# Enhanced thermal entanglement in an anisotropic Heisenberg *XYZ* chain

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The thermal entanglement in the Heisenberg $XYZ$ chain is investigated in the presence of an external magnetic field $B$. In the two-qubit system, the critical magnetic field $B_c$ is increased by introducing the interaction of the $z$ component of two neighboring spins $J_z$. This interaction not only improves the critical temperature $T_c$, but also enhances the entanglement for a particular fixed $B$. We also analyze the pairwise entanglement between nearest neighbors in three qubits. The pairwise entanglement, for a fixed $T$, can become strong by controlling $B$ and $J_z$.

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*Introduction.* Entanglement is an important resource in quantum information [1]. The ideal case in which quantum computing and quantum communication are put into use is to find an entanglement resource in solid system at a finite temperature. The Heisenberg model is a simple but realistic and extensively studied solid-state system [2,3]. Recently, it has been found that the Heisenberg interaction is not localized in spin system. It can be realized in quantum dots [4], nuclear spins [5], cavity QED [6,7]. This effective Hamiltonian can be used for quantum computation [8] and controlled-NOT gate [7]. The thermal entanglement in an isotropic Heisenberg spin chain has been studied in the absence [15] and in the presence of an external magnetic field $B$ [9,10,14]. The entanglement of the two-qubit isotropic Heisenberg system decreases with increasing $T$ and vanishes beyond a critical value $T_c$ [9,10], which is independent of $B$. Pairwise entanglement in the $N$-qubit isotropic Heisenberg system in certain degree can be increased by increasing the temperature or the external field $B$ [9]. An anisotropic $XY$ Heisenberg spin chain has been investigated in the case of $B=0$ [10] and $B\neq 0$ [11]. For a two-qubit anisotropic Heisenberg $XY$ chain, one is able to produce entanglement for finite $T$ by adjusting the magnetic-field strength [11]. However, the entanglement by increasing $T$ or $B$, in the two-qubit anisotropic Heisenberg $XY$ chain [11] or in the $N$-qubit isotropic Heisenberg chain [9], is very weak. How to produce strong entanglement is worth studying.

On the other hand, we have not found any work regarding the two-qubit or the $N$-qubit anisotropic $XYZ$ Heisenberg chain in the presence of magnetic field. Although the $N$-qubit Heisenberg chain has been studied [12,9], in Ref. [12] the authors studied the maximum possible nearest-neighbor entanglement for ground state in a ring of $N$ qubits, and in Ref. [9] they just investigated the case of the isotropic $N$-qubit Heisenberg chain. In this paper, we study the entanglement of the two-qubit anisotropic Heisenberg $XYZ$ chain and the pairwise entanglement of the three-qubit anisotropic Heisenberg $XYZ$ chain. Introducing the interaction of the $z$-component of two neighboring spins not only improves the critical temperature $T_c$ but also enhances the entanglement for fixed $B$ and $T$ in particular regions. In the case of the anisotropic three-qubit Heisenberg $XYZ$ chain, the effect of partial anisotropy $\gamma$ makes the revival phenomenon more apparent than in the two-qubit chain; for a fixed $T$, one can obtain a robust entanglement by controlling $B$ and $J_z$.

The Hamiltonian of the $N$-qubit anisotropic Heisenberg $XYZ$ model in an external magnetic field $B$ is [11]

$$H=\frac{1}{2}\sum_{i=1}^{N}\left[J_x\sigma_i^x\sigma_{i+1}^x+J_y\sigma_i^y\sigma_{i+1}^y+J_z\sigma_i^z\sigma_{i+1}^z+B(\sigma_i^z+\sigma_{i+1}^z)\right],\qquad(1)$$

where $\vec{\sigma}_j=(\sigma_j^x,\sigma_j^y,\sigma_j^z)$ is the vector of Pauli matrices and $J_i(i=x,y,z)$ is the real coupling coefficient. The coupling coefficient $J_i$ of arbitrary nearest-neighbor two qubits is equal in value. For the spin interaction, the chain is said to be antiferromagnetic for $J_i>0$ and ferromagnetic for $J_i<0$.

For a system in equilibrium at temperature $T$, the density operator is $\rho=Z^{-1}\exp(-H/k_BT)$, where $Z=\mathrm{Tr}[\exp(-H/k_BT)]$ is the partition function and $k_B$ is the Boltzmann constant. For simplicity, we write $k_B=1$. The entanglement of two qubits can be measured by the concurrence $C$ which is written as $C=\max(0,2\max\{\lambda_i\}-\Sigma_{i=1}^{4}\lambda_i)$ [13,16,17], where $\lambda_i$ are the square roots of the eigenvalues of the matrix $R=\rho S\rho^*S$, $\rho$ is the density matrix, $S=\sigma_1^y\otimes\sigma_2^y$ and * stands for the complex conjugate. The concurrence is available, no matter whether $\rho$ is pure or mixed.

*The two-qubit Heisenberg XYZ chain.* Now, we consider the Hamiltonian for an anisotropic two-qubit Heisenberg $XYZ$ chain in an external magnetic field $B$. The Hamiltonian can be expressed as

$$H=J(\sigma_1^+\sigma_2^-+\sigma_1^-\sigma_2^+)+J\gamma(\sigma_1^+\sigma_2^++\sigma_1^-\sigma_2^-)+(J_z/2)\,\sigma_1^z\sigma_2^z+(B/2)\,(\sigma_1^z+\sigma_2^z),\qquad(2)$$

where $\sigma^{\pm}=\frac{1}{2}(\sigma^x\pm i\sigma^y)$ are raising and lowering operators respectively, and $J=(J_x+J_y)/2$, $\gamma=(J_x-J_y)/(J_x+J_y)$. The parameter $\gamma$ $(0<\gamma<1)$ measures the anisotropy (partial anisotropy) in the $XY$ plane. When the Hamiltonian of the system has the form of Eq. (2), in the standard basis $\{|00\rangle,|01\rangle,|10\rangle,|11\rangle\}$, the density matrix of the system can be written as

$$\rho_{12}=\begin{pmatrix}u_1&0&0&v\\0&w&z&0\\0&z&w&0\\v&0&0&u_2\end{pmatrix}.\qquad(3)$$

 

These nonzero matrix elements can be calculated through

$$u_1=\mathrm{Tr}(|00\rangle\langle 00|\rho),\quad u_2=\mathrm{Tr}(|11\rangle\langle 11|\rho),$$

$$w=\mathrm{Tr}(|01\rangle\langle 01|\rho),\quad v=\mathrm{Tr}(|00\rangle\langle 11|\rho),$$

$$z=\mathrm{Tr}(|01\rangle\langle 10|\rho). \tag{4}$$

The square roots of the eigenvalues of the matrix $R$ are $\lambda_{1,2}=|w\pm z|$, $\lambda_{3,4}=|\sqrt{u_1u_2}\pm v|$. Therefore, we can calculate the concurrence.

The eigenvalues and eigenstates of $H$ are easily obtained as $H|\Psi^{\pm}\rangle=(-J_z/2\pm J)|\Psi^{\pm}\rangle$, $H|\Sigma^{\pm}\rangle=(J_z/2\pm\eta)|\Sigma^{\pm}\rangle$, with the eigenstates $|\Psi^{\pm}\rangle=(1/\sqrt{2})(|01\rangle\pm|10\rangle)$, $|\Sigma^{\pm}\rangle=[1/\sqrt{2\eta(\eta\mp B)}][(\eta\mp B)|00\rangle\pm J\gamma|11\rangle]$, where $\eta=\sqrt{B^2+(J\gamma)^2}$. One can notice that the eigenstates are the same as the case of $J_z=0$ [11]. Because the bases $|01\rangle$ and $|10\rangle$ are the two degenerate eigenstates of $\sigma_1^z\sigma_2^z$ with eigenvalue $-1$, the superposition of the two degenerate states $|01\rangle$ and $|10\rangle$ still is the eigenstate of $\sigma_1^z\sigma_2^z$, that is, $|\Psi^{\pm}\rangle$ is the eigenstate of $J_z=0$ as well as that of $J_z\neq 0$. The same reason accounts for $|\Sigma^{\pm}\rangle$ both as an eigenstate of Eq. (2) and as that of the case of $J_z=0$ . From Eq. (4), tracing the eigenstates, we obtain the square roots of the eigenvalues of the matrix $R$,

$$\lambda_{1,2}=Z^{-1}e^{\beta J_z/2}e^{\pm\beta J},$$

$$\lambda_{3,4}=Z^{-1}e^{-\beta J_z/2}\left|\sqrt{1+\left(\frac{J\gamma}{\eta}\sinh\beta\eta\right)^2}\mp\frac{J\gamma}{\eta}\sinh\beta\eta\right|, \tag{5}$$

where the partition function $Z=2(e^{-J_z/2T}\cosh\beta\eta+e^{\beta J_z/2}\cosh\beta J)$. Because the concurrence is invariant under the substitutions $J\to -J$ and $\gamma\to-\gamma$ [11], we will consider the cases $J>0$ and $0<\gamma<1$. But with substitution $J_z\to -J_z$, the concurrence is variant. We choose $J_z>0$, and we will state the reason later.

We first review the circumstance of the anisotropic Heisenberg $XY$ chain, which is analyzed in Ref. [11]. At $T=0$, there exists a critical magnetic field $B_c$. As $B$ crosses $B_c$, the concurrence $C$ drops suddenly and then undergoes a "revival" for sufficiently large $\gamma$. However, we noticed that $B_c$ decreases with the increase of the anisotropic parameter $\gamma$. Although with the increase of $\gamma$ the critical temperature $T_c$ is improved, the entanglement, when temperature is in the revival region, is very weak.

With $\gamma=0.3$, we show the concurrence as a function of $B$ and $T$ for two values of $J_z$ in Fig. 1. For $J_z=0$ [Fig. 1(a)] corresponding to the circumstance of the anisotropic Heisenberg $XY$ chain [11], one can observe a revival phenomenon and weak entanglement in the revival region. For the convenience of representation, we define the main region in which the concurrence $C$ keeps its constant and maximal values. Comparing Fig. 1(a) with 1(b), we find that with the increasing $J_z$, the main region is extended in terms of $B$ and $T$, i.e., the critical magnetic field $B_c$ is broadened and the critical temperature $T_c$ in the main region is improved. That is to say, the range of concurrence $C$ keeping its constant and maximal values is extended in terms of $B$ and $T$, so that we can obtain strong entanglement in the extended range.

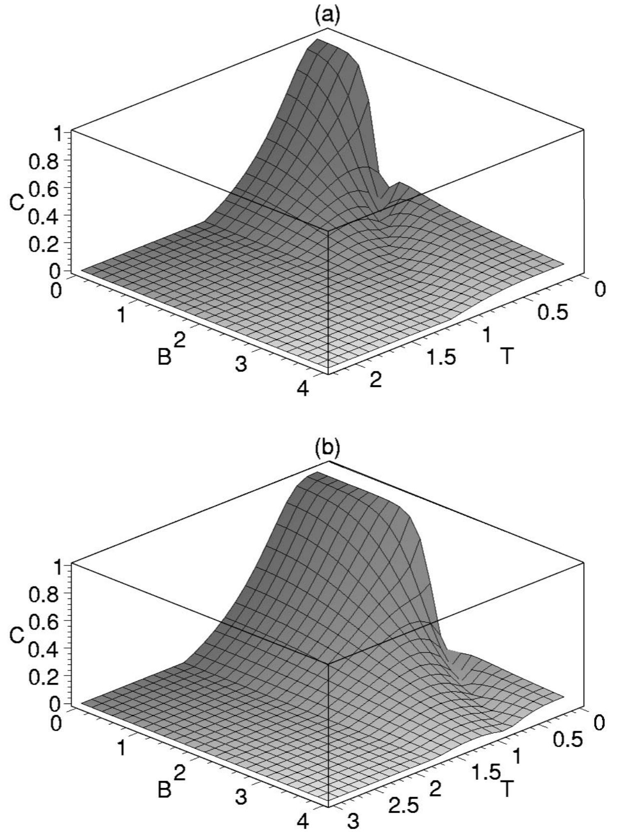


FIG. 1. Concurrence in the two-qubit Heisenberg $XYZ$ chain is plotted vs $T$ and $B$, where (a) $J_z=0$, (b) $J_z=0.9$. For all plotted $J=1.0$, $\gamma=0.3$.

We can understand the effect of $J_z$ on $B_c$ from the case of $T=0$. For $T=0$ under the condition of $J_z\leqslant J$, $C$ can be written analytically as

$$C(T=0)=\begin{cases}1 & \text{for } \eta<J+J_z,\\ (1-J\gamma/\eta)/2 & \text{for } \eta=J+J_z,\\ J\gamma/\eta & \text{for } \eta>J+J_z.\end{cases} \tag{6}$$

The parameters $J$, $\eta$, and $\gamma$ are independent of $J_z$ in the case of two interacting qubits. Comparing Eq. (6) with Eq. (6) of Ref. [11], we can see clearly that if $J_z$ is positive, $J_z$ makes the intersection points of the piecewise function shift. In this paper, we consider the case of $J_z>0$. Figure 2 shows the concurrence at $T=0$ for three values of positive $J_z$. It shows clearly that the concurrence drops sharply at a finite value of the magnetic field $B$, which is called the critical magnetic field $B_c$, at which the quantum phase transition occurs [11]. But with the increase of $J_z$, $B_c$ is increased. The interaction of the $z$ component of two neighboring spins $J_z$ causes a shift in the locations of the phase transitions. Namely, the presence of positive $J_z$ increases the region over which the concurrence C attains its maximum value. This result means that in larger region of $B$ and $T$, we can obtain stronger entanglement. The effect of $J_z$ is different from that of $\gamma$ on changing

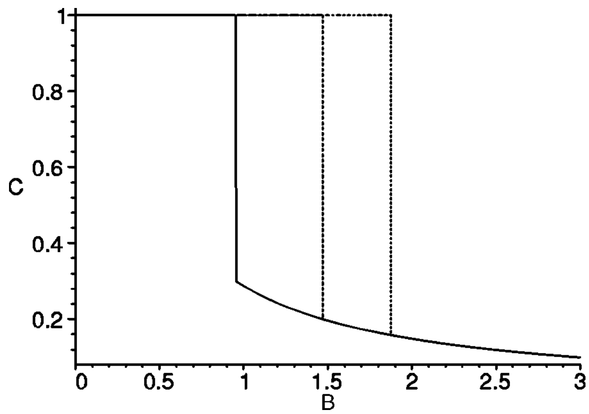


FIG. 2. Concurrence in the two-qubit Heisenberg $XYZ$ chain vs $B$ at zero temperature for various values of $J_z$ with $\gamma=0.3$ and $J=1.0$. From left to right, $J_z$ equals 0, 0.5, 0.9, respectively.

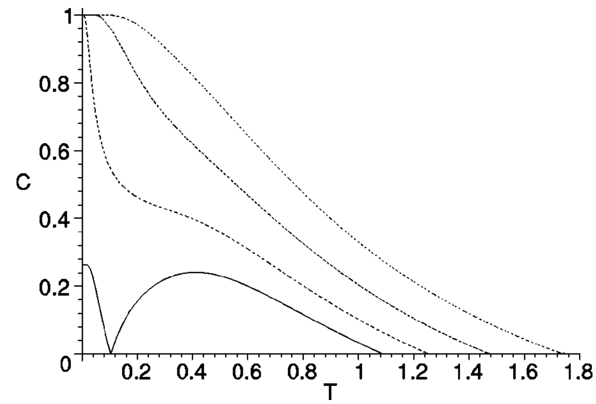


FIG. 3. Concurrence in the two-qubit Heisenberg $XYZ$ chain is plotted vs $T$. For all plotted $J=1.0$, $B=1.1$, $\gamma=0.3$. From top to bottom, $J_z$ equals 0.9, 0.5, 0.2, 0, respectively.

$B_c$. In the case of $J_z=0$ [11], although with the increase of $\gamma$ the critical temperature $T_c$ is increased, the larger the values of $\gamma$, the smaller the critical magnetic field $B_c$. Here, introducing the $z$-component interaction of two neighboring spins not only extends the critical magnetic field $B_c$ but also improves the critical temperature $T_c$ and the entanglement (we will further show it in Fig. 3).

Let us consider the concurrence changing with temperature for different values of $J_z$ in a fixed $B(B=1.1)$. We plot it in Fig. 3 with $\gamma=0.3$. We notice the existence of a critical temperature $T_c$ at which the entanglement vanishes. Obviously, $T_c$ is improved monotonously with the increase of $J_z$. Under the condition $J_z=0$ (corresponding to the $XY$ model [11]), the concurrence exhibits a revival phenomenon, but the maximal values of entanglement in both areas are small. If we introduce $J_z$, the critical external magnetic field $B_c$ becomes larger so that $B=1.1$ is less than $B_c$ (the critical magnetic field when $J_z=0.2,0.5$ or $J_z=0.9$), and thus we observe the maximal value of entanglement 1. In the temperature range $0<T<1.725$, the larger the value of $J_z$, the stronger the entanglement. Therefore, $J_z$ not only improves the critical temperature $T_c$, but also enhances the entanglement for particular fixed $B$ and $\gamma$.

*The pairwise entanglement in three qubits.* The calculation of pairwise entanglement in $N$ qubits is very complicated due to the anisotropy in the Heisenberg $XYZ$ chain. Here we just calculate the pairwise entanglement in three qubits to show the effects of $J_z$. We now solve the eigenvalue problems of the three-qubit $XYZ$ Hamiltonian. We list the eigenvalues and the corresponding eigenvectors as follows:

$$E_{1,2}=-J-\frac{J_z}{2}+B:|\Phi_{1,2}\rangle=\pm\frac{1}{2}\left(1\mp\frac{1}{\sqrt{3}}\right)|110\rangle+\frac{1}{\sqrt{3}}|101\rangle\mp\frac{1}{2}\left(1\pm\frac{1}{\sqrt{3}}\right)|011\rangle,$$

$$E_{3,4}=J+\frac{J_z}{2}-B\pm\eta_-:|\Phi_{3,4}\rangle=\frac{1}{\sqrt{2\eta_-[\eta_-\pm(J_z-2B-J)]}}\left[(J_z-2B-J\pm\eta_-)|000\rangle+J\gamma\sum_{n=0}^{2}\Upsilon^n|110\rangle\right],$$

$$E_{5,6}=-J-\frac{J_z}{2}-B:|\Phi_{5,6}\rangle=\pm\frac{1}{2}\left(1\mp\frac{1}{\sqrt{3}}\right)|010\rangle+\frac{1}{\sqrt{3}}|100\rangle\mp\frac{1}{2}\left(1\pm\frac{1}{\sqrt{3}}\right)|001\rangle,$$

$$E_{7,8}=J+\frac{J_z}{2}+B\pm\eta_+:|\Phi_{7,8}\rangle=\frac{1}{\sqrt{2\eta_+[\eta_+\pm(J_z+2B-J)]}}\left[(J_z+2B-J\pm\eta_+)|111\rangle+J\gamma\sum_{n=0}^{2}\Upsilon^n|010\rangle\right], \qquad (7)$$

where $\eta_\pm=\sqrt{(J_z-J\pm2B)^2+3(J\gamma)^2}$ and $\Upsilon$ is the cyclic right shift operator [15]. The reduced density matrix of two nearest-neighbor qubits in the $N$-qubit system also has the form of Eq. (3). Employing Eq. (4) and tracing on the basis of eigenstates shown in Eq. (7), one can get the density matrices $\mu_1$, $\mu_2$, $w$, $z$, $v$, and then further obtain the concurrence. Here we do not write the expressions of $\lambda_i$ because they are very long. We will directly plot some curves to show the effect of $J_z$ on enhancing entanglement.

Figure 4 shows the concurrence as a function of $B$ and $T$

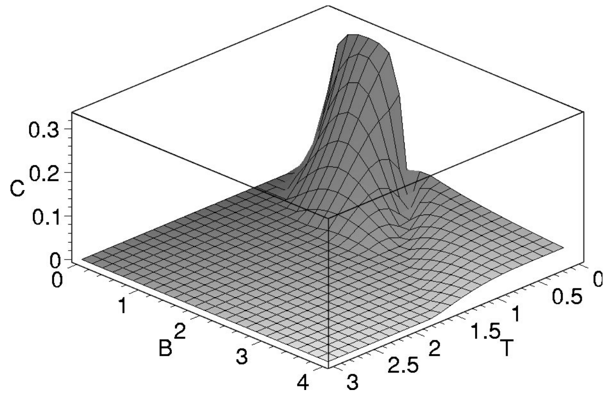


FIG. 4. Pairwise entanglement in the three-qubit Heisenberg $XYZ$ chain is plotted as a function of $T$ and $B$, where $\gamma=0.3$, $J=1.0$, $J_z=0.9$.

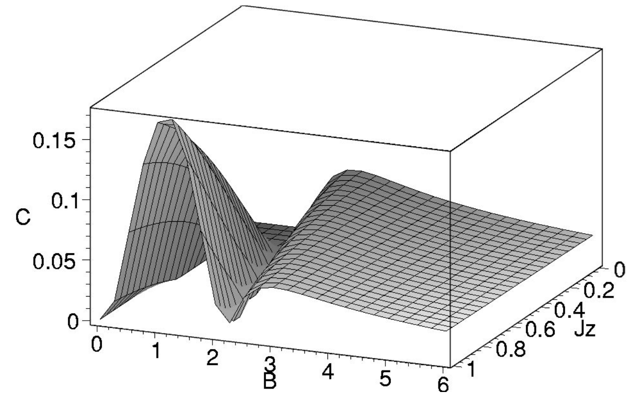


FIG. 5. Pairwise entanglement is plotted as a function of $B$ and $J_z$, where $T=0.6$, $J=1.0$, $\gamma=0.3$.

with $\gamma=0.3$, $J_z=0.9$, and $J=1.0$ in the three-qubit $XYZ$ Heisenberg chain. We see that with the same $\gamma=0.3$, the effect of partial anisotropy $\gamma$ makes the revival phenomenon more apparent than in the two-qubit chain. When $B=4$ in Fig. 1, the largest critical temperature $T_c$ produced by $\gamma$ is about 1.0 [Fig. 1(a)]; due to the restrain of $J_z$, the maximum temperature only caused by $\gamma$ is below 0.8 [Fig. 1(b)]. However, in the three-qubit system if $B=4$ with the same set of parameters, comparing Fig. 1(b) with Fig. 4, the critical temperature $T_c$ in the revival region almost equals 1.8. The stronger effect of $\gamma$ implies that if we aim to obtain a strong entanglement, we can decrease $\gamma$ properly and increase $J_z$; otherwise increasing $\gamma$ can make the revival phenomenon more evident. Of course, the coupling constant $J_z$ also increases the magnetic field $B_c$ and expand the region of concurrence keeping constant in terms of $B$ and $T$ as it does in the two-qubit (due to lack of space, we do not plot it here) .

For $T=0.6$, Fig. 5 shows concurrence as a function of $B$ and $J_z$. There is no entanglement for $B=0$, which corresponds to Fig. 4. If $J_z$ is below a certain value, in case of Fig. 5 the value is about 0.2, the entanglement appears in an area corresponding to the revival one [11] on condition that the magnetic field is larger than a certain value, and the certain value of $B$ is increased with the increase of $J_z$. But, if $J_z$ is larger than 0.2, there are two areas showing entanglement, and the entanglement appearing in the lower range of $B$ can be much stronger than that in the higher magnetic field. In the lower range of $B$, for a certain $B$, the larger the value of $J_z$ the large concurrence. Thus, in the $N$-qubit $XYZ$ system, for a fixed $T$, one can obtain a robust entanglement by controlling $B$ and $J_z$.

*Conclusion.* The thermal entanglement in an anisotropic $XYZ$ Heisenberg chain is investigated. Through analyzing the two-qubit system, we find that with the increase of $J_z$, the critical magnetic field $B_c$ is increased; the coupling along $Z$ not only improves the critical temperature $T_c$ but also enhances the entanglement for a certain fixed $B$. We also analyze the entanglement between two nearest neighbors in three qubits and find that the effect of the partial anisotropy is more evident than that in the two-qubit system. The pairwise entanglement exhibits an interesting phenomenon. For a certain fixed $B$, if the coupling constant $J_z$ is small, the pairwise entanglement only exists in the relative strong magnetic field $B$ and the entanglement is weak. By increasing $J_z$, in the lower range of $B$, one can obtain a strong entanglement. Therefore, interaction constant of the $z$ component of two neighboring spins $J_z$ plays an important role in enhancing entanglement and in improving the critical temperature.

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