# Effects of the Next-Nearest-Neighbor Interaction on the Entanglement of the Heisenberg XX Chain*

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**Abstract** The pairwise entanglement of the Heisenberg XX chain with next-nearest-neighbor (NNN) interactions was investigated by using the concurrence measure. The results show that for the nearest-neighbor sites, the entanglement may be improved or suppressed depending on the magnitudes of the NNN coupling constant $J$, while for the next-nearest-neighbor sites, it always increases with the increase of $|J|$. The critical temperature $T_c$ decreases with the increase of $J$ for the nearest-neighbor entanglement and increases with the increase of $|J|$ for the next-nearest-neighbor entanglement, respectively. We also show that the general Heisenberg XX model still can be used to create the entangled W states of three and four qubits, and that the presence of NNN coupling has no effect on the creation of four-qubit W states, while it shifts the instant of time at which the three-qubit W states are created.

**Key words** Heisenberg XX chain, next-nearest-neighbor interaction, thermal entanglement

## 1 Introduction

Entanglement is a unique quantum property that does not exist classically. It has attracted much attention in recent years due to its central role in quantum communication[1, 2] and information processing[3], such as quantum teleportation[1], superdense coding[4], quantum cryptographic key distribution[2], etc. Particularly, in the field of condensed-matter physics, the entanglement of the quantum spin systems was intensively investigated[5—13] with the measure of the entanglement formation, namely, the concurrence $C$ (see below). However, as far as we know, most discussions mentioned above merely focused on the models with the nearest-neighbor (NN) interactions, and the next-nearest-neighbor (NNN) interaction has seldom been taken into account. In fact, there are some quasi-one-dimensional and two-dimensional antiferromagnetic (AFM)[14] spin models that manifest such interactions. Therefore, it is worthwhile to include these interactions in the studies of spin chain entanglement.

In this paper, we study pairwise entanglement between the nearest neighbors and that between the next-nearest neighbors in a spin-1/2 antiferromagnetic Heisenberg XX chain with the nearest-neighbor coupling constant $J_1$ and the next-nearest-neighbor coupling constant $J_2$. We quantify it by means of the concurrence[15, 16], which is defined as $C=\max\{\lambda_1-\lambda_2-\lambda_3-\lambda_4,0\}$, where the $\lambda_i$'s are the square roots of the eigenvalues of the product matrix $R=\rho_{ij}\tilde{\rho}_{ij}$ in the decreasing order. The spin-flipped density matrix is defined by $\tilde{\rho}_{ij}=(\sigma_i^y\otimes\sigma_j^y)\rho_{ij}^*(\sigma_i^y\otimes\sigma_j^y)$. For a system with temperature $T$ at thermal equilibrium, the density matrix is characterized by $\rho(T)=Z^{-1}\exp(-\hat{H}/k_{\rm B}T)$, where $Z=\mathrm{Tr}\,[\exp(-\hat{H}/k_{\rm B}T)]$ is

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the partition function and $k_{\rm B}$ is the Boltzmann's constant and has been set to 1 hereafter. The reduced density matrix $\rho_{ij}$ is obtained by tracing out all other qubits from $\rho(T)$.

## 2 General formalism

The Hamiltonian for the spin-1/2 Heisenberg XX chain we studied in this paper is described by

$$\hat{H} = \sum_{n=1}^{N}(\sigma_n^x\sigma_{n+1}^x+\sigma_n^y\sigma_{n+1}^y)+ J\sum_{n=1}^{N}(\sigma_n^x\sigma_{n+2}^x+\sigma_n^y\sigma_{n+2}^y). \quad (1)$$

where we have set the NN coupling constant $J_1$ to 1 and the NNN coupling constant $J_2$ to $J$ for reason of succinct presentation. The periodic boundary condition is imposed, so that $N+1\equiv 1$, $N+2\equiv 2$. The topology of the chain being studied is illustrated in Fig. 1, which can also be considered a two-chain lattice with diagonal, or "zigzag" couplings.

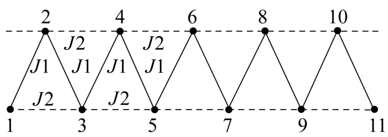


Fig. 1. Schematic picture of the zigzag spin chain.

The model we studied has the symmetry of translational invariance, and also it is easy to check that the commutator $[\hat{H}, S^z]$=0 (rotation symmetry about the $z$-axis); all these guarantee that the reduced density matrix for the subspace of any two spins has the form

$$\rho_{ij}=\begin{pmatrix} u^+ & 0 & 0 & 0 \\ 0 & \omega & z & 0 \\ 0 & z & \omega & 0 \\ 0 & 0 & 0 & u^- \end{pmatrix}, \quad (2)$$

in the standard basis $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$. Here $S^z=\sum_{i=1}^{N}(\sigma_i^z/2)$ are the collective spin operators. The elements of the reduced density matrix (2) are related to various correlation functions $G^{\alpha\beta}=\langle\sigma_i^\alpha\sigma_j^\beta\rangle$ ($\alpha,\ \beta=x,\ y,\ z$) and the magnetization per site $\bar{M}=\langle\sum_{i=1}^{N}\sigma_i^z\rangle/N$ as

$$\begin{aligned} u^{\pm} &= \frac{1}{4}(1+G^{zz}\pm 2\bar{M}) \\ z &= \frac{1}{4}(G^{xx}+G^{yy}) \end{aligned}, \quad (3)$$

The fact $[\hat{H},\ S^z]$=0 guarantees that $G^{xx}=G^{yy}$, so the corresponding concurrence quantifying the entanglement of arbitrary two spins is readily obtained as

$$C=\max\{|G^{xx}|-\frac{1}{2}\sqrt{(1+G^{zz})^2-4\bar{M}^2},0\}. \quad (4)$$

## 3 Entanglement of the ground states

### 3.1 Ground-state entanglement

To observe the effects of the next-nearest- neighbor (NNN) exchange interactions on the entanglement of the ground states, we give our numerical simulation results as follows. We first consider the case of the nearest-neighbor entanglement, which is plotted as a function of $J$ for $N$=6,7,$\cdots$,10 in Fig. 2(a). Apparently, with the increasing value of $J$, the concurrence $C_{\rm n}$ (the subscript n denotes the nearest-neighbor entanglement) firstly increases monotonously and arrives at a certain maximum value, then decays off gradually and drops to zero suddenly when $J$ reaches a critical point $J_{\rm c}$. The singularities are mainly caused by the energy level-crossing at these points. Also one can find from Fig. 2(a) that for any number $N$, the frustrated NNN exchange interactions can be used to enhance the entanglement between the nearest-neighbor sites at some special parameter regions of $J$, which implies that the presence of interactions with a third party does not always suppress the entanglement between the original biparties; sometimes it may improve the entanglement. Moreover, we note that the curves for entanglement in the case of even and odd $N$ converge rapidly as $N$ increases, which can be understood from the fact that for large $N$, it should not make a difference to the nearest-neighbor entanglement whether we add or subtract a qubit somewhere far along the chain.

For entanglement of the next-nearest-neighbor sites, as can be seen from Fig. 2(b), there is no entanglement if $|J|$ is below some certain values, which means a weak NNN exchange interaction still cannot induce entanglement between the next-nearest-neighbor sites. However, if the frustrated NNN exchange interaction is strong enough, the entanglement may be enhanced with the increase of $|J|$ except the case of $N$=6.

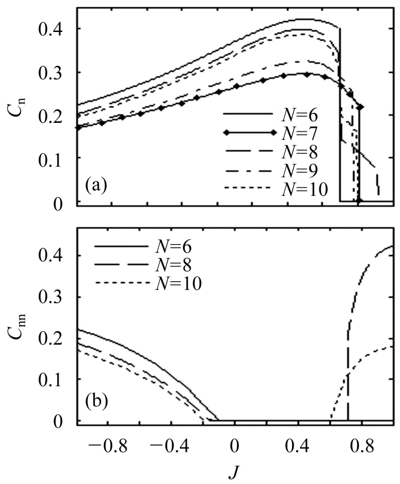


Fig. 2. Concurrence versus the next-nearest-neighbor coupling constant $J$ at zero absolute temperature. (a) entanglement of the nearest-neighbor spins; (b) entanglement of the next-nearest-neighbor spins.

### 3.2 Generation of the entangled W states

The Heisenberg XX model with only the nearest-neighbor exchange interactions can be used to generate the entangled W states of the form $|W_N\rangle=(1/\sqrt{N})(\mathrm{e}^{\mathrm{i}\theta_1}|100\cdots0\rangle+\mathrm{e}^{\mathrm{i}\theta_2}|010\cdots0\rangle+\mathrm{e}^{\mathrm{i}\theta_3}|001\cdots0\rangle+\cdots+\mathrm{e}^{\mathrm{i}\theta_N}|000\cdots1\rangle)$ for three and four qubits[5]. However, when the frustrated next-nearest-neighbor interaction is present, can such states still be generated, or do the NNN interactions have any effect on the generation of the so-called W states? In order to see this explicitly, let us first rewrite the Hamiltonian (1) as

$$\hat{H} = 2\left[\sum_{n=1}^{N}(\sigma_n^+\sigma_{n+1}^- + \sigma_{n+1}^+\sigma_n^-) + J\sum_{n=1}^{N}(\sigma_n^+\sigma_{n+2}^- + \sigma_{n+2}^+\sigma_n^-)\right]. \tag{5}$$

where $\sigma^{\pm}=(\sigma^x \pm \mathrm{i}\sigma^y)/2$ are the raising and lowering operators, respectively.

Then if we prepare the initial state of the system with the first spin pointing up and all other spins pointing down (i.e., the initial state of the system is $\sigma_1^+|0\rangle^{\otimes N}$), following the procedures of Ref. [5], the state vector at time $t$ is easily obtained as

$$|\Psi(t)\rangle = \sum_{n=1}^{N} b_n(t)\sigma_n^+|0\rangle^{\otimes N}, \tag{6}$$

where

$$b_n(t) = \frac{1}{N}\sum_{k=1}^{N}\exp\left[\mathrm{i}\frac{2k(n-1)\pi}{N} - \mathrm{i}t\left(\cos\frac{2k\pi}{N} + J\cos\frac{4k\pi}{N}\right)\right]. \tag{7}$$

From Eq. (7), the probability at time $t$ for state $\sigma_n^+|0\rangle^{\otimes N}$ is obtained as

$$p(n,N,t) = |b_n(t)|^2, \tag{8}$$

For the case of $N$=3 and $N$=4, after a straightforward calculation, the expressions of $p(n,N,t)$ are given by

$$\begin{aligned} p(1,3,t) &= \frac{1}{9}[5+4\cos(6+6J)t] \\ p(2,3,t) &= p(3,3,t) = \frac{1}{9}[2-2\cos(6+6J)t] \end{aligned}, \tag{9}$$

and

$$\begin{aligned} p(1,4,t) &= \cos^4(2t) \\ p(2,4,t) &= \frac{1}{4}\sin^2(4t) \\ p(3,4,t) &= \frac{1}{4}[1+\cos^2(4t)-2\cos(4t)\cos(8Jt)] \\ p(4,4,t) &= \frac{1}{4}[1+\cos^2(4t)-2\cos(4t)\sin(8Jt)] \end{aligned}. \tag{10}$$

As everyone knows, in order to generate the so-called entangled W states, the equality $p(n,N,t)=1/N$ must be satisfied, which gives the following solutions

$$\begin{aligned} t_n &= \frac{(1+3n)\pi}{9(1+J)} \quad \text{or} \\ t_n &= \frac{(2+3n)\pi}{9(1+J)} \quad (n=0,1,2,\cdots) \end{aligned}, \tag{11}$$

and

$$t_n = \frac{(1+2n)\pi}{8} \quad (n=0,1,2,\cdots). \tag{12}$$

for $N$=3 and 4, respectively.

Apparently, the three-qubit and four-qubit entangled W states can be generated by only one-time evolution of the Heisenberg XX model. However, the instant of time at which the three-qubit entangled W states are generated is changed by the presence of the NNN exchange interactions compared with the case that only interacts via the NN interactions, while it has no effect on the generation of the four-qubit entangled W states.

Further studies show that we can't generate entangled W states more than four qubits with this model, no matter whether the frustrated NNN interactions are present or not.

## 4 Thermal entanglement

Raising the temperature mixed the ground states with other states, depending on the relative magnitudes of the parameters involved, the effects of the NNN coupling on the pairwise entanglement may be different. To observe these clearly, we determine the dependence of the concurrence on the NNN coupling constant $J$ and the environment temperature $T$.

We begin by considering the entanglement of the nearest-neighbor sites, which is plotted as a function of $J$ and $T$ for $N$=10 in Fig. 3(a). One can observe that when the frustrated NNN coupling constant $J>0.7$, there is no entanglement at any temperature $T$. This indicates that a strong antiferromagnetic frustrated NNN coupling generally suppresses the pairwise entanglement between the nearest-neighbor spins in the Heisenberg XX model. When the NNN coupling constant $J<0.7$, at any fixed temperature $T$, the concurrence $C_{\rm n}$ initially increases with the increase of $J$, and then arrives at a certain maximum value before it decays off to zero as $J$ reaches a critical point $J_{\rm c}$. And as is shown in Fig. 3(a), $J_{\rm c}$ decreases with the increase of the temperature $T$.

Also it is worthwhile to note that there exists a threshold temperature $T_{\rm th}$ (about 0.8 for $N$=10) at which the concurrence $C_{\rm n}$ obtains its maximum value when $J$=0. At this critical point, the nearest-neighbor entanglement is always suppressed when the NNN exchange interaction is present, while for $T<T_{\rm th}$, it is always suppressed when $J<0$, and for $T>T_{\rm th}$, it is always suppressed when $J>0$.

The next-nearest-neighbor entanglement as a function of $J$ and $T$ for $N$=10 is shown in Fig. 3(b). It is clear that the entanglement only occurs when $J<-0.2$ or $J>0.6$, and at these two regions, it always increases with the increasing value of $|J|$ at any temperature $T$. The fact that there is no next-nearest-neighbor entanglement for $-0.2<J<0.6$ may be regarded as evidence to support the argument that even the presence of a weak NNN exchange interaction still cannot induce entanglement between the next-nearest-neighbor spins.

Fig. 3 also shows that the concurrence $C_{\rm n}$ and $C_{\rm nn}$ ($C_{\rm nn}$ denotes the next-nearest-neighbor entanglement) always decrease with the increase of the temperature $T$, which means the thermal fluctuation usually suppresses the pairwise entanglement in the one-dimensional Heisenberg XX model.

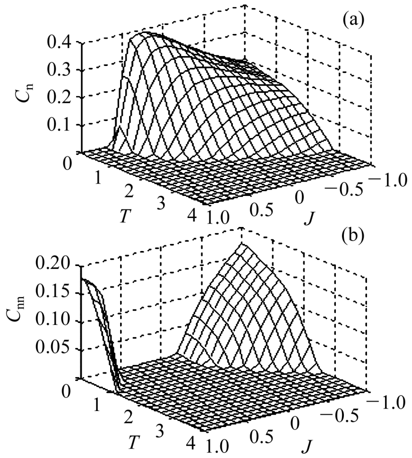


Fig. 3. Concurrence versus both next-nearest-neighbor coupling constant $J$ and temperature $T$ for $N$=10. (a) entanglement of the nearest-neighbor spins; (b) entanglement of the next-nearest-neighbor spins.

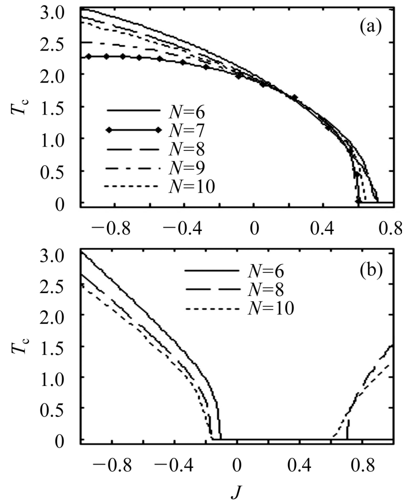


Fig. 4. Critical temperature $T_{\rm c}$ versus the next-nearest-neighbor coupling constant $J$. (a) entanglement of the nearest-neighbor spins; (b) entanglement of the next-nearest-neighbor spins.

In Fig. 4 we give the dependence of the critical temperature $T_c$ (above which the entanglement vanishes) on the NNN coupling constant $J$. Clearly, for entanglement of the nearest neighbors, $T_c$ always decreases with the increase of $J$ and drops to zero at the neighborhood of $J$=0.65; and there is a cross point around $J$=0.2. For entanglement of the next-nearest neighbors, $T_c$ firstly keeps its constant value of zero, and then increases with the increase of $|J|$.

## 5 Conclusion

In this paper, we investigated the pairwise entanglement of the Heisenberg XX model in the presence of the next-nearest-neighbor exchange interactions. Through calculating the concurrence of the system, we show that the nearest-neighbor entanglement may be enhanced or suppressed depending on the magnitudes of the NNN coupling constant $J$, while the next-nearest-neighbor entanglement always increases with the increase of $|J|$. The critical temperature $T_c$ above which the entanglement vanishes is also studied, and the results show that $T_c$ declines with the increase of $J$ for entanglement of nearest neighbors, and rises with the increase of $|J|$ for entanglement of the next-nearest neighbors.

By solving the XX model, we also show that the existence of the NNN coupling shifts the instant of time at which the three-qubit entangled W states are generated, while it has no effect on the generation of the four-qubit entangled W states.

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# 次近邻相互作用对Heisenberg XX链纠缠影响的研究*


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**摘要** 研究了存在次近邻相互作用(耦合)时Heisenberg XX链的纠缠特性. 结果表明对近邻格点, 随着耦合常数$J$的变化, 次近邻相互作用的存在可能使其纠缠度增大或者减小; 而对次近邻格点, 引进次近邻相互作用却可以产生纠缠, 并且使其随着$|J|$的增大而增大. 近邻格点间纠缠存在的临界温度$T_c$随着$J$的增大而降低, 次近邻格点间纠缠存在的临界温度$T_c$随着$|J|$的增大而升高. 此外对纠缠W态的制备, 次近邻相互作用的存在还使得三量子位情形时W态产生的时刻改变, 而对于四量子位情形却没有影响.



**关键词** Heisenberg XX链 次近邻相互作用 热纠缠

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