Thermal entanglement of the Ising–Heisenberg diamond chain with Dzyaloshinskii–Moriya interaction*

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We investigate the thermal entanglement in a spin-1/2 Ising–Heisenberg diamond chain, in which the vertical Heisenberg spin dimers alternate with single Ising spins. Due to the fact that the Dzyaloshinskii–Moriya (DM) interaction contributes to unusual and interesting magnetic properties in actual materials, and moreover it plays a significant role in the degree of the entanglement of the Heisenberg quantum spin systems, we focus on the effects of different DM interactions, including D_z and D_x, on the thermal entanglement of the Heisenberg spin dimer. The concurrence, as a measure of spin dimer entanglement, is calculated for different values of exchange interactions, DM interaction, external magnetic field, and temperature. It is found that the critical temperature and the critical magnetic field corresponding to the vanishing of entanglement increase with DM interaction, and the entanglement revival region gets larger by increasing DM interaction, thus DM interaction favors the formation of the thermal entanglement. It is observed that different DM interaction parameters (D_z and D_x) have remarkably different influences on the entanglement. Different from the case D_z, there is the non-monotonic variation of the concurrence with temperature in the case D_x, and additionally the DM interaction D_x can induce the entanglement near zero temperature in the case that the antiferromagnetic Ising-type interaction constant is larger than the antiferromagnetic Heisenberg interaction constant. It is also shown that for the same value of DM interaction the critical magnetic field of the case D_x is larger than that of the case D_z.

Keywords: thermal entanglement, Ising–Heisenberg diamond chain, Dzyaloshinskii–Moriya interaction

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1. Introduction

Entanglement is a fundamental feature of the quantum mechanics, and it is also a potential valuable resource for quantum information processing. As one of the simplest quantum systems which exhibit rich entanglement features, the Heisenberg spin chain is regarded as a natural candidate in the solid state proposals of realizing quantum computing.[1] Considering that thermal fluctuation suppresses quantum effects, the concept of thermal entanglement was introduced to refer to the idea that the effects of temperature should be viewed as the external control in the preparation of entangled states.[2,3] Up to now, considerable theoretical studies have been done on the thermal entanglement of the Heisenberg spin chains,[4–14] and moreover the experimental observations of thermal entanglement have also been reported for some magnetic materials.[15–18]

The diamond Heisenberg spin chain, in which the vertical spin dimers alternate with single spins to form one-dimensional lattices composed of diamond-shaped units, is a kind of important and interesting model in the the studies of the Heisenberg spin chains. Since Takano *et al.* first studied theoretically the ground state of an ideal diamond spin chain in 1996,[19] the theoretical research of the diamond chain has attracted much attention due to rich physical properties as a consequence of the mutual interplay between quantum fluctuations and geometric frustration.[20–25] In these theoretical works, several modifications of the ideal diamond chain have been proposed, such as the distorted diamond chain, the frustrated diamond chain, and the generalized diamond chain. In 2003, the experimental results reported by Kikuchi *et al.* showed that the natural mineral azurite $Cu_3(CO_3)_2(OH)_2$ formed by the spin-1/2 Cu^{2+} ions can be regarded as an actual material for a diamond chain model.[26] Later on, the 1/3 magnetization plateau in the azurite $Cu_3(CO_3)_2(OH)_2$ was observed experimentally.[27,28] Since then, the physics properties of the azurite $Cu_3(CO_3)_2(OH)_2$, as diamond chain compound, have been investigated on the experimental side with considerable interest.[29,30] Kikuchi *et al.* discussed the magnetic anisotropy observed in the magnetization results of azurite, and proposed that the most plausible origin of the magnetic anisotropy is the Dzyaloshinskii–Moriya (DM) interaction since there is no point symmetry in the azurite and the single-ion anisotropy vanishes in spin-1/2 Cu^{2+} magnetic systems.[27,28] Additionally, Rule *et al.* also analyzed the important influence of DM interaction on the ordered magnetic moment structure of the azurite.[30]

We note that the rigorous theoretical treatment of geo-

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metrically frustrated quantum Heisenberg diamond chains is a very difficult task due to a non-commutability of spin operators involved in these models. To overcome the mathematical difficulties, a novel class of the simplified versions was proposed.[31–33] In this simplified model called the geometrically frustrated Ising–Heisenberg diamond chain, the Ising spins locate at the nodal sites and the Heisenberg spin dimers are on the interstitial decorating sites of the diamond chain (see Fig. 1). The ground-state phase diagram, the magnetization, the susceptibility, and the thermodynamics of the Ising–Heisenberg diamond chains have already been theoretically examined.[34–38] Furthermore, the thermal entanglement properties of several kinds of Ising–Heisenberg diamond models, such as spin-$1/2$ generalized symmetrical Ising–Heisenberg diamond chain,[39] Ising–*XXZ* diamond chain,[40] Ising–*XYZ* diamond chain,[41] and the mixed spin-$1/2$ and spin-1 Ising–Heisenberg diamond chain,[42] have been investigated recently.

The aforementioned DM interaction, which arises from spin–orbit coupling and describes the super-exchange between the interacting spins, was first introduced as anisotropic antisymmetric exchange interactions to explain weak ferromagnetism of the antiferromagnetic crystals.[43,44] Some antiferromagnetic materials described by DM interaction exhibit unusual and interesting magnetic properties due to quantum fluctuation in the presence of an applied magnetic field. Additionally, it has been found that the DM interaction plays a significant role in the degree of the entanglement of the Heisenberg quantum spin systems.[45–48] It was found that DM interaction may increase the critical temperature for a two-qubit *XX* spin chain,[45] and may excite the entanglement and teleportation fidelity for a two-qubit *XXX* spin chain.[46] It was also shown that the entanglement can be efficiently controlled by DM interaction parameter for the two-qubit *XXZ* spin model.[47] Recently, the mutual effect of DM interaction and transverse magnetic field on the thermal entanglement for an infinite one-dimensional spin-$1/2$ *XX* model has been studied.[48] Motivated by the importance of DM interaction in actual materials such as the azurite $Cu_3(CO_3)_2(OH)_2$, in this paper we will focus on the effect of DM interaction between Heisenberg spins in the dimer on the thermal entanglement of a spin-$1/2$ Ising–Heisenberg diamond chain. The effects of DM interaction will be discussed according to two different directions of the $\boldsymbol{D}$ vector of DM interaction, respectively. In one case it is assumed that the $\boldsymbol{D}$ vector is perpendicular to both the Heisenberg spin dimer bond and to the chain (i.e., $\boldsymbol{D} = D_z\boldsymbol{e}_z$), and the other it is assumed that the $\boldsymbol{D}$ vector is along the direction of the Heisenberg dimer bond (i.e., $\boldsymbol{D} = D_x\boldsymbol{e}_x$). We will calculate the concurrence as a measure of Heisenberg spin dimer entanglement. According to the argument of Ananikian *et al.*,[39] each Heisenberg spin dimer interacts with its neighboring dimer through the classical Ising-type interaction, then the states of two adjacent dimers become disentangled. Thus, the calculation of the concurrence can be performed for each Heisenberg spin dimer separately. The concurrence will be constructed for different values of exchange interactions, DM interaction, external magnetic field, and temperature. The critical temperatures and the critical magnetic fields via different DM interaction and exchange interactions will also be obtained, respectively. It will be shown that different DM interaction parameters (D_z and D_x) have remarkably different influences on the entanglement near zero temperature and the critical temperature and magnetic field.

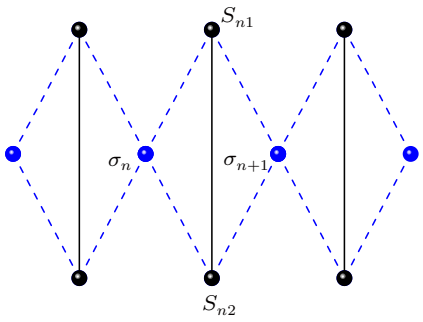


Fig. 1. (color online) Schematic representation of the spin-$1/2$ Ising–Heisenberg diamond chain. The black circle $\mathbf{S}_{n1}$ represents Heisenberg spin, and the blue circle σ_n represents Ising spin. The black solid line corresponds to Heisenberg interaction, while the blue dashed line to Ising interaction.

2. Model and method

We consider a spin-$1/2$ Ising–Heisenberg diamond chain model with DM interaction in the presence of an external magnetic field. The model consists of the nodal Ising spins alternating with vertical Heisenberg spin dimers (see Fig. 1). Let us write the total Hamiltonian of the model as a sum over cluster Hamiltonian $H = \sum_{n=1}^{N} H_n$, where each cluster Hamiltonian H_n involves all the interaction terms within the n-th diamond-shaped cluster

$$\begin{aligned} H_n \;=\; & J_0\boldsymbol{S}_{n1}\cdot\boldsymbol{S}_{n2} + J(\sigma_n^z+\sigma_{n+1}^z)(S_{n1}^z+S_{n2}^z) \\ & + \boldsymbol{D}\cdot(\boldsymbol{S}_{n1}\times\boldsymbol{S}_{n2}) - h\left(S_{n1}^z+S_{n2}^z+\frac{\sigma_n^z+\sigma_{n+1}^z}{2}\right). \quad (1) \end{aligned}$$

Here, $\boldsymbol{S}_n$ denotes the Heisenberg spin-$1/2$ operator, and σ_n^z is the Ising spin, $J_0 > 0$ is the antiferromagnetic Heisenberg interaction constant, and $J > 0$ labels the antiferromagnetic Ising-type interaction, $\boldsymbol{D}$ is the DM vector coupling parameter accounting for DM interaction between Heisenberg spins in the dimer. The last term in the Hamiltonian (1) determines the Zeeman energy of the Heisenberg and Ising spins in an external magnetic field h oriented along the z axis. Since each Ising spin belongs simultaneously to two clusters, there is a factor of 1/2 for the Ising spin in the last term of the Hamiltonian (1). To see the effect of the anisotropic parameter $\boldsymbol{D}$, in the following discussion, we will consider two different directions

of the $\boldsymbol{D}$ vector, namely assuming $\boldsymbol{D} = D_z \boldsymbol{e}_z$ and $\boldsymbol{D} = D_x \boldsymbol{e}_x$, respectively.

Here, we calculate the concurrence C as a measure of entanglement between Heisenberg spins in the dimer. The concurrence is defined as[49,50]

$$C = \max\{\lambda_1 - \lambda_2 - \lambda_3 - \lambda_4, 0\}, \tag{2}$$

where the quantities λ_i are the square roots of the eigenvalues of the operator

$$\rho = \rho_{S_{12}} \left(\sigma^y_{S_1} \otimes \sigma^y_{S_2}\right) \rho^*_{S_{12}} \left(\sigma^y_{S_1} \otimes \sigma^y_{S_2}\right) \tag{3}$$

in descending order ($\rho_{S_{12}}$ is the reduced density matrix of the Heisenberg spin dimer and $\sigma^y_{S_1}$ is the Pauli operator). The values of the concurrence are ranged from zero to one when quantum states are changed from unentangled to maximally entangled states. The cluster state at thermal equilibrium is described by the density matrix $\rho_n(T) = \exp(-\beta H_n)/Z_n$, where $\beta = 1/k_{\mathrm{B}}T$ (k_{B} is the Boltzmann's constant that we henceforth will take equal to 1, and T is the temperature) and $Z_n = \mathrm{Tr}\left[\exp(-\beta H_n)\right]$ is the partition function.

3. Thermal entanglement of Heisenberg spin dimer

3.1. The case with $\boldsymbol{D}$ vector along the z axis

In this section, we assume that the $\boldsymbol{D}$ vector of DM interaction in Hamiltonian (1) is along the z axis, i.e., $\boldsymbol{D} = D_z \boldsymbol{e}_z$. As mentioned above, the states of neighboring Heisenberg spin dimers are disentangled due to a classical character of the coupling between them via the Ising spin.[39] Thus, we can calculate the concurrence for each of the dimers individually. We consider the n-th cluster consisting of Heisenberg spin dimer (S_{n1} and S_{n2}) and two Ising spins (σ_n and σ_{n+1}), and would like to emphasize that each Ising spin belongs simultaneously to two clusters. Then, the sixteen eigenvalues of the n-th cluster Hamiltonian $H_n(1)$ can be given as

$$\begin{aligned}
&E_0 = E_1 = \frac{1}{4}(-4h + J_0),\ E_2 = E_3 = \frac{1}{4}(4h + J_0),\\
&E_4 = E_5 = \frac{1}{4}(-J_0 - 2\gamma),\ E_6 = E_7 = \frac{1}{4}(-J_0 + 2\gamma),\\
&E_8 = \frac{1}{4}(-2h - 4J + J_0),\ E_9 = \frac{1}{4}(2h - 4J + J_0),\\
&E_{10} = \frac{1}{4}(-6h + 4J + J_0),\ E_{11} = \frac{1}{4}(6h + 4J + J_0),\\
&E_{12} = \frac{1}{4}(-2h - J_0 - 2\gamma),\ E_{13} = \frac{1}{4}(2h - J_0 - 2\gamma),\\
&E_{14} = \frac{1}{4}(-2h - J_0 + 2\gamma),\ E_{15} = \frac{1}{4}(2h - J_0 + 2\gamma),
\end{aligned}$$

where $\gamma = \sqrt{D_Z^2 + J_0^2}$, and the corresponding eigenvectors are expressed as

$$\begin{aligned}
&|\psi_0\rangle = |1011\rangle,\quad |\psi_1\rangle = |1110\rangle,\\
&|\psi_2\rangle = |0001\rangle,\quad |\psi_3\rangle = |0100\rangle,\\
&|\psi_4\rangle = \frac{1}{\sqrt{2}}\left(\mathrm{e}^{\mathrm{i}\theta}|1001\rangle - |0011\rangle\right),\\
&|\psi_5\rangle = \frac{1}{\sqrt{2}}\left(\mathrm{e}^{\mathrm{i}\theta}|1100\rangle - |0110\rangle\right),\\
&|\psi_6\rangle = \frac{1}{\sqrt{2}}\left(\mathrm{e}^{\mathrm{i}\theta}|1001\rangle + |0011\rangle\right),\\
&|\psi_7\rangle = \frac{1}{\sqrt{2}}\left(\mathrm{e}^{\mathrm{i}\theta}|1100\rangle + |0110\rangle\right),\\
&|\psi_8\rangle = |1010\rangle,\quad |\psi_9\rangle = |0101\rangle,\\
&|\psi_{10}\rangle = |1111\rangle,\quad |\psi_{11}\rangle = |0000\rangle,\\
&|\psi_{12}\rangle = \frac{1}{\sqrt{2}}\left(\mathrm{e}^{\mathrm{i}\theta}|1101\rangle - |0111\rangle\right),\\
&|\psi_{13}\rangle = \frac{1}{\sqrt{2}}\left(\mathrm{e}^{\mathrm{i}\theta}|1000\rangle - |0010\rangle\right),\\
&|\psi_{14}\rangle = \frac{1}{\sqrt{2}}\left(\mathrm{e}^{\mathrm{i}\theta}|1101\rangle + |0111\rangle\right),\\
&|\psi_{15}\rangle = \frac{1}{\sqrt{2}}\left(\mathrm{e}^{\mathrm{i}\theta}|1000\rangle + |0010\rangle\right),
\end{aligned}$$

where $\theta = \arctan(J_0/D_Z)$. It is noted that here the sequence of the standard basis vectors of the Hilbert space associated with the n-th cluster is defined as $\{S_{n1}, \sigma_{n+1}, S_{n2}, \sigma_n\}$.

The density matrix ρ_n describing the n-th cluster state at temperature T is written as

$$\rho_n = \frac{1}{Z_n}\sum_{i=0}^{15} \mathrm{e}^{-\beta E_i}|\psi_i\rangle\langle\psi_i|, \tag{4}$$

with the partition function Z_n

$$\begin{aligned}
Z_n &= \mathrm{Tr}\left[\sum_{i=0}^{15} \mathrm{e}^{-\beta E_i}|\psi_i\rangle\langle\psi_i|\right]\\
&= 8\,\mathrm{e}^{\frac{1}{4}J_0\beta}\cosh^2\left(\frac{h}{4}\beta\right)\cosh\left(\frac{\gamma}{2}\beta\right)\\
&\quad + \mathrm{e}^{-\frac{1}{4}J_0\beta}\left[4\cosh(h\beta) + 2\,\mathrm{e}^{J\beta}\cosh\left(\frac{h}{2}\beta\right)\right.\\
&\quad \left. + 2\,\mathrm{e}^{-J\beta}\cosh\left(\frac{3h}{2}\beta\right)\right].
\end{aligned} \tag{5}$$

We construct the reduced density matrix $\rho_{S_{12}}$ describing the Heisenberg spin dimer $\{S_{n1}, S_{n2}\}$ by tracing out two Ising spins $\{\sigma_{n+1}, \sigma_n\}$ in the n-th cluster. In the basis vectors $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$, the reduced density matrix $\rho_{S_{12}}$ can be given by

$$\rho_{S_{12}} = \frac{1}{Z_n}\begin{pmatrix} u & 0 & 0 & 0\\ 0 & w & y & 0\\ 0 & y^* & w & 0\\ 0 & 0 & 0 & v \end{pmatrix}, \tag{6}$$

where

$$\begin{aligned}
u &= \mathrm{e}^{-\frac{1}{4}J_0\beta}\left(2\mathrm{e}^{h\beta} + \mathrm{e}^{\left(\frac{1}{2}h+J\right)\beta} + \mathrm{e}^{\left(\frac{3}{2}h-J\right)\beta}\right),\\
v &= \mathrm{e}^{-\frac{1}{4}J_0\beta}\left(2\mathrm{e}^{-h\beta} + \mathrm{e}^{\left(-\frac{1}{2}h+J\right)\beta} + \mathrm{e}^{\left(-\frac{3}{2}h-J\right)\beta}\right),
\end{aligned}$$

$$y = -4\mathrm{e}^{\mathrm{i}\theta}\,\mathrm{e}^{\frac{1}{4}J_0\beta}\cosh^2\left(\frac{h}{4}\beta\right)\sinh\left(\frac{\gamma}{2}\beta\right),$$

$$w = 4\mathrm{e}^{\frac{1}{4}J_0\beta}\cosh^2\left(\frac{h}{4}\beta\right)\cosh\left(\frac{\gamma}{2}\beta\right).$$

The square roots of the four eigenvalues of the operator ρ defined in Eq. (3) are calculated

$$\lambda_1 = \frac{w+|y|}{Z_n},\ \lambda_2 = \frac{w-|y|}{Z_n},\ \lambda_3 = \lambda_4 = \frac{\sqrt{uv}}{Z_n}, \tag{7}$$

so the concurrence as a measure of Heisenberg spin dimer entanglement is given by

$$C = \frac{2}{Z_n}\max\left\{|y| - \sqrt{uv}, 0\right\}. \tag{8}$$

We can discuss the effects of DM interaction on the thermal entanglement of the Heisenberg spin dimer by calculating the concurrence (8). Firstly, we consider the case without the magnetic field (i.e., $h = 0$). In Fig. 2, the variations of concurrence C with the temperature T for different values of D_z are plotted in three different cases (i.e., $J - J_0 < 0$, $J - J_0 = 0$, and $J - J_0 > 0$). Disregarding the DM interaction (i.e., letting $D_z = 0$), one can obtain results presented by the black solid lines, which are consistent with the results of the previous literature.[39] For the case with $J_0 = 1$ and $J = 0.5$ (see Fig. 2(a)), the concurrence C is equal to 1 at zero temperature, monotonically decreases with temperature increasing and reaches zero at the critical temperature T_c corresponding to the vanishing of entanglement. Considering the effect of DM interaction, it is found that the critical temperature T_c increases with $|D_z|$. For instance, $T_c = 0.867$, 0.887, 0.941, 1.022, and 1.123, for $D_z = 0$, 0.25, 0.5, 0.75 and 1.0, respectively. It is also seen that at a fixed temperature (lower than the critical temperature) the concurrence value increases with the DM interaction. The variation of T_c with D_z is shown in Fig. 3, where the black dotted line corresponds to the case with $J_0 = 1$ and $J = 0.5$. It is concluded that the DM interaction favors the formation of thermal entanglement. This consequence is due to the fact that DM interaction induces the quantum correlation between two Heisenberg spins in the dimer, when the DM interaction is turned on, the low-lying excited states tend to the more correlated.[48]

Figure 2(b) shows the case with $J_0 = 1$ and $J = 1$. When $D_z = 0$, the concurrence C starts from $1/3$ other than 1 at $T = 0$, and then with temperature increasing it gradually deceases to zero at the critical temperature $T_c = 0.693$.[39] When the DM interaction is considered, the concurrence C near zero temperature (e.g., $T = 0.005$) increases with $|D_z|$, and gradually reaches its maximum values of 1. The variation of the concurrence C with D_z at $T = 0.005$ is shown in Fig. 4, where the red dotted line corresponds to the case with $J_0 = 1$ and $J = 1$. In this case, the maximum entangled state with $C = 1$ appears when the DM interaction parameter $|D_z|$ is larger than 0.4. In Fig. 3, it is shown that the critical temperature T_c (red dashed-line) also increases with $|D_z|$, but T_c of the case with $J = 1$ is smaller than that of the case with $J = 0.5$ for the same value of the DM interaction parameter D_z.

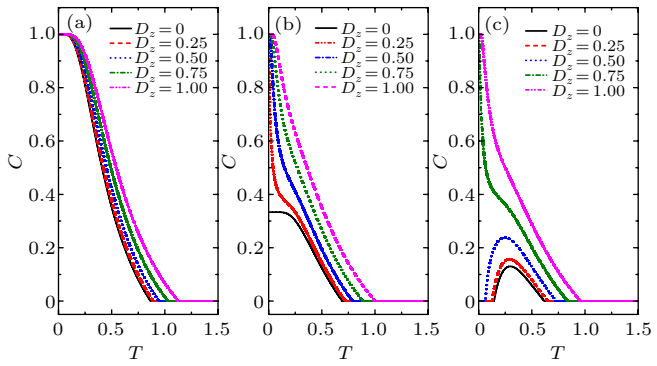


Fig. 2. (color online) The concurrence C versus the temperature T for different values of D_z with $h = 0$, $J_0 = 1$, and (a) $J = 0.5$; (b) $J = 1$; (c) $J = 1.1$.

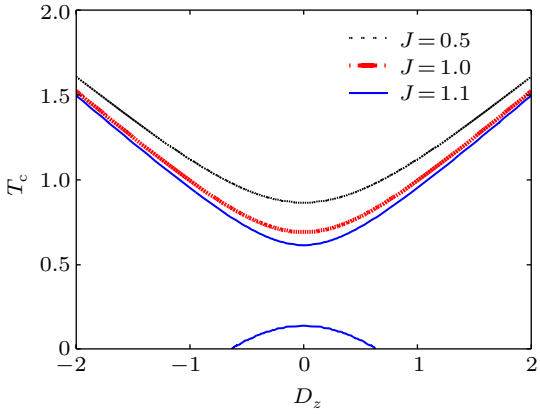


Fig. 3. (color online) The dependence of the critical temperature T_c on D_z for different values of J with $h = 0$ and $J_0 = 1$.

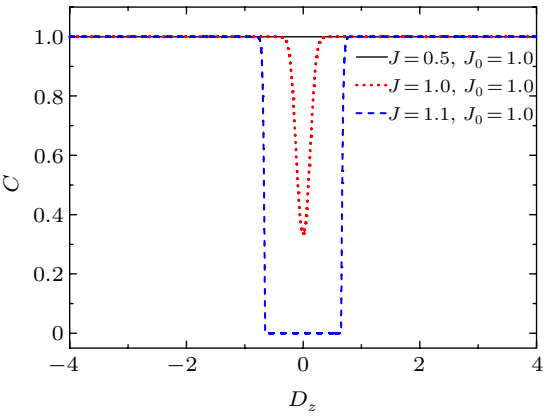


Fig. 4. (color online) The dependence of the concurrence C at $T = 0.005$ on D_z for different values of J with $h = 0$ and $J_0 = 1$.

The third case ($J - J_0 > 0$, e.g., $J_0 = 1$ and $J = 1.1$) is plotted in Fig. 2(c). In the case of $D_z = 0$, the Heisenberg spin dimer is not entangled (i.e., the concurrence $C = 0$) at $T = 0$.

By increasing the temperature from zero, the Heisenberg spin dimer remains unentangled up to the first critical temperature $T_{c1} = 0.145$. As soon as the temperature increases from T_{c1}, the concurrence $C > 0$ (i.e., the thermal entanglement regains, that is so-called entanglement revival) and takes a maximum value and then decreases and reaches zero at the second critical temperature $T_{c2} = 0.617$. The existence of the first critical temperature arises from mixing the entangled excited states with the unentangled ground state due to thermal fluctuations, while sufficiently large thermal fluctuations will destroy all quantum correlations so that the second critical temperature occurs. It is observed that with $|D_z|$ increasing, T_{c1} gradually decreases to zero, while T_{c2} increases. Thus, the width of the temperature interval within which the Heisenberg spin dimer becomes entangled (i.e., the concurrence $C > 0$) gets larger by increasing $|D_z|$. As a result, different from the first two cases ($J = 0.5$ and $J = 1$), there are two critical temperature lines for the case with $J_0 = 1$ and $J = 1.1$ in Fig. 3 (shown by two blue solid lines). Further, from blue solid lines in Fig. 3 it is found that if $|D_z|$ is larger than 0.663, the DM interaction can induce the entanglement at $T = 0$. In fact, at zero temperature, when $|D_z| < |D_z^*| = 2\sqrt{J(J - J_0)}$ the ground state contains twofold degenerate states $|\psi_8\rangle$ and $|\psi_9\rangle$, which are unentangled states with $C = 0$ since these states are factorable. However, when $|D_z| > |D_z^*|$, the ground state becomes fourfold degenerate, containing $|\psi_4\rangle$, $|\psi_5\rangle$, $|\psi_{12}\rangle$, and $|\psi_{13}\rangle$, which are the maximum entangled states in the subspace of the Heisenberg spin dimer, corresponding to the concurrence $C = 1$. Thus, there exists the quantum phase transition from unentangled state to maximum entangled state at zero temperature by changing the DM interaction parameter D_z. In Fig. 4, it is shown by the blue dashed-line that the concurrence C sharply changes from 0 to 1 at the critical DM interaction parameter value $|D_z^*| = 0.663$.

Now, we proceed to study the role of the magnetic field h on the thermal entanglement with the DM interaction D_z. The variations of concurrence C with the magnetic field h for different values of D_z at temperature $T = 0.1$ are plotted in Fig. 5. Figure 5(a) shows the case with $J - J_0 < 0$ (here, $J_0 = 1$ and $J = 0.5$). With $|h|$ increasing, the concurrence C gradually decreases to zero, and moreover the critical magnetic field $|h_c|$ corresponding to the vanishing of entanglement increases with $|D_z|$. For instance, $|h_c| = 2.25$, 2.40, and 2.81, for $D_z = 0.5$, 1.0, and 2.0, respectively. Here, it is assumed that C with the value less than 10^{-3} corresponds to the entanglement disappearing. The dependence of the critical magnetic field h_c on D_z is shown in Fig. 6, in which the black dashed-line corresponds to the case with $J_0 = 1$ and $J = 0.5$.

The case with $J_0 = 1$ and $J = 1$ is shown in Fig. 5(b). When $D_z = 0$, with increasing the magnetic field h the concurrence C firstly increases from 0.333 to a maximum 0.493, and then gradually vanishes. It is found that this maximum of the concurrence C increases with $|D_z|$ up to 1. For instance, the maximums of C are 0.639, 0.887, and 0.998 for $D_z = 0.5$, 1.0, and 2.0, respectively. Likewise, the critical magnetic field $|h_c|$ also increases with $|D_z|$, but $|h_c|$ of the case with $J = 1$ (also see red dotted line in Fig. 6) is higher than that of the case with $J = 0.5$ for the same value of the DM interaction parameter D_z.

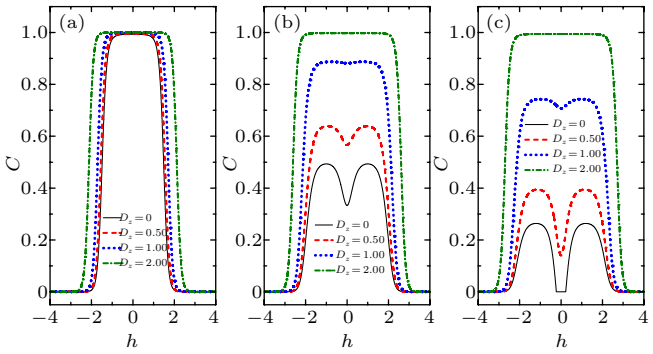


Fig. 5. (color online) The concurrence C versus the magnetic field h for different values of D_z with $T = 0.1$, $J_0 = 1$, and (a) $J = 0.5$; (b) $J = 1$; (c) $J = 1.1$.

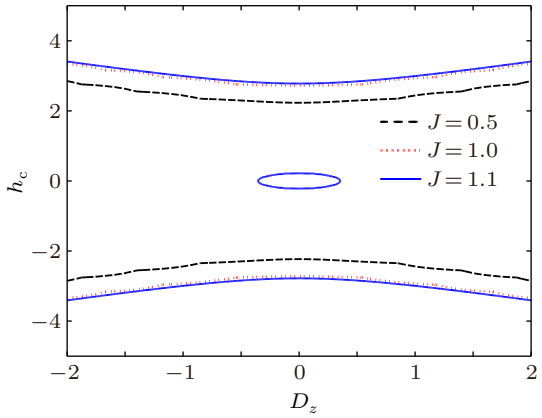


Fig. 6. (color online) The dependence of the critical magnetic field h_c on D_z for different values of J with $J_0 = 1$ and $T = 0.1$. (Here, it is assumed that C with the value less than 10^{-3} corresponds to the entanglement disappearing.)

Figure 5(c) shows the case with $J_0 = 1$ and $J = 1.1$. In the absence of the DM interaction D_z and the magnetic field h, the concurrence C is zero and Heisenberg spin dimer is unentangled. By increasing $|h|$ from zero, Heisenberg spin dimer still keeps unentangled up to the first critical magnetic field $|h_{c1}| = 0.23$. When the magnetic field increases from $|h_{c1}|$, the thermal entanglement (at $T = 0.1$) revives, and the concurrence C takes a maximum value 0.264 at $|h| = 1.20$, and then gradually deceases to zero at the second critical magnetic field $|h_{c2}| = 2.78$. As mentioned above, when $D_z = 0$ and $h = 0$, the ground state contains twofold degenerate states $|\psi_8\rangle$ and $|\psi_9\rangle$, which are unentangled states. At $T = 0.1$, with increasing the magnetic field due to admixture of entangled excited states into the mix state, the thermal entanglement regains at the first critical magnetic field $|h_{c1}|$. The existence of

the second critical magnetic field is completely natural, since sufficiently large magnetic field will induce the ground state to be factorable state $|\psi_{10}\rangle = |1111\rangle$ or $|\psi_{11}\rangle = |0000\rangle$. It is seen that with $|D_z|$ increasing, $|h_{c1}|$ gradually decreases to zero, while $|h_{c2}|$ increases. Thus, for the case with $J_0 = 1$ and $J = 1.1$, distinct from the first two cases with $J = 0.5$ and $J = 1$, the dependence of the critical magnetic field h_c on the DM interaction parameter D_z is presented by three blue solid lines in Fig. 6.

3.2. The case with $\boldsymbol{D}$ vector along the x axis

In this section we shall study the case that the $\boldsymbol{D}$ vector of DM interaction in the Hamiltonian (1) is along the x axis, i.e., $\boldsymbol{D} = D_x \boldsymbol{e}_x$. In principle, the problem of 4-qubit spin models can be solved analytically. However, for the case with the $\boldsymbol{D}$ vector along the x axis the analytical expressions of eigenfunctions and the corresponding eigenvalues of the Hamiltonian (1) are too complex to be compactly given. Thus, in order to obtain explicit physical results, we resort to a numerical calculation method based on the standard process given above.

First, we shall start with discussion of the thermal entanglement in the absence of a magnetic field (i.e., $h = 0$). Figure 7 shows the variations of concurrence C with the temperature T for different values of D_x according to three different cases, i.e., $J - J_0 < 0$, $J - J_0 = 0$, and $J - J_0 > 0$. For the case with $J_0 = 1$ and $J = 0.5$ (see Fig. 7(a)), due to the effect of the DM interaction D_x, the maximum of the concurrence C is not located at zero temperature any more, but shifts to a finite T value, and moreover is smaller than 1. For instance, the maximum of the concurrence C is 0.964 at $T = 0.115$ for $D_x = 1.0$. This non-monotonic variation of C with T in the case with the $\boldsymbol{D}$ vector along the x axis is obviously different from the case with the $\boldsymbol{D}$ vector along the z axis. For the cases with $J - J_0 = 0$ and $J - J_0 > 0$, the concurrence C increases with D_x, and the non-monotonic variation of C with T is also observed (see Figs. 7(b) and 7(c)).

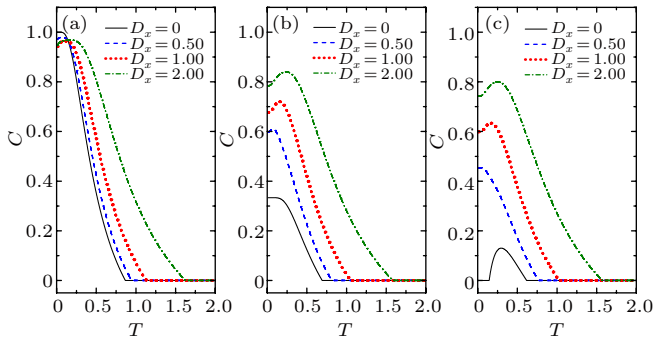


Fig. 7. (color online) The concurrence C versus the temperature T for different values of D_x with $h = 0$, $J_0 = 1$, and (a) $J = 0.5$; (b) $J = 1$; (c) $J = 1.1$.

After the concurrence reaches the maximum, it decreases gradually with temperature increasing and vanishes at the critical temperature T_c. The dependence of the critical temperature T_c on D_x for different values of J is plotted in Fig. 8. Compared with the case D_z (see Fig. 3), the effect of D_x on the thermal entanglement has a distinct property in the case with $J - J_0 > 0$ (see blue solid line in Fig. 8), in which the DM interaction D_x can induce the entanglement characterized by a nonzero concurrence near zero temperature. Specifically, for very small $|D_x|$, there exist three critical temperature values in the case with $J_0 = 1$ and $J = 1.1$.

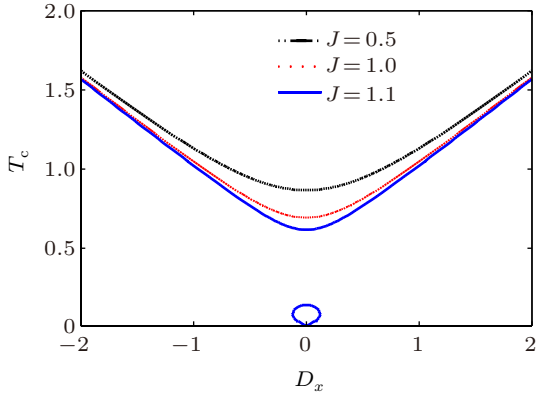


Fig. 8. (color online) The dependence of the critical temperature T_c on D_x for different values of J with $h = 0$ and $J_0 = 1$.

Additionally, the dependence of the concurrence C on D_x for different values of J near zero temperature (e.g., $T = 0.01$) is shown in Fig. 9. For the case with $J_0 = 1$ and $J = 0.5$, with $|D_x|$ increasing, the concurrence C firstly decreases from 1 to a minimum of 0.940 at $|D_x| = 1.29$, and then gradually increases, while for the case with $J - J_0 \geq 0$, it is observed that the concurrence C increases with $|D_x|$. The results given by Fig. 9 (for the DM interaction D_x) are obviously different from those of the case D_z (see Fig. 4).

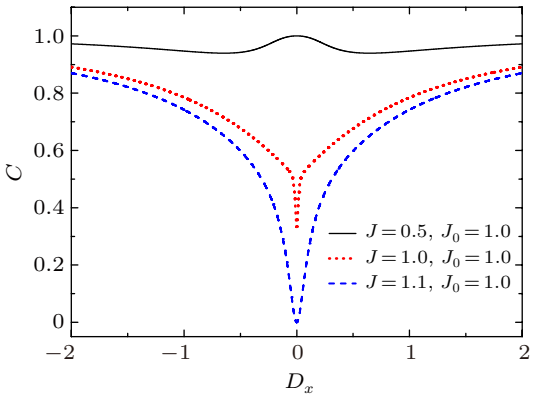


Fig. 9. (color online) The dependence of the concurrence C at $T = 0.01$ on D_x for different values of J with $h = 0$ and $J_0 = 1$.

Now, we concentrate on the thermal entanglement in the presence of a magnetic field. The variations of concurrence C (at $T = 0.1$) with the magnetic field h for different values of D_x are plotted in Fig. 10. Figure 10(a) shows the case with

$J - J_0 < 0$ (here, $J_0 = 1$ and $J = 0.5$). Due to the effect of D_x, with $|h|$ increasing, the concurrence C firstly increases to a maximum, and then gradually decreases to zero. Likewise, the critical magnetic field $|h_c|$ increases with $|D_x|$, and the variation of h_c with D_x is also shown in Fig. 11 (here, the black dashed line corresponds to the case with $J_0 = 1$ and $J = 0.5$). It is found that for the same value of the DM interaction the critical magnetic field $|h_c|$ of the case D_x is higher than that of the case D_z.

Figures 10(b) and 10(c) show the cases with $J - J_0 = 0$ and $J - J_0 > 0$, respectively. Compared with the case D_z (see Figs. 5(b) and 5(c)), the concurrence C shows a different variation tendency in Figs. 10(b) and 10(c). At $T = 0.1$, for the case with $J - J_0 > 0$, there exist two critical magnetic fields $|h_{c1}|$ and $|h_{c2}|$ ($|h_{c1}| < |h_{c2}|$) without the DM interaction (see black solid line in Fig. 10(c)). With $|D_x|$ increasing, the first critical magnetic field $|h_{c1}|$ gradually decreases, while the second critical magnetic field $|h_{c2}|$ increases (see blue solid lines in Fig. 11). Noted that for the same value of the DM interaction, $|h_{c1}|$ of the case D_x is smaller than that of the case D_z, but $|h_{c2}|$ of the case D_x is higher than that of the case D_z.

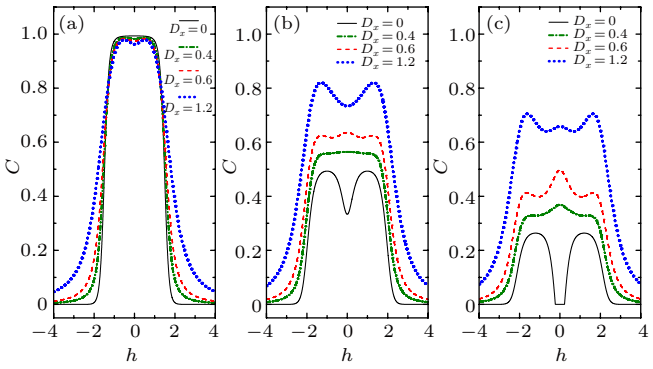


Fig. 10. (color online) The concurrence C versus the magnetic field h for different values of D_x with $T = 0.1$, $J_0 = 1$, and (a) $J = 0.5$; (b) $J = 1$; (c) $J = 1.1$.

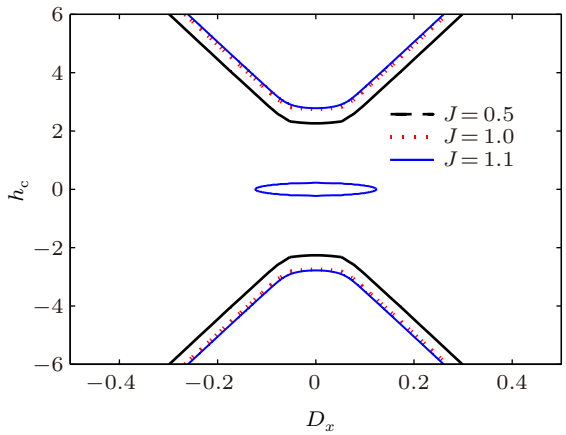


Fig. 11. (color online) The dependence of the critical magnetic field h_c on D_x for different values of J with $J_0 = 1$ and $T = 0.1$. (Here, it is assumed that C with the value less than 10^{-3} corresponds to the entanglement disappearing).

4. Conclusions

In summary, the thermal entanglement of a spin-1/2 Ising–Heisenberg diamond chain with the DM interaction between Heisenberg spins has been investigated. As is well known, the DM interaction plays a significant role in the degree of the entanglement of the Heisenberg quantum spin systems. In this paper, we are concerned with the effects of different DM interaction parameters, relating to variations of direction and amplitude of the $\boldsymbol{D}$ vector, on the thermal entanglement of the Heisenberg spin dimer. Two cases, i.e., z-component DM interaction parameter (D_z) and x-component DM interaction parameter (D_x), are discussed respectively. In the absence/presence of magnetic field, the concurrence as a measure of spin dimer entanglement is calculated. The variations of the concurrence with different values of exchange interactions, DM interaction, external magnetic field, and temperature are shown. The critical temperatures and the critical magnetic fields via different DM interaction parameters and exchange interactions are also obtained, respectively. It is found that the DM interaction favors the formation of thermal entanglement. Furthermore, it is shown that different DM interaction parameters (D_z and D_x) have remarkably different influences on the entanglement near zero temperature and the critical temperature and magnetic field.

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