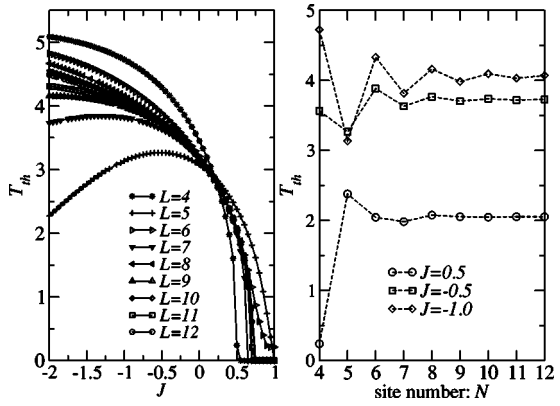

FIG. 3. Threshold temperature of the concurrence of the nearest-neighbor sites C_1 as a function of J for different lattices. Clearly, it converges quickly as L exceeds 10.

We plotted our numerical results for the threshold temperature for the case of next-nearest neighbors in Fig. 4. We can see that there is no entanglement at any temperature T and any coupling J when $L=6$. This is because the system can be partitioned into two parts for $L=6$, i.e., the part of sites $\{1,3,5\}$ and that of $\{2,4,6\}$. For each part, the next-nearest-neighbor interaction does not assist the entanglement of formation because of the inside frustration. For other cases, the threshold temperature exhibits "down-down-up-up" behavior as the number of sites increases, which differs from that of the nearest-neighbor sites completely, and it converges rapidly after L exceeds 10. We can therefore reasonably assume that the threshold temperature of a system with $L=12$ is sufficient to capture the feature of the infinite system. As is well known, in spin-1/2 systems, the nearest-neighbor superexchange interaction is estimated in the order of 1000 K. Our result shows that the threshold temperature is above that magnitude. Thus the entanglement of formation for spin systems may always exist at room temperature.

As we indicated before, the entanglement of a small system can well characterize the behavior of a large system. We plotted the thermal concurrence for nearest neighbors versus the temperature and the interaction J in Fig. 5. The thermal

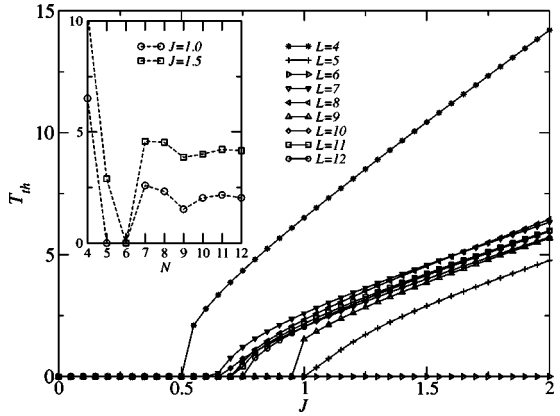

FIG. 4. Threshold temperature of the concurrence between the next-nearest-neighbor sites C_2 as a function of J for different lattices. Clearly, it converges quickly as L exceeds 10.

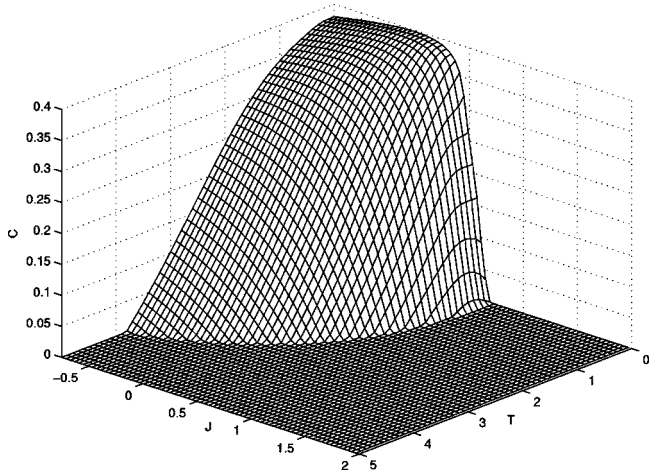

FIG. 5. The curved surface of thermal concurrence C_1 between the nearest-neighbor sites as a function of the temperature and the next-nearest-neighbor interaction J. Here $L=12$.

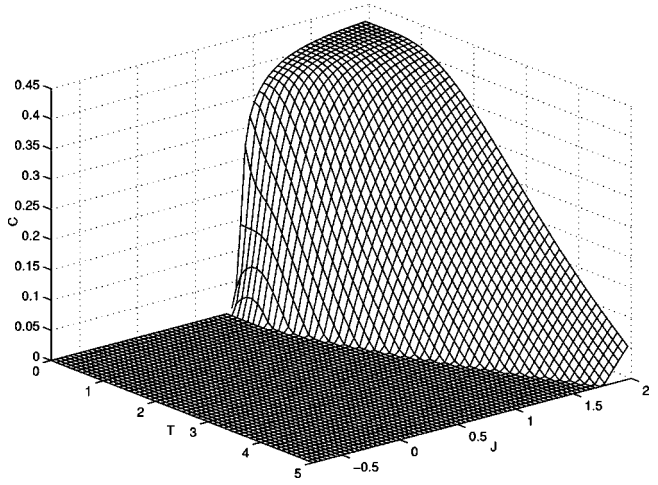

FIG. 6. The curved surface of thermal concurrence C_2 between the next-nearest-neighbor sites as a function of the temperature and the next-nearest-neighbor interaction J. Here $L=12$.

fluctuation usually suppresses the pairwise entanglement. However, around $J=0.6$ where the ground-state concurrence tends to zero, thermal fluctuations may enhance the concurrence. In Fig. 6, we gave the results of the thermal concurrence for the next-nearest neighbors. From Fig. 6, we observe that no next-nearest-neighbor spin entanglement occurs at any temperature as long as J is smaller than a threshold value J_{th}, while for $J>J_{th}$, thermal fluctuation suppresses it in most regions.

V. SUMMARY AND DISCUSSION

In this work, we studied the entanglement features of the Heisenberg chain in the presence of next-nearest-neighbor coupling. Both the entanglement between nearest-neighbor sites and that between next-nearest-neighbor sites are calculated for the ground state and for finite temperatures, respectively. We found that the frustrated interaction $J>0$ suppresses the nearest-neighbor concurrence substantially, while it induces the entanglement of formation between the next-nearest-neighbor sites. Naturally, one expects that the entanglement between spins located at site i and j will arise from a sufficiently large interaction between the two spins. However, this may not be true. Take the Haldane-Shastry model [27,28] as an example. This is a soluble model describing the long-range spin interaction $H=\Sigma_{nm} J_n\sigma_m\sigma_{m+n}$ with $J_n=J_0/[2\sin^2(n\pi/N)]$. Its correlation function $\langle\sigma_0\sigma_n\rangle$ decreases rapidly as n increases and the concurrence between any pair of two sites is zero. This example demonstrates that the concurrence is a unwonted resource in condensed matter physics. We also noted that the interaction with a third party generally suppresses the entanglement between the original biparties, regardless of whether the coupling is ferromagnetic or antiferromagnetic.

We also investigated the entanglement arising from thermal fluctuations at a finite temperature. The threshold temperature of the entanglement was calculated for systems with different sizes. We found that the dependence of T_{th} on J for systems with an even number of sites differs from that with an odd number of sites. Except in the region around $J=0.6$, the thermal fluctuation usually suppresses the entanglement at finite temperatures.

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