I. INTRODUCTION

Recently, much attention has been focused on the entanglement in the spin systems $\{1, 2, 3, 4, 5, 6, 7\}$ and indistinguishable particle systems $\{8\}$ due to the recently-discovered importance of entanglement in the quantum theory $\{9, 10\}$. These systems typically include transverse field Ising model and anisotropic Heisenberg model. And the studies not only reveal the non-trivial behavior of entanglement in the phenomenon of condensed matter physics, such as quantum phase transition $\{11, 12\}$, but also shed new light on the quantum physics. However, most of the previous works on the spin chain mainly focused on the model with the nearest spin exchange interaction. And in most cases, the entanglement of formation between two spin qubits vanishes unless the two sites are at most next-nearest neighbors $\{11\}$. Thus it is interesting to investigate the problem when other kinds of interaction besides the nearest-neighbor one exist, such as next-nearest-neighbor interaction. This is not merely a pure theoretical consideration, whereas, there does exist some quasi-one-dimensional compounds, such as CuGeO$_3$ $\{13\}$ and NaV$_2$O$_5$ $\{14\}$, manifesting strong evidence of the presence of such interaction.

In this paper, we study the pairwise entanglement of the nearest-neighbor sites and of the next-nearest-neighbor sites in a Heisenberg chain with the next-nearest-neighbor exchange both at finite temperatures and the ground state. The entanglement of formation, i.e., the concurrence $\{15\}$ is used to quantify these two quantities. In the following section, we first introduce the model, then show that the entanglement of formation can be calculated either from the ground state energy at $T = 0$ or from the partition function at finite $T$. In section III, we study the properties of the entanglement at the ground state, and discuss some special cases. Our results show that the presence of the interaction between the next-nearest-neighbor sites does not enhance the entanglement between the nearest-neighbor sites, regardless it is a ferromagnetic or antiferromagnetic coupling.

In section IV the thermal concurrences of a 12-site system as well as the threshold temperature with different size’s systems are investigated. Finally, a brief summary and discussions are given in section V.

II. THE MODEL FORMULATION

The Hamiltonian of a Heisenberg chain with the next-nearest-neighbor interaction and periodic boundary conditions reads

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

$$\sigma_1 = \sigma_{L+1},$$

(1)

where $L$ is the number of lattice sites, $\sigma_j = (\sigma^x_j, \sigma^y_j, \sigma^z_j)$ denote Pauli matrices of a spin at $j$th site, and $J$ is a dimensionless parameter characterizing the interaction strength between the next-nearest-neighbor sites. The Hamiltonian is obviously invariant under translation, and moreover, it has SU(2) symmetry, which manifests the spin conservation. Thus the reduced density matrix between the arbitrary two sites takes the form

$$\rho_{jl} = \frac{1}{4} \begin{pmatrix} u^{+} & 0 & 0 & 0 \\ 0 & w_1 & z & 0 \\ 0 & z^* & w_2 & 0 \\ 0 & 0 & 0 & u^- \end{pmatrix}$$

(2)

in the standard basis $|00\rangle, |01\rangle, |10\rangle, |11\rangle$, and the corresponding concurrence has already been given $\{1\}$

$$C = 2 \max \left[ 0, |z| - \sqrt{u^{+}u^-} \right].$$

(3)

The entities of the reduced density matrix $\{2\}$ can be calculated from correlation functions $G$, for the present model, they are

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

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

(4)
where $G^{\alpha\beta} = \langle \sigma^\alpha \sigma^\beta \rangle$. Hence the concurrence of arbitrary two sites is given by

$$C = \frac{1}{2} \max \left[ 0, 2|G^{zz}| - G^{zz} - 1 \right],$$  \hspace{1cm} (5)

where the SU(2) symmetry has been taken into account. According to statistical physics, the correlation function of the next-nearest-neighbor sites at finite temperatures is

$$G^{zz}_2(T) = -\frac{T}{3Z} \frac{\partial Z}{\partial J},$$  \hspace{1cm} (6)

where $Z$ is the partition function and the subscript 2 denotes distance between two sites (so does the subscript 1 given below). At the ground state, by the Hellmann-Feynman theorem, we have

$$G^{zz}_2 \bigg|_{T=0} = \frac{1}{3} \frac{dE(J)}{dJ}. $$  \hspace{1cm} (7)

Then the correlation function of neighboring sites is evaluated as

$$G^{zz}_1 = \frac{E}{3L} - JG^{zz}_2,$$  \hspace{1cm} (8)

where $E = \langle H \rangle$ is the internal energy of the system. Hence the key point is to study the two-site correlation function for the next-nearest neighbors.

III. GROUND STATE CONCURRENCE

As is well known, the exact results of the Hamiltonian \cite{1} for general $J$ have not yet been obtained except for some special points. At $J = 0$, the exact solution for the ground state and excited states has been well studied by the Bethe-ansatz method, and the correlation function $G^{zz}_1$ is simply $E/3L$, thus the thermal concurrence can be expressed in terms of the internal energy and it equals to 0.386 for the ground state. When $J = 1/2$, the ground state consists of an equal-weight superposition of the two nearest-neighbor valence bond state\cite{16}:

$$\begin{align*}
|\psi_1\rangle &= [1, 2][3, 4] \cdots [L - 1, L] \\
|\psi_2\rangle &= [L, 1][2, 3] \cdots [L - 2, L - 1]
\end{align*}$$  \hspace{1cm} (9)

where

$$[i, j] = \frac{1}{\sqrt{2}} (|0\rangle_i |1\rangle_j - |1\rangle_i |0\rangle_j).$$  \hspace{1cm} (10)

Hence the ground state concurrence can be simply written as

$$C = \left( \frac{1}{2} + \frac{1}{2L/2} \right) \left( 2 + \frac{(-1)^{L/2}}{2L/2-2} \right)^{-1},$$  \hspace{1cm} (11)

which becomes 1/4 in the thermodynamic limit.

In general case, however, we need to solve the eigenvalue problem of the Hamiltonian for finite-size system numerically. It can be shown that the ground state of the system for $J < 0$ is antiferromagnetic\cite{17}, while for $J > 0$, many numerical results suggested that the ground state is antiferromagnetic for finite chain\cite{18}. Thus we only need to work in the invariant subspace spanned by those states with equal number of down spins and up spins, i.e., $S_{\text{total}}^{z} = 0$. For example, if $L = 10$, the dimension of the subspace is 252. This subspace should include the eigenstate 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.

We show the correlation function of the nearest-neighbor sites $G_1$ and that of the next-nearest-neighbor sites $G_2$ in Fig. 1 and the corresponding $C_{1(2)}$ in Fig. 2. From those two figures, we see that $G_1$ reaches a minimum at $J = 0$, which means that the presence of the interaction $J$ between the next-nearest-neighbor sites does...
not enhance the antiferromagnetic correlation between the nearest-neighbor sites, regardless it is a ferromagnetic or antiferromagnetic coupling. From this point of view, we deem that the presence of interaction with the third party generally suppresses the entanglement between original bi-parties. This fact obviously leads to a maximum value of the concurrence $C_1$ at $J = 0$. Moreover, in the region of antiferromagnetically frustrated coupling $J > 0$, the concurrence $C_1$ is strongly affected by the value of $J$, especially around $J = 1/2$, as the antiferromagnetic correlation of $G_1$ is dramatically broken by the frustration effect. And $C_1$ then will be suppressed down to zero quickly at a critical point $J_c$. On the contrary, the correlation function $G_2$, as well as the concurrence $C_2$, between the next-nearest-neighbor sites behave completely in a different way. From the Hamiltonian, we can easily conclude that the frustrated interaction $J > 0$ helps the formation of antiferromagnetic correlation $G_2$, thus it is an obviously conclusion that $C_2$ is an increasing function of $J$, as shown in Fig. 2. Moreover, we can also see from the figures that the concurrence as well as the correlation function are not smoothly continuous for all value of $J$. We interpret this phenomena as a consequence of the ground-state level crossing around $J = 1/2$ for finite-size systems.

IV. THERMAL CONCURRENCE AND THRESHOLD TEMPERATURE

At finite temperatures, the density matrix of the system is the summation of all states with its Boltzmann weight. Therefore, in the $T \to \infty$ limit, the density matrix consists of an uniform distribution in the state space, which leads to a vanishing $G^{\infty}$. From Eq. 5, we then have a zero entanglement. Thus the thermal fluctuations at high temperature always suppresses the pairwise entanglement, namely, the concurrence is a decreasing function of the temperature. So it is natural to expect that there exists a threshold temperature $T_{th}$ at which the concurrence vanishes. In this section, we start with the dependence of threshold temperature on the size of the system and coupling constant.

We use numerical method to determine the threshold temperature for the system of $L = 4, 5, \ldots, 12$. The results for the concurrence of the nearest-neighbor sites are presented in Fig. 3 from which we observe the finite size effect of the threshold temperature. We find that the threshold temperature converge quickly as $L$ increases, this is due to the fact that the concurrence here is expressed in terms of the two-site correlation function of the nearest-neighbor sites, or from the other point, simply the internal energy. And for system’s energy, a smallish system, such as $L > 12$, can well describe the physical properties of the thermodynamic system. So we conclude that the system up to $L = 12$ is sufficient to describe the threshold temperature for the infinite system. We also observe that the system of even (or odd) number sites manifest different properties. If $J < 0$, the threshold temperature of even-number-site system is larger than that of odd-number-site system, which is very similar to the results of traditional isotropic Heisenberg model. This is because a ferromagnetic $J$ does not frustrate the tendency of singlet formation between nearest-neighbor sites. If $J > 0$, however, the situation becomes different, merely due to the frustration. From the left plot of Fig. 4 we see that the line of $L = 5$ crosses the other lines around $J = 0.125$, so does $L = 4$. Consequently, the threshold temperature of the nearest-neighbor sites is not always a decreasing function of $J$, the exceptions include $L = 5$ and $L = 7$. For large system, it is expected to vanish around $J = 0.7$.

In Fig. 4 we present our numerical result of the threshold temperature of the concurrence between the next-nearest-neighbor sites. We see that for the case of $L = 6$, there is no entanglement at any temperature and $J$. It is because that if $L = 6$, the system can be divided into two parts, including sites $\{1, 3, 5\}$ and $\{2, 4, 6\}$, respectively. For each closed part, the frustrated interaction does not assist the entanglement of formation because...
As we pointed out before, the entanglement of a smallish system can well represent the behavior of a large system. We show the thermal concurrence of nearest-neighbor sites as a function of the temperature and the interaction $J$ in Fig. 6. Generally, the thermal fluctuation suppresses the pairwise entanglement. Around $J = 0.6$, the concurrence tends to zero at the ground state, the thermal fluctuation may enhance it. In Fig. 6 we show the results of thermal concurrence of the next-nearest-neighbor sites, from which we can see that there is no entanglement at any temperature if $J < J_c$. While at $J > J_c$, the thermal frustration also generally breaks the entanglement except in a small region of $J \rightarrow J_c$.

V. SUMMARY AND DISCUSSION

In this paper, we studied the entanglement between the nearest-neighbor sites as well as the next-nearest-neighbor sites in a Heisenberg chain with the next-nearest-neighbor interaction both at the ground state and finite temperatures. We found that the presence of a frustrated interaction $J > 0$ will induce the entanglement of formation between the next-nearest-neighbor sites. Thus, the entanglement in spin system stems from sufficiently large interaction between two sites. However, physically, the long-range interaction usually decreases as the distance increases. A typical example is the Haldane-Shastry model [20, 21], which is modelled by $H = \sum_{nm} J_{nm} \sigma_m \sigma_{m+n}$ with $J_{nm} = J_0/2 \sin^2(n\pi/N)$. Its correlation function $\langle \sigma_n \sigma_{n+m} \rangle$ also decreases rapidly as $n$ increases, which results in a zero concurrence even between the nearest-neighbor sites. It is therefore believed that the concurrence is unwanted resources in realistic condensed matter. We also found that the presence of the interaction with third party generally suppresses the entanglement between original bi-parties, regardless it is ferromagnetic or antiferromagnetic.

At finite temperature, we studied the entanglement by considering the thermal fluctuation. The threshold temperature of the entanglement was discussed for different system sizes. We found that $T_{th}$ shows different properties for the system with even and odd number sites, and it converges quickly when the number of sites exceeds 10. The thermal fluctuation generally suppresses the entanglement at finite temperatures except in some region, i.e., around $J = 0.6$, where it may enhance the entanglement.

This work is supported by the Earmarked Grant for Research from the Research Grants Council (RGC) of the HKSAR, China (Project CUHK 4246/01P & 4037/02P), and NSF China No.10225419 & No. 90103022.

[1] K. M. O’Connor and W. K. Wootters, Phys. Rev. A 63, 052302 (2001).
[2] P. Zanardi, Phys. Rev. A 65, 042101(2002).
[3] L.F. Santos, Phys. Rev. A 67, 062306 (2003).
[4] X. Wang, Phys. Lett. A 281, 101(2001).
[5] X. Wang, and P. Zanardi, Phys. Lett. A 301, 1(2002).
[6] Y. Sun, Y. Chen, and H. Chen, Phys. Rev. A 68, 044301 (2003).
[7] S. J. Gu, H. Q. Lin, and Y. Q. Li, Phys. Rev. A 68, 042330 (2003).
[8] P. Zanardi, and X. Wang, J. Phys. A 35, 7947 (2002).
[9] M. A. Nilesen and I. L. Chuang, Quantum Computation and Quantum Information (Cambridge University Press, Cambridge, England, 2000)
[10] See review article by C. H. Bennett and D. P. Divincenzo, Nature 404, 247 (2000).
[11] A. Osterloh, Luigi Amico, G. Falci and Rosario Fazio, Nature 416, 608 (2002).
[12] G. Vidal, J. I. Latorre, E. Rico, and A. Kitaev, Phys. Rev. Lett. 90, 227902 (2003).
[13] M. Hase, I. Terasaki, and K. Uchinokura, Phys. Rev. Lett. 70, 3651 (1993).
[14] J. W. Bray et al., in Extended Linear Chain Compounds, edited by J. S. Miller (Plenum, New Youk, 1993), Vol. 3, pp. 353-415.
[15] W. K. Wootters, Phys. Rev. Lett. 80, 2245 (1998).
[16] C. K. Majumdar, J. Phys. C 3, 911 (1969).
[17] E. Lieb and D. Mattis, J. Math. Phys. 3, 749 (1962).
[18] H. P. Bader and R. Schilling, Phys. Rev. B 19, 3556 (1979).
[19] X. Wang, Phys. Rev. A 66, 044305 (2002).
[20] F. D. M. Haldane, Phys. Rev. Lett. 60, 635 (1988).
[21] B. S. Shastry, Phys. Rev. Lett. 60, 639 (1988).