Entanglement properties in $\left( \frac{1}{2}, 1 \right)$ mixed-spin Heisenberg systems

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Abstract

By using the concept of negativity, we investigate entanglement in $\left( \frac{1}{2}, 1 \right)$ mixed-spin Heisenberg systems. We obtain the analytical results of entanglement in small isotropic Heisenberg clusters with only nearest-neighbor (NN) interactions up to four spins and in the four-spin Heisenberg model with both NN and next-nearest-neighbor (NNN) interactions. For more spins, we numerically study effects of temperature, magnetic fields, and NNN interactions on entanglement. We study in detail the threshold value of the temperature, after which the negativity vanishes.

Keywords: Negativity; Entanglement

1. Introduction

Entanglement, an essential feature of the quantum mechanics, has been introduced in many fields of physics. In the field of quantum information, the entanglement has played a key role. The study of entanglement properties in many-body systems have attracted much attention [1–29]. The Heisenberg chains, widely studied in the condensed matter field, display rich entanglement features and have many useful applications such as in the quantum state transfer [30].

Most of the systems considered in previous studies are spin-half systems as there exists a good measure of entanglement of two spin-halves, the concurrence [31], which is applicable to an arbitrary state of two spin halves. On the other hand, the entanglements in mixed-spin or higher spin systems are not well-studied due to the lack of good operational entanglement measures. There are several initial studies along this direction [32–34], however these works are restricted to the case of two particles.

For the case of higher spins, a non-entangled state has necessarily a positive partial transpose according to the Peres–Horodecki criterion [35]. In the case of two spin halves, and the case of $\left( \frac{1}{2}, 1 \right)$ mixed spins, fortunately, a positive partial transpose is also sufficient. Thus, the sufficient and necessary condition for entangled state in $\left( \frac{1}{2}, 1 \right)$ mixed spin systems is that it has a negative partial transpose. This allows us to investigate entanglement features of the mixed spin system.

The Peres–Horodecki criterion give a qualitative way for judging whether the state is entangled or not. The quantitative version of the criterion was developed by Vidal and Werner [36]. They presented a measure of

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entanglement called negativity that can be computed efficiently, and the negativity does not increase under local manipulations of the system. The negativity of a state $\rho$ is defined as

$$N(\rho) = \sum_i |\mu_i|,$$

where $\mu_i$ is the negative eigenvalue of $\rho^{T_1}$, and $T_1$ denotes the partial transpose with respect to the first system. The negativity $N$ is related to the trace norm of $\rho^{T_1}$ via

$$N(\rho) = \frac{\|\rho^{T_1}\|_1 - 1}{2},$$

where the trace norm of $\rho^{T_1}$ is equal to the sum of the absolute values of the eigenvalues of $\rho^{T_1}$. In this paper, we will use the concept of negativity to study entanglement in $(\frac{1}{2}, 1)$ mixed-spin systems.

As shown in most previous works, models with the NN exchange interactions are considered and it is not easy to have pairwise entanglement between the NNN spins [9,10]. It is true that there exist some quasi-one-dimension compounds offering us systems with NNN interactions. Bose and Chattopadhyay [37] and Gu et al. [38] have investigated entanglement in spin-half Heisenberg chain with NNN interactions. In our paper here, we study entanglement properties not only in the $(\frac{1}{2}, 1)$ mixed-spin systems only with NN interactions, but also in the system with NNN interactions.

Entanglement in a system with a few spins displays general features of entanglement with more spins. For instance, in the anisotropic Heisenberg model with a large number of qubits, the pairwise entanglement shows a maximum at the isotropic point [38]. This feature was already shown in a small system with four or five qubits [39]. So, the study of small systems is meaningful in the study of entanglement as they may reflect general features of larger or macroscopic systems. Also, due to the limitation of our computation capability, we only concentrate on small systems such as 4, 5 and 6-spin models.

The paper is organized as follows. In Section 2, we study the systems with only NN interactions. The analytical results of negativity for the cases of two and three spins are given. The relation between entanglement and the macroscopic thermodynamical function, the internal energy is revealed. Also we numerically compute the negativity in more general mixed-spin models up to eight spins, and consider the effects of magnetic fields in this section. In Section 3, the system with NNN interaction is discussed. For the four-spin case, we analytically calculate the eigenenergy of the system from which we get the analytical results of the negativity of the NN spins. We numerically study negativities versus NNN exchanging coupling, and the case of finite temperature is also considered. For larger system up to eight-spin system, we get some numerical results. The conclusion is given in Section 4.

2. Entanglement in Heisenberg chain only with nearest-neighbor interaction

2.1. Analytical results of Entanglement in Heisenberg models

We study entanglement of states of the system at thermal equilibrium described by the density operator $\rho(T) = \exp(-\beta H)/Z$, where $\beta = 1/k_B T$, $k_B$ is the Boltzmann’s constant, which is assumed to be one throughout the paper, and $Z = \text{Tr}(\exp(-\beta H))$ is the partition function. The entanglement in the thermal state is called thermal entanglement.

We consider two kinds of spins, spin $\frac{1}{2}$ and 1, alternating on a ring with antiferromagnetic exchange coupling. The Hamiltonian is given by

$$H_0 = \sum_{i=1}^{N/2} (s_i \cdot S_i + S_i \cdot s_{i+1}) \quad (N \in \text{even})$$

and

$$H_0 = \sum_{i=1}^{(N-1)/2} (s_i \cdot S_i + S_i \cdot s_{i+1}) + s_{(N+1)/2} \cdot s_{i} \quad (N \in \text{odd}),$$
where \( s_i \) and \( S_i \) are spin-\( \frac{1}{2} \) and spin-1 operators, respectively. The exchange interactions exist only between nearest neighbors, and they are of the same strength which are set to one. We adopt the periodic boundary condition. In Fig. 1, we give the schematic representation of the above Hamiltonian. Next, we first consider the models with two and three spins, and aim at getting analytical results of entanglement.

### 2.1.1. Two-spin case

For the two-spin case, the Hamiltonian (3) reduces to \( H_0 = s_1 \cdot S_1 \). To have a matrix representation of the Hamiltonian, we choose the following basis

\[
| -\frac{1}{2}, -1 \rangle, | \frac{1}{2}, 0 \rangle, | -\frac{1}{2}, 1 \rangle, | \frac{1}{2}, -1 \rangle, | -\frac{1}{2}, 0 \rangle, | \frac{1}{2}, 1 \rangle,
\]

where \(|m, M\rangle\) is the eigenstate of \( s_z \) and \( S_z \) with the corresponding eigenvalues given by \( m \) and \( M \), respectively.

In the above basis, the Hamiltonian can be written as a block-diagonal form with the dimension of each block being at most 2 \( \times \) 2. Thus, the density matrix \( \rho_{12} \) for the thermal state is obtained as

\[
\rho_{12} = \begin{pmatrix}
a_1 & 0 & 0 & 0 & 0 & 0 \\
0 & a_2 & b_1 & 0 & 0 & 0 \\
0 & b_1 & a_3 & 0 & 0 & 0 \\
0 & 0 & 0 & a_4 & b_2 & 0 \\
0 & 0 & 0 & b_2 & a_5 & 0 \\
0 & 0 & 0 & 0 & 0 & a_6
\end{pmatrix},
\]

with the partition function and the matrix elements given by

\[
Z = 2e^\beta + 4e^{-(1/2)\beta},
\]

\[
a_1 = a_6 = e^{-(1/2)\beta} / Z,
\]

\[
a_2 = a_5 = \frac{1}{6},
\]

\[
a_3 = a_4 = \frac{1}{3}(2e^\beta + e^{-(1/2)\beta}) / Z,
\]

\[
b_1 = b_2 = \frac{\sqrt{2}}{3}(e^{-(1/2)\beta} - e^\beta) / Z,
\]

\[
= \sqrt{2}(a_1 - a_2).
\]

Fig. 1. Schematic representation of the mixed spin Hamiltonian for the number of spins from 2 to 5.
After the partial transpose with respect to the first spin-half subsystem, we can get $\rho_{12}^{T_1}$

$$
\rho_{12}^{T_1} = \begin{pmatrix}
a_1 & b_2 & 0 & 0 & 0 & 0 \\
b_2 & a_2 & 0 & 0 & 0 & 0 \\
0 & 0 & a_3 & 0 & 0 & 0 \\
0 & 0 & 0 & a_4 & 0 & 0 \\
0 & 0 & 0 & 0 & a_5 & b_1 \\
0 & 0 & 0 & 0 & b_1 & a_6
\end{pmatrix},
$$

(12)

which is still of the block-diagonal form, and computation of its eigenvalues is straightforward. There are only two eigenvalues which are possibly negative. The negativity is thus given by

$$
N(\rho_{12}) = \frac{1}{4} \max \left[ 0, \sqrt{(a_1 - a_2)^2 + 4b_2^2 - a_1 - a_2} \right] + \frac{1}{4} \max \left[ 0, \sqrt{(a_5 - a_6)^2 + 4b_1^2 - a_5 - a_6} \right].
$$

(13)

Substituting Eqs. (7)–(11) leads to the analytical result of negativity

$$
N(\rho) = \max \left[ 0, \sqrt{(a_1 - a_2)^2 + 4b_2^2 - a_1 - a_2} \right] \\
= 2 \max [0, a_2 - 2a_1] \\
= \frac{1}{3} \max \left[ 0, \frac{e^{\beta} - 4e^{-(1/2)\beta}}{e^{\beta} + 2e^{-(1/2)\beta}} \right],
$$

(14)

where the second equality follows from Eq. (11).

We can see that the negativity is a function of the single parameter $\beta$. In the limit of $T \to 0$, the negativity becomes $\frac{1}{3}$ and the ground state is entangled. From Eq. (14), it is direct to check that the negativity is a monotonically decreasing function when temperature increases. After a certain threshold value of the temperature, the entanglement disappears. This threshold value $T_{th}$ can be obtained as

$$
T_{th} = \frac{3}{4 \ln 2} \approx 1.0820.
$$

(15)

For a ring of spin-half particles interacting via the Hisenberg Hamiltonian, it was shown that the pairwise thermal entanglement is determined by the internal energy [40]. It is natural to ask if similar relations exist in the present mixed-spin system. The internal energy can be obtained from the partition function as

$$
U = -\frac{1}{Z} \frac{\partial Z}{\partial \beta}.
$$

(16)

Substituting Eq. (7) into the above equation leads to

$$
U = \frac{-e^{\beta} + e^{-(1/2)\beta}}{e^{\beta} + 2e^{-(1/2)\beta}}.
$$

(17)

From Eqs. (14) and (17), we obtain a quantitative relation between the negativity and the internal energy

$$
N(\rho) = \frac{1}{3} \max [0, -1 - 2U].
$$

(18)

The above equation builds a connection between the microscopic entanglement and the macroscopic thermodynamical function, the internal energy. The internal energy completely determine the thermal entanglement. From the equation, we can also read that the thermal state becomes entangled if and only if the internal energy $U < -\frac{1}{2}$. Since $U = \langle H \rangle = \langle S_1 \cdot S_1 \rangle$, we have

$$
N(\rho) = \frac{1}{3} \max [0, -1 - 2\langle S_1 \cdot S_1 \rangle],
$$

(19)

which is consistent with the result obtained in Ref. [32] by the group-theoretical technique.
2.1.2. Three-spin case

We now consider the three-spin case and the schematic representation of the corresponding Hamiltonian is given by Fig. 1. In this situation, there are two types of pairwise entanglement, the entanglement between spin \( \frac{1}{2} \) and spin \( 1 \) and the entanglement between two spin halves.

The eigenvalue problem can be solved analytically, and after tracing out the third spin-half system the reduced density matrix \( \rho_{12} \) is still of the same form as in Eq. (6) with matrix elements given by

\[
a_1 = \left( \frac{5}{2} e^{-(5/4)\beta} + \frac{3}{4} e^{(3/4)\beta} \right) / Z,
\]

\[
a_2 = \left( \frac{5}{4} e^{-(5/4)\beta} + e^{(3/4)\beta} + \frac{1}{2} e^{(7/4)\beta} \right) / Z,
\]

\[
a_3 = \left( \frac{5}{12} e^{-(5/4)\beta} + \frac{5}{4} e^{(3/4)\beta} + \frac{1}{4} e^{(7/4)\beta} \right) / Z,
\]

\[
b_1 = \left( \frac{5\sqrt{2}}{12} e^{-(5/4)\beta} - \frac{\sqrt{2}}{4} e^{(3/4)\beta} - \frac{1}{6} e^{(7/4)\beta} \right) / Z,
\]

\[
Z = 5 e^{-(5/4)\beta} + 6 e^{(3/4)\beta} + e^{(7/4)\beta}.
\]  

Substituting the above equations to Eq. (13) leads to the negativity

\[
\mathcal{N}(\rho_{12}) = \max[0, -\frac{10}{3} e^{-(5/4)\beta} - e^{(3/4)\beta} + \frac{1}{3} e^{(7/4)\beta}] / Z.
\]  

It is evident that the negativity becomes \( \frac{1}{3} \) in the limit of \( T \to 0 \). From the expression of the negativity, the threshold value of temperature after which the entanglement vanishes can be estimated as

\[
T_{th} \approx \frac{1}{\ln 3.2719} \approx 0.7609.
\]

To examine the entanglement between two spin halves, we trace out the spin 1 system and get the reduced density matrix \( \rho_{13} \) as follows

\[
\rho_{13} = \begin{pmatrix}
a_1 & 0 & 0 & 0 \\
0 & a_2 & b & 0 \\
0 & b & a_2 & 0 \\
0 & 0 & 0 & a_1
\end{pmatrix},
\]

with the matrix elements given by

\[
a_1 = \left( \frac{5}{2} e^{-(5/4)\beta} + e^{(3/4)\beta} + \frac{1}{2} e^{(7/4)\beta} \right) / Z,
\]

\[
a_2 = \left( \frac{5}{4} e^{-(5/4)\beta} + 2 e^{(3/4)\beta} + \frac{1}{6} e^{(7/4)\beta} \right) / Z,
\]

\[
b = \left( \frac{5\sqrt{2}}{12} e^{-(5/4)\beta} - \frac{\sqrt{2}}{4} e^{(3/4)\beta} - \frac{1}{6} e^{(7/4)\beta} \right) / Z.
\]

After taking the partial transpose, we can get \( \rho_{13}^T \)

\[
\rho_{13}^T = \begin{pmatrix}
a_1 & 0 & 0 & b \\
0 & a_2 & 0 & 0 \\
0 & 0 & a_2 & 0 \\
b & 0 & 0 & a_1
\end{pmatrix}.
\]

Then, the negativity is readily obtained as

\[
\mathcal{N}(\rho_{13}) = \max[0, |b| - a_1].
\]
It is straightforward to check that the negativity is always zero. Or, from another way, all the eigenvalues of the matrix $\rho_{13}^T$ are obtained as

$$\lambda_1 = \left(\frac{5}{6}e^{-5\beta/4} + \frac{1}{6}e^{7\beta/4}\right)/Z,$$

$$\lambda_2 = \left(\frac{5}{6}e^{-5\beta/4} + 2e^{3\beta/4} + \frac{1}{6}e^{7\beta/4}\right)/Z,$$

$$\lambda_3 = \lambda_4 = \alpha_2. \quad (27)$$

Obviously the negativity vanishes here, in other words there is no entanglement between the two spin halves. The ground-state negativity $\mathcal{N}_{12} = \mathcal{N}(\rho_{12}) = \frac{1}{4}$ and $\mathcal{N}_{13} = \mathcal{N}(\rho_{13}) = 0$, here $\mathcal{N}_{12}$ denotes the negativity between the first and second spin on the chain and $\mathcal{N}_{13}$ denotes the one between the first and third spin. The equation above can be obtained from the non-degenerate ground state given by:

$$|\psi_0\rangle = \frac{\sqrt{6}}{6}(|\frac{1}{2}, 0, -\frac{1}{2}\rangle + |\frac{1}{2}, 0, \frac{1}{2}\rangle) - \frac{\sqrt{3}}{2}(|\frac{1}{2}, -1, \frac{1}{2}\rangle + |\frac{1}{2}, 1, -\frac{1}{2}\rangle). \quad (28)$$

It is interesting to see that the ground-state entanglement between the spin half and spin 1 in the three-spin case is the same as that in the two-spin case.

Due to the SU(2) symmetry in our system, there are following relations between correlation functions and negativities [32]

$$\mathcal{N}_{12} = -\frac{1}{4} - \frac{3}{4} \langle s_1 \cdot s_1 \rangle,$$

$$\mathcal{N}_{23} = -\frac{1}{4} - \frac{3}{4} \langle s_2 \cdot s_2 \rangle,$$

$$\mathcal{N}_{31} = -\frac{1}{4} - \langle s_2 \cdot s_1 \rangle, \quad (29)$$

where we have removed the max function in the negativity, implying that the negative value of $\mathcal{N}$ indicates no entanglement. Then, we have the relation between the internal energy and the negativities

$$U = -\frac{3}{4} - \mathcal{N}_{13} - \frac{3}{4}\left(\mathcal{N}_{12} + \mathcal{N}_{23}\right)$$

$$= -\frac{3}{4} - \mathcal{N}_{13} - 3\mathcal{N}_{12}. \quad (30)$$

The second equality follows from the exchange symmetry, namely, the Hamiltonian is invariant when exchanging two spin halves. So, for the three-spin case, the internal energy is related to two negativities.

To apply the above result, we consider the ground-state properties ($T = 0$). The Hamiltonian can be rewritten as

$$H = \frac{1}{4}[\langle s_1 + s_1 + s_2 \rangle^2 - s_1^2 - S_1^2 - s_2^2]. \quad (31)$$

Then, by the angular momentum coupling theory, the ground-state energy is obtained as $E_0 = -\frac{7}{4}$. Substituting the ground-state energy and $\mathcal{N}_{12} = \frac{1}{4}$ to Eq. (30), we obtain $\mathcal{N}_{13} = -\frac{1}{4}$, indicating that there exists no entanglement between two spin halves. Also we can understand this phenomena in the picture of a valence bond solid. By regarding the spin 1 as made of two symmetrized spin halves, it is straightforward that the ground state of the ring with two spin $\frac{1}{2}$ and a spin 1 is as approximately two singlets between each spin $\frac{1}{2}$ and the subspins of the spin 1. Obviously, that is why there is on entanglement left between the two spin $\frac{1}{2}$.

2.1.3. The case of even $N$ spins

Except for the SU(2) symmetry in the system, there exists exchange symmetry for the case of even spins. For instance, in the four-spin model, the Hamiltonian is invariant when exchanging two spin halves or two spin ones. Thus, for even-spin model, the entanglements between the two nearest-neighbor spins and the correlation functions $\langle s_i \cdot s_j \rangle$ are independent on index $i$. Therefore, the internal energy per spin is equal to the correlation function $\langle s_i \cdot s_j \rangle$

$$u = U/N = \langle s_1 \cdot s_1 \rangle. \quad (32)$$
From Eqs. (29) and (32), we have

\[ N_{12} = -\frac{1}{3} - \frac{2}{3} u. \] (33)

This equation indicates that for the case of even spins the entanglement between two nearest neighbors is solely determined by the internal energy per spin. And for the case of zero temperature, the entanglement is determined by the ground-state energy. The less the energy, the more the entanglement.

We now apply the above result to the study of ground-state entanglement. We rewrite the four-spin Hamiltonian as follows

\[ H = \frac{1}{2} [(s_1 + S_1 + s_2 + S_2)^2 - (s_1 + s_2)^2 - (S_1 + S_2)^2]. \] (34)

Then, by the angular momentum coupling theory, we obtain the ground-state energy per site \( e_0 = E_0/4 = -\frac{1}{6} \). Thus, from Eq. (33), we have \( N_{12} = \frac{1}{6} \). For \( N \geq 5 \), it is hard to get analytical results, but by many numerical methods the ground energy of our mixed-spin system even to the thermodynamic limit can be obtained [41], using the result of third-order spin-wave theory the ground energy of per spin \( u = -0.727161 \), we got the negativity \( N_{12} = 0.1514 \) to the case of the size of system \( N \to \infty \). That means when the size of the mixed-spin system becomes much large, the entanglement of ground state goes to be steady.

2.2. Numerical results

Having obtained analytical results of entanglement in the Heisenberg model with a few spins, we now numerically examine the entanglement behaviors in more general Hamiltonian including more spins and magnetic fields.

2.2.1. Entanglement versus temperature

We consider the entanglement versus temperature for different number of spins \( N \), and the numerical results are plotted in Figs. 2 and 3. It is clear to see that the ground state exhibits maximal entanglement, and with the increase of temperature, the entanglement monotonically decreases until it reaches zero. The decrease of entanglement is due to the mixture of less entangled excited states when increasing the temperature. The existence of the threshold temperature is also evident. For the case of even number of sites (Fig. 2), the
threshold temperature decreases with the increase of $N$. In contrast to this behavior, for the case of odd number of spins, as seen from Fig. 3, the threshold temperature increases with the increase of $N$.

Here we should take more attention to the Fig. 2. As you know, the properties of the very large systems must be close to the even spins system. So although due to the limitation of our numerical methods we only calculated as large as 8 spins, in the Fig. 2 the cases of 6 and 8-spin show us that the behavior of entanglement between NN spin becomes nearly consistent. At very low temperature, the negativity goes to the steady value of about 0.1514 which is just the result got from Eq. (33) based on the numerical result of [41] to the thermodynamic limit. We can see that the entanglement in small system up to 8 spins even can exhibits some general properties. So that, from the results of Fig. 2, at finite temperature, the threshold temperature may be going to a steady value at last without changing no matter how the size of the system increasing. And the value is around 0.937, which can be seen as a general property of the entanglement in our system.

### 2.2.2. Effects of magnetic fields

We now examine the effect of magnetic fields on entanglement. The Heisenberg Hamiltonian with a magnetic field along $z$ direction is given by

$$H_1 = H_0 + B \sum_{i=1}^{N/2} (s_{iz} + S_{i,z}) \quad (N \in \text{even}).$$

(35)

For $N = 2$, the analytical result of negativity can be obtained (see Appendix A).

In Fig. 4, we plot the negativity versus the magnetic field at a low temperature. For the two-spin case, with the increase of the magnetic field, the negativity rapidly reach a platform, and then after a certain magnetic field $B_{th}$, it jumps down to zero, indicating no entanglement. When $B = 0$, the ground state is two-fold degenerate with $N = \frac{1}{2}$. For a small $B > 0$, the system is no longer degenerate, and the ground state is given by

$$|\psi_0\rangle = \frac{\sqrt{2}}{\sqrt{3}} |\frac{1}{2}, -1\rangle - \frac{\sqrt{2}}{\sqrt{3}} |\frac{1}{2}, -\frac{1}{2}\rangle,$$

(36)

which is of the Schmidt form. For a state written as its Schmidt form

$$|\psi\rangle = \sum_n c_n |e_n\rangle |f_n\rangle,$$

(37)
the negativity is obtained as \[ N = \frac{1}{2} \left[ \left( \sum_n C_n \right)^2 - 1 \right] \] (38)

Here, \( C_n \) are the Schmidt coefficients, and \(|e_n\rangle \) and \(|f_n\rangle \) are bases for subsystems 1 and 2, respectively. Applying this formula to the ground state, we immediately have \( N = \frac{\sqrt{3}}{2} \). When \( B = B_{th} = \tfrac{3}{2} \), the ground state is two-fold degenerate, and when \( B > B_{th} \) the ground state becomes non-degenerate and the corresponding wave function is given by

\[
|\psi_0\rangle = | - \tfrac{1}{2}, -1 \rangle,
\]

which is obviously of no entanglement. Then, the ground-state negativity forms a platform when \( 0 < B < B_{th} \). The jump of negativity at \( B = B_{th} \) is due to the level crossing. For \( N > 2 \), the effects of magnetic fields on entanglement can be also explained by level crossing. For instance, for \( N = 4 \), there are two level crossing, and the entanglement displays two jumps.

### 3. Effects of next-nearest-neighbor interactions on entanglement

In the study of condensed matter physics, frustrated systems are recognized as the ones with lots of interesting properties. So here we want to discover how the entanglement as a characteristic behaves in the frustrated system. It is well known that frustration in a system may be caused by the topology of the lattice or induced by the inclusion of further-neighbor interactions. In this section, we will study the frustrated system with both the NN and NNN interactions, and the entanglement will modified by changing the NNN interaction and temperature. It should be pointed out that the frustrated system of us is more composite as there are three kinds of sublattices corresponding to spin 1, \( \tfrac{1}{2} \), spin \( \tfrac{1}{2} \)s and spin 1s combined together, so the system must contains plenty entanglement properties. The Hamiltonian can be expressed as

\[
H = J_1 \sum_{i=1}^{N/2} (s_i \cdot s_i + S_i \cdot S_{i+1}) + J_2 \sum_{i=1}^{N/2} (s_i \cdot s_{i+1} + S_i \cdot S_{i+1}),
\]

(40)
where the $s_i$ and $S_i$ are spin-$\frac{1}{2}$ and spin-1 operators in the $i$th cell. $J_1$ characterizes the NN exchange coupling and $J_2$ the NNN coupling. We consider the antiferromagnetic interaction by taking $J_1, J_2 > 0$. $N$ is the total number of spins and here we choose it be even. Also we adopt the periodic boundary condition.

### 3.1. Four-spin model

#### 3.1.1. Eigenenergy and ground-state entanglement

The model with four spins is the simplest model with NNN interactions. We first solve the eigenvalue problem of this model. The key step is to write the four-spin Hamiltonian in the following form,

$$ H = \frac{1}{2}[J_1 S_1^2 + (2J_2 - J_1)[(s_1 + s_2)^2 + (S_1 + S_2)^2] - 2J_2(s_1^2 + s_2^2 + S_1^2 + S_2^2)], \quad (41) $$

where $S = S_1 + S_2 + s_1 + s_2$ denotes the total spin. From the above form, by angular momentum coupling theory, one can readily obtain all eigenvalues of the system as

$$ E_1 = J_2 n(n+1) - \frac{11}{2} J_2, $$

$$ E_2 = n J_1 + n(n+1) J_2 - \frac{7}{2} J_2, $$

$$ E_3 = - J_1 + n(n+1) J_2 - \frac{7}{2} J_2, $$

$$ E_4 = -(n+1) J_1 + n(n+1) J_2 - \frac{7}{2} J_2, \quad (42) $$

where parameter $n = 0, 1, 2$ in expressions $E_1$ and $E_2$ and $n = 1, 2$ in expressions $E_3$ and $E_4$, respectively. Then, from Eq. (42), we may find the ground-state energy as

$$ E_{GS} = \begin{cases} 
-3J_1 + \frac{5}{2} J_2 & \text{when } 0 < J_2 < J_1/4, \\
-2J_1 - \frac{7}{2} J_2 & \text{when } J_1/4 < J_2 < J_1/2, \\
-11J_2 & \text{when } J_2 > J_1/2.
\end{cases} \quad (43) $$

Clearly, there are two level-crossing points, which will greatly affect behaviors of ground-state entanglement.

From Eq. (41), it is obvious that in addition to the SU(2) symmetry, there also exists an exchange symmetry, namely, exchanging two spin halves or two spin ones yields invariant Hamiltonian. Then, the correlator $\langle s_i \cdot S_j \rangle$ between any NN spins are the same. Therefore, we can get the correlator $\langle s_i \cdot S_j \rangle$ from the ground-state energy via the Hellmann–Feynman theorem.

When $0 < J_2 < J_1/4$, after applying the Hellmann–Feynman theorem to the ground-state energy, we obtain

$$ \langle s_1 \cdot S_1 \rangle = \frac{1}{4} \frac{\partial E_0}{\partial J_1} = -\frac{3}{4}. \quad (44) $$

Due to the SU(2) symmetry in our system, we have the following relation between the negativity and the correlator $\langle s_1 \cdot S_1 \rangle$ [32],

$$ \mathcal{N}_{1/2,1} = \max\{0, -\frac{1}{2} - \frac{3}{2} \langle s_1 \cdot S_1 \rangle\}, \quad (45) $$

where we use $\mathcal{N}_{1/2,1}$ to denote the negativity between the NN spins. Thus we obtain

$$ \mathcal{N}_{1/2,1} = \frac{1}{8}. \quad (46) $$

In other regions, we find that $\mathcal{N}_{1/2,1} = 0$ for $J_2 > J_1/4$.

From the above analytical results, we can find that when the NNN interaction $J_2$ is strong enough to the value $J_2 = 0.25$, the entanglement of the NN spins will be destroyed absolutely.

Having studied ground-state entanglement, now we make a short discussion of entanglement of excited states. We consider the first excited state. In the region $J_1/4 < J_2 < 3J_1/8$, the first excited energy is given by

$$ E_1 = -3J_1 + \frac{5}{2} J_2, \quad (47) $$

from that we can get $\langle s_1 \cdot S_1 \rangle = -\frac{1}{8}$ and $N_{1/2,1} = \frac{1}{8}$. While in the rest region the negativity of the first excited state is zero.
3.1.2. Thermal entanglement

Next, we consider the thermal entanglement. From Eq. (42), the partition function can be obtained as

\[
Z = 5e^{-(1/2)\beta J_2} + 6e^{(7/2)\beta J_2} + e^{(1/2)\beta J_2} + e^{-(5/2)\beta J_2}(7e^{-2\beta J_1} + 5e^{\beta J_1} + 3e^{3\beta J_1}) \\
+ e^{(3/2)\beta J_2}(5e^{-\beta J_1} + 3e^{\beta J_1} + e^{2\beta J_1}),
\]

(48)

The correlator \(\langle s_1 \cdot s_1 \rangle\) at finite temperature can be computed from the partition function via the following relation

\[
\langle s_1 \cdot s_1 \rangle = -\frac{1}{4\beta Z} \frac{\partial Z}{\partial J_1}.
\]

(49)

Substituting (48) to Eq. (49) yields

\[
\langle s_1 \cdot s_1 \rangle = -\frac{1}{4Z} [e^{-(5/2)\beta J_2}(-14e^{-2\beta J_1} + 5e^{\beta J_1} + 9e^{3\beta J_1}) + e^{(3/2)\beta J_2}(-5e^{-\beta J_1} + 3e^{\beta J_1} + 2e^{2\beta J_1})].
\]

(50)

After substituting the above equation into (45), we may get analytical expression of the negativity \(N_{1/1,1}\) at finite temperatures. The negativity is a function of \(J_1, J_2\) and \(T\). That means the two kinds of interaction and some external parameters such as temperature may affect the entanglement remarkably which will be shown in our following numerical results.

**Low-temperature case:** We now make numerical calculations of entanglement to the case at low temperature close to ground state. We take \(J_1 = 1\) in all the following plots. In our system there exist three kinds of negativity, the negativity \(N_{1/2,1}\) between spin-1 and spin-1/2, \(N_{1/2,1/2}\) between two spin-1/2, and \(N_{1,1}\) between two spin-1.

In Fig. 5, we plot the negativity versus \(J_2\) in four-spin system at a low temperature of \(T = 0.008\). It is clear to see that \(N_{1/2,1}\) keeps a value about 0.5 when \(J_2 < 0.25\) and after that the \(N_{1/2,1}\) vanishes. This behavior of entanglement is consistent with analytical results. It is natural to see that introducing the NNN exchange interaction will suppress the entanglement of NN spins, and at last completely erase the entanglement. In comparison with \(N_{1/2,1}\), the negativities \(N_{1,1}\) and \(N_{1/2,1/2}\) behave distinctly. We see that the \(N_{1,1}\) increases quickly by two steps corresponding to the two special points of \(J_2 = 0.25\) and \(0.5\). And \(N_{1/2,1/2}\) displays a jump to a steady value of 0.5 near \(J_2 = 0.5\).
In our mixed-spin system with NNN interaction $J_2$, the increasing strength of $J_2$ must change the ground energy and ground states. From the insert figure of Fig. 5, we can clearly see the energy level crossing at the special points of $J_2 = \frac{1}{4}$ and $\frac{1}{2}$, which means the ground states changes at the points. Simply to know that the entanglement must change there. On another hands, in our frustrated system there exist three kinds sublattices. As $J_2$ increasing, the configuration of the system changes in the process from the main sublattice of NN spins to another main sublattice of NNN spins. Following that, the entanglement must behave differently. So let us see the result again. When $J_2 < \frac{1}{4}$, the sublattice consists of spin $\frac{1}{4}$ and 1 is main, the entanglement between two spin 1s and spin $\frac{1}{8}$ may be suppressed. Until $J_2 \geq \frac{1}{4}$, the spin 1s sublattice becomes main in the system, and then $\mathcal{N}_{1,1} = \frac{1}{2}$ which is just like the case of four-spin frustrated system only consists of spin 1s which is studied in reference [12], and the entanglement of spin 1s suppresses all the other ones. When $J_2 \geq \frac{1}{5}$, the two kinds sublattices of spin 1s and spin $\frac{1}{8}$s may be treated nearly self-existent. The $\mathcal{N}_{1,1} = 1$ is the same as the case of four-spin-1 frustrated system [12], and the $\mathcal{N}_{1/2,1/2} = 0.5$ is the same as the case of four-spin-$\frac{1}{2}$ frustrated system. $J_2 = \frac{1}{2}$ is a critical point in the frustrated spin-$\frac{1}{2}$ system [42].

**Entanglement versus $J_2$ and $T$:** As temperature increases the entanglement will decrease due to the mixing of less entangled excited states to the thermal state. It is obvious that there exists a threshold temperature after which the negativity is zero. In the frustrated system, there exists the parameter $J_2$, and with its increase, the negativity $\mathcal{N}_{1/2,1}$ will decrease to zero, while $\mathcal{N}_{1,1}$ and $\mathcal{N}_{1/2,1/2}$ increase from zero to their maxima. So it is clear that there exists a competition between the thermal fluctuation and the NNN interaction $J_2$.

In Fig. 6, we show the negativity $\mathcal{N}_{1/2,1}$ versus the temperature and $J_2$. Clearly, the thermal fluctuation suppresses the entanglement as $\mathcal{N}_{1/2,1}$ decreases from its maximum to zero at the temperature about $T = 1.082$. On the $J_2 - T$ plane, there is a curve along which the negativity just turns to be zero. It is possible to consider that the curve describes the threshold temperature $T_{th}$ versus $J_2$. $T_{th}$ does not behave as a monotonous function of the $J_2$, and it displays a peak at about $T = 0.178$, which is in big contrast with the case of non-mixed qubit systems [38].

Next, we consider the entanglement between NNN spins. In Fig. 7, we plot the negativity $\mathcal{N}_{1/2,1/2}$ as a function of the temperature and $J_2$. We can see that, only in the region $J_2 > 0.5$, $\mathcal{N}_{1/2,1/2}$ has non zero value. The thermal fluctuation all along suppresses the entanglement. So, from the curve lying on the $J_2 - T$ plane, we may find that the stronger the $J_2$ is, the higher the threshold temperature will be. In Fig. 8, we plot the negativity $\mathcal{N}_{1,1}$ versus $T$ and $J_2$. In the region of $J_2 < 0.25$, $\mathcal{N}_{1,1}$ is zero at any temperature. When $J_2 > 0.25$, the increasing NNN exchange interaction $J_2$ enhances the negativity and exhibits two particular flat roofs. With the temperature rises, $\mathcal{N}_{1,1}$ is suppressed to zero.

![Fig. 6. Negativity $\mathcal{N}_{1/2,1}$ versus both the exchange interaction coefficient $J_2$ and the temperature in the four-spin system.](image-url)
From Figs. 6–8, we show the properties of entanglement of NN and NNN spins affected by both the temperature and NNN interaction. Obviously, the thermal fluctuation suppresses the entanglement. At high temperature all the entanglement will be destroyed absolutely. And the NNN interaction may erase the NN entanglement, while enhance the NNN entanglement. This is the general property of the entanglement in our system. By the way, by using the concept of negativity here we should notice that, because $N_{1,1} > 0$ only gives a sufficient condition for entangled state, we cannot definitely say that the state in the area of zero negativity is not entangled, but we can make sure the negativity can materialize main property of entanglement of spin 1s.

3.2. Numerical results of negativity for more spins

In this section, we present numerical results of negativity for more spins, and first consider the low-temperature case.
3.2.1. Low-temperature case

In Fig. 9, we plot the negativity versus $J_2$ for the case of six spins at a lower temperature. The negativity $\mathcal{N}_{1/2,1}$ behaves as a decreasing function of $J_2$. It decreases to zero at about $J_2 = 0.27$, which is the special point corresponding to the energy level crossing. On the contrary, around the point $J_2 = 0.27$, $\mathcal{N}_{1,1}$ jumps up to a nonzero value, and then increases gradually until approaching the limit about $\frac{1}{3}$. The behavior of $\mathcal{N}_{1,1}$ is

![Fig. 9. Negativity versus the exchange interaction $J_2$ at the temperature $T = 0.02$ in six-spin system. The ground and the first two excited energy levels versus the $J_2$ are inserted in the plot.](image)

![Fig. 10. Negativity versus the exchange interaction $J_2$ at the temperature $T = 0.02$ in eight-spin system. The ground and the first three excited energy levels versus the $J_2$ are inserted.](image)
similar with the six-spin-1 frustrated system in [12], which may imply that, after \( J_2 \) gets some special point the NNN sublattices behave their own properties. Which has also been seen in Fig. 5. And in Fig. 9, there are not some platforms just like Fig. 5, because the ground energy is not linear function of \( J_2 \) as the case of four-spin case in Fig. 5, which is shown in the insert figure. But the energy crossing still happens.

We also see that \( N_{1/2,1/2} \) is zero all the time. It can be understood as follows. In the six-site system there are three spin halves with the NNN interaction constitute a triangular sublattice. An antiparallel pair of spin halves has the lowest interaction energy \(-J_2\), while a pair of parallel spin halves has the energy \(+J_2\). In a triangular lattice all the three spin pairs cannot be simultaneously antiparallel in the ground state [43]. Just because of this intrinsical frustration both with the absolute symmetric position of the three qubits, no one of the spin triangle has enough capability to be entangled with another one. And by calculation it is easy to be proved true [5].

The negativity versus \( J_2 \) in the eight-site case is shown in Fig. 10. \( N_{1/2,1/2} \) decreases in two processes corresponds to \( J_2 = 0.25 \) and \( 0.55 \). And \( N_{1,1} \) behaves two steps, just like the four-spin case of our system. All the special points where the negativities changed remarkably are all corresponding to the energy crossing and the strange behavior of negativity between \( J_2 = 0.55 \) to \( J_2 = 0.67 \) may due to the too close energy levels, which can be seen in the insert figure. That means the change of ground energy greatly affects the entanglement. Similar to the 4 and 6-spin case above, when \( J_2 \) is larger than some critical value, negativities in the sublattices of spin \( \frac{1}{2} \) and spin \( 1 \) behave just as that in their own frustrated systems. \( N_{1,1} \) at last goes to \( \frac{1}{4} \) and \( N_{1/2,1/2} \) goes to \( \frac{2}{3} \).

3.2.2. Entanglement versus \( J_2 \) and \( T \)

Now, we present the entanglement versus \( J_2 \) and \( T \) in the six-spin model. The NN negativity \( N_{1/2,1/2} \) is shown in Fig. 11. We may find that the entanglement only exists in the region approximately \( T < 0.925 \) and \( J_2 < 0.418 \). We give the NNN negativity \( N_{1,1} \) in Fig. 12. In the region of \( J_2 < 0.282 \), there is no negativity \( N_{1,1} \) at any temperature. The threshold \( T_{th} \) is increased by the increasing \( J_2 \), which is similar to the four-spin case.

4. Conclusion

In conclusion, we have studied the entanglement properties of the \( (\frac{1}{2}, 1) \) mixed-spin systems described by the Heisenberg model. In the systems only with NN exchange interactions, for two-spin and three-spin cases analytical results of the negativity have been obtained, which facilitate our discussions of entanglement. The analytical expression of threshold temperature after which the entanglement vanishes are obtained for the

![Fig. 11. Negativity \( N_{1/2,1/2} \) versus both the exchange interaction \( J_2 \) and the temperature in the six-spin system.](image-url)
two-site case. For the case of even number of particles, it has been found that the pairwise thermal entanglement is solely determined by the internal energy, and thus builds an interesting relation between the microscopic quantity, entanglement, and the macroscopic thermal dynamical function, the internal energy in the mixed-spin systems. And by using the numerical results of ground energy in very large system, we can know how about the entanglement in thermodynamic limit system. And the analytical results are accordant well with the numerical results. After that we have numerically studied the effects of different finite temperature and magnetic fields on entanglement. As a conclusion, the thermal fluctuation suppresses the entanglement, and entanglement may change evidently at some critical points of magnetic field.

In the systems also with NNN interactions, by applying the angular momentum coupling method, we obtained analytical results of all the eigenenergies of the four-spin system, based on which the negativity of the NN spins has been obtained. We also considered the excited-state entanglement. The analytical results of negativity at finite temperature has been given. We have numerically studied the effects of the NNN interaction on the NN entanglement and NNN entanglement. It is natural to see that the NNN interaction suppresses the NN entanglement, and enhances the NNN entanglement. We found that after some special values of \( J_2 \) the sublattices consisted of NNN spins become main station, and the negativities of NNN spins display some properties just as in non mixed-spin frustrated systems. At finite temperature, the thermal fluctuation suppresses both the NN entanglement and the NNN entanglement. The threshold temperature \( T_{th} \) are studied. The entanglement displays some peculiar properties, which are quite different from those of the spin-half model. These are due to inherent mixed-spin character of our system. It is more interesting to study entanglements in other mixed systems and explore some universal properties, which are under consideration.

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**Appendix A. Two-site Heisenberg model with a magnetic field**

The Hamiltonian of the two-site Heisenberg model with a magnetic field is written explicitly as

\[
H_1 = s_{1x} \otimes S_{2x} + s_{1y} \otimes S_{2y} + s_{1z} \otimes S_{2z} + B(s_{1z} + S_{2z}).
\]
Following the same way as the discussions of Section 2.1, the density matrix of the thermal state is given by Eq. (6) with the matrix elements

\[ a_1 = a_6 e^{3bB} = e^{(\beta/2)(3B-1)}, \]

\[ a_5 = a_2 e^{\beta B} = \frac{1}{2} e^{\beta B/2} (e^{\beta} + 2e^{-\beta/2}), \]

\[ a_4 = a_3 e^{\beta B} = \frac{1}{2} e^{\beta B/2} (2e^{\beta} + e^{-\beta/2}), \]

\[ b_2 = b_1 e^{\beta B} = -\frac{\sqrt{3}}{2} e^{\beta B/2} (e^{\beta} - e^{-\beta/2}), \]

(A1)

and the partition function

\[ Z = e^{(\beta/2)(3B-1)} + e^{-(\beta/2)(3B+1)} + e^{(1/4)\beta} \cosh\left(\frac{3\beta}{4}\right) \cosh\left(\frac{\beta B}{2}\right). \]

(A2)

Having obtained the analytical expressions of the matrix, we directly obtain the negativity after substituting the matrix elements to Eq. (13).

References