Thermal entanglement in molecular spin rings*

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The thermal entanglement in the triangular molecular spin ring with Dzyaloshinskii–Moriya interaction is studied. The concurrences of arbitrary two spins of the triangular molecular spin ring for various cases are evaluated. The tendency of the concurrence with Dzyaloshinskii–Moriya interaction and temperature is analysed and discussed. We note that the concurrence arrives at its maximum in the regime with the large Dzyaloshinskii–Moriya interaction and low temperature, and gradually decreases to zero with the increase of temperature. The concurrence has different features for the ferromagnetic and antiferromagnetic cases. For completeness, we also numerically calculate the concurrence of spin rings with $N > 3$ spins and analyse their behaviours.

Keywords: thermal entanglement, molecular spin ring, concurrence

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1. Introduction

Entanglement is one of the most essential features of quantum mechanics which make it different from the classical mechanics, and provides a fundamental resource in quantum information processing. Due to its essential features and potential applications, entanglement has been extensively studied in the last decade.[1−6] Entanglement is involved in many key discoveries and applications, including quantum cryptography,[7] quantum dense coding,[8] quantum teleportation,[9] and quantum computation.[10,11] Entanglement also helps physicists to further understand many physical phenomena such as super-radiance,[12] superconductivity,[13] disordered systems.[14] Entanglement theory has given support for numerical methods, such as the density matrix renormalisation group,[15] and the design of new efficient simulation strategies for many-body systems.[16]

Spin model is a promising candidate for quantum information processing. Therefore, many efforts are made to study the entanglement in spin model in recent years. Reference [17] has studied the entanglement in a quantum mixed-spin chain of arbitrary spin S and 1/2, found that the entanglement is witnessed by the magnetic susceptibility and given the bound of pairwise entanglement. References [18]–[20] have studied the relations between entanglement and quantum phase transition in spin chains. Reference [21] has studied the pairwise entanglement of the ground state for an alternating XY spin chain with the next-nearest neighbouring interaction. Reference [22] has obtained the exact solution of a Yang–Baxter spin-1/2 chain and discussed the behaviours of the pairwise entanglement. Recently, thermal entanglement in spin model has drawn much attention of physicists. Literature has reported the research on the thermal entanglement in spin model. Reference [23] has studied the thermal entanglement in a two-qubit XX model with a magnetic field and in a two-qubit XY model. The behaviour of thermal entanglement of a two-qubit XY model under a magnetic field has been analysed.[24,25] The thermal entanglement of a two-qubit XY with an in-plane magnetic field and a two-qubit XX model with an nonuniform magnetic field,[26] a two-qubit isotropic Heisenberg model with a nonuniform magnetic field,[27] a two-qubit XXZ model with a nonuniform magnetic field,[28] a two-qubit XY model with a nonuniform magnetic field[29] have been studied. The thermal entanglements of a two-qubit XY model with Dzyaloshinskii–Moriya interaction under a magnetic field,[30] and of two-qubit XXZ and XYZ models with Dzyaloshinskii–Moriya interaction[31,32] have been studied. The thermal entanglements of a three-qubit XY model under a nonuniform magnetic field[33] and a four-qubit XY model under a uniform magnetic field[34] have been investigated. Reference [35] has investigated the thermal entanglement in XY models with the structures of a 2×2 square lattice and a 3×3 square lattice. In addition, the thermal entanglement in a two-qutrit spin-1 chain has also been

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studied.[36−38]

Molecular magnets have been intensively studied due to their pronounced quantum characteristics. They are especially promising for the implementation of quantum information processing. Recently, the $\{Cu_3\}$-type molecular spin ring was realised.[39] The triangular molecular spin ring might be the best candidate for observing a peculiar quantum magnetisation induced by spin chirality. However, the entanglement properties of molecular spin rings have not yet investigated. In this paper, we study the thermal entanglement of the triangular molecular spin ring. We evaluate the concurrences of the system for different cases. Furthermore, we analyse and discuss the features of the thermal entanglement for different cases. For the sake of completeness, we also numerically calculate the concurrence for $N > 3$ spin rings and compare their behaviours.

2. Model

First, we consider the triangular molecular spin ring as shown in Fig. 1. we assume that the XXZ-type exchange interaction and the z-component of the Dzyaloshinskii–Moriya interaction are present between spins.

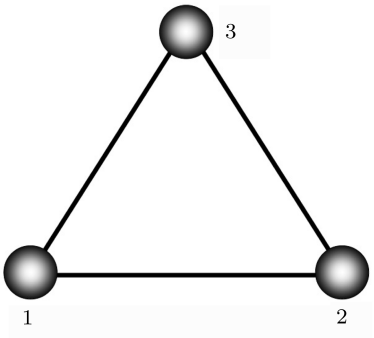


Fig. 1. Schematic of triangular molecular spin ring.

The Hamiltonian of the triangular molecular spin ring can be written as

$$H = J\sum_{i=1}^{3}(\sigma_i^x\sigma_{i+1}^x + \sigma_i^y\sigma_{i+1}^y) + J_z\sum_{i=1}^{3}\sigma_i^z\sigma_{i+1}^z + D_z\sum_{i=1}^{3}(\sigma_i^x\sigma_{i+1}^y - \sigma_i^y\sigma_{i+1}^x), \quad (1)$$

where J and J_z are the exchange coupling constants, D_z is the z component of the Dzyaloshiskii–Moriya interaction parameter. Here, we assume $\sigma_4^x = \sigma_1^x, \sigma_4^y = \sigma_1^y$ and $\sigma_4^z = \sigma_1^z$. In the basis $\{|\uparrow\uparrow\uparrow\rangle, |\uparrow\uparrow\downarrow\rangle, |\uparrow\downarrow\uparrow\rangle, |\uparrow\downarrow\downarrow\rangle, |\downarrow\uparrow\uparrow\rangle, |\downarrow\uparrow\downarrow\rangle, |\downarrow\downarrow\uparrow\rangle, |\downarrow\downarrow\downarrow\rangle\}$, Hamiltonian (1) can be rewritten in the matrix form as

$$\boldsymbol{H} = \begin{pmatrix} 3J_z & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -J_z & 2J+2\mathrm{i}D_z & 2J-2\mathrm{i}D_z & 0 & 0 & 0 & 0 \\ 0 & 2J-2\mathrm{i}D_z & -J_z & 2J+2\mathrm{i}D_z & 0 & 0 & 0 & 0 \\ 0 & 2J+2\mathrm{i}D_z & 2J-2\mathrm{i}D_z & -J_z & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -J_z & 2J+2\mathrm{i}D_z & 2J-2\mathrm{i}D_z & 0 \\ 0 & 0 & 0 & 0 & 2J-2\mathrm{i}D_z & -J_zh & 2J+2\mathrm{i}D_z & 0 \\ 0 & 0 & 0 & 0 & 2J+2\mathrm{i}D_z & 2J-2\mathrm{i}D_z & -J_z & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3J_z \end{pmatrix}. \quad (2)$$

The eigenstates of Hamiltonian (2) are

$$|\phi_1\rangle = |\uparrow\uparrow\uparrow\rangle, \quad (3)$$

$$|\phi_2\rangle = \frac{1}{\sqrt{3}}(|\uparrow\uparrow\downarrow\rangle + |\uparrow\downarrow\uparrow\rangle + |\downarrow\uparrow\uparrow\rangle), \quad (4)$$

$$|\phi_3\rangle = \frac{1}{\sqrt{3}}(|\uparrow\uparrow\downarrow\rangle + \mathrm{e}^{-\mathrm{i}2\pi/3}|\uparrow\downarrow\uparrow\rangle + \mathrm{e}^{\mathrm{i}2\pi/3}|\downarrow\uparrow\uparrow\rangle), \quad (5)$$

$$|\phi_4\rangle = \frac{1}{\sqrt{3}}(|\uparrow\uparrow\downarrow\rangle + \mathrm{e}^{\mathrm{i}2\pi/3}|\uparrow\downarrow\uparrow\rangle + \mathrm{e}^{-\mathrm{i}2\pi/3}|\downarrow\uparrow\uparrow\rangle), \quad (6)$$

$$|\phi_5\rangle = \frac{1}{\sqrt{3}}(|\uparrow\downarrow\downarrow\rangle + |\downarrow\uparrow\downarrow\rangle + |\downarrow\downarrow\uparrow\rangle), \quad (7)$$

$$|\phi_6\rangle = \frac{1}{\sqrt{3}}(|\uparrow\downarrow\downarrow\rangle + \mathrm{e}^{-\mathrm{i}2\pi/3}|\downarrow\uparrow\downarrow\rangle + \mathrm{e}^{\mathrm{i}2\pi/3}|\downarrow\downarrow\uparrow\rangle), \quad (8)$$

$$|\phi_7\rangle = \frac{1}{\sqrt{3}}(|\uparrow\downarrow\downarrow\rangle + \mathrm{e}^{\mathrm{i}2\pi/3}|\downarrow\uparrow\downarrow\rangle + \mathrm{e}^{-\mathrm{i}2\pi/3}|\downarrow\downarrow\uparrow\rangle), \quad (9)$$

$$|\phi_8\rangle = |\downarrow\downarrow\downarrow\rangle, \quad (10)$$

and the corresponding eigenvalues are

$$E_1 = 3J_z, \tag{11}$$
$$E_2 = -J_z + 4J, \tag{12}$$
$$E_3 = -J_z - 2J + 2\sqrt{3}D_z, \tag{13}$$
$$E_4 = -J_z - 2J - 2\sqrt{3}D_z, \tag{14}$$
$$E_5 = -J_z + 4J, \tag{15}$$
$$E_6 = -J_z - 2J + 2\sqrt{3}D_z, \tag{16}$$
$$E_7 = -J_z - 2J - 2\sqrt{3}D_z, \tag{17}$$
$$E_8 = 3J_z. \tag{18}$$

Here, $|\phi_1\rangle$ and $|\phi_8\rangle$ are separable states, $|\phi_2\rangle$ and $|\phi_5\rangle$ are W-type states, and $|\phi_3\rangle, |\phi_4\rangle, |\phi_6\rangle, |\phi_7\rangle$ can be regarded as the generalised W states.

At thermal equilibrium, the density matrix of the triangular molecular spin ring is

$$\boldsymbol{\rho} = \frac{1}{Z}\exp(-\beta H), \tag{19}$$

where $Z = \mathrm{tr}[\exp(-\beta H)]$ is the partition function of the system and $\beta = 1/k_{\mathrm{B}}T$ with k_{B} being the Boltzmann's constant and T being the temperature. For convenience, we set $k_{\mathrm{B}} = 1$ in our work. Substituting Eq. (2) into Eq. (19), we obtain the expression of the density matrix as follows:

$$\boldsymbol{\rho} = \frac{1}{Z}\begin{pmatrix} w & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & u & v^* & v & 0 & 0 & 0 & 0 \\ 0 & v & u & v^* & 0 & 0 & 0 & 0 \\ 0 & v^* & v & u & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & u & v^* & v & 0 \\ 0 & 0 & 0 & 0 & v & u & v^* & 0 \\ 0 & 0 & 0 & 0 & v^* & v & u & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & w \end{pmatrix} \tag{20}$$

with

$$w = \mathrm{e}^{-3\beta J_z}, \tag{21}$$
$$u = \frac{1}{3}\mathrm{e}^{\beta J_z + 2\beta J}[\mathrm{e}^{-6\beta J} + 2\cosh(2\sqrt{3}\beta D_z)], \tag{22}$$
$$v = \frac{1}{3}\mathrm{e}^{\beta J_z + 2\beta J}[\mathrm{e}^{-6\beta J} - \cosh(2\sqrt{3}\beta D_z) - \mathrm{i}\sqrt{3}\sinh(2\sqrt{3}\beta D_z)], \tag{23}$$

and

$$Z = 2\mathrm{e}^{-3\beta J_z} + 2\mathrm{e}^{\beta(J_z - 4J)} + 2\mathrm{e}^{\beta(J_z + 2J - 2\sqrt{3}D_z)} + 2\mathrm{e}^{\beta(J_z + 2J + 2\sqrt{3}D_z)}. \tag{24}$$

In order to calculate the thermal entanglement of arbitrary two qubits in the triangular molecular spin ring, we need the reduced density matrix of the two qubits. Without loss of the generality, we choose to trace out the third spin. In the basis $\{|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle\}$, the reduced density matrix can be expressed by

$$\boldsymbol{\rho}_{12} = \mathrm{tr}_3\rho = \frac{1}{Z}\begin{pmatrix} w+u & 0 & 0 & 0 \\ 0 & 2u & 2v^* & 0 \\ 0 & 2v & 2u & 0 \\ 0 & 0 & 0 & w+u \end{pmatrix}. \tag{25}$$

The entanglement of formation is often employed as an entanglement measure of mixed states.[3] The entanglement of formation is a monotonically increasing function of parameter 'concurrence' C, which ranges from 0 for an untangled state to 1 for a maximally entangled state. Thus, we can use the concurrence C to measure the entanglement of a mixed state. The concurrence is a function of the density matrix and is defined as[6]

$$C(\boldsymbol{\rho}_{12}) = \max\left(0, 2\max\lambda_i - \sum_{i=1}^{4}\lambda_i\right), \tag{26}$$

where λ_i are the square roots of the eigenvalues of the matrix

$$R = \boldsymbol{\rho}_{12}(\boldsymbol{\sigma}_1^y \otimes \boldsymbol{\sigma}_2^y)\boldsymbol{\rho}_{12}^*(\boldsymbol{\sigma}_1^y \otimes \boldsymbol{\sigma}_2^y) \tag{27}$$

with $\boldsymbol{\sigma}_i^y$ being the Pauli matrix and the asterisk referring to the complex conjugate.

Substituting Eq. (25) into Eq. (27), we obtain the expression of the matrix $\boldsymbol{R}$ as follows:

$$\boldsymbol{R} = \frac{1}{Z^2}\begin{pmatrix} (w+u)^2 & 0 & 0 & 0 \\ 0 & 4(u^2+|v|^2) & 8uv & 0 \\ 0 & 8uv^* & 4(u^2+|v|^2) & 0 \\ 0 & 0 & 0 & (w+u)^2 \end{pmatrix}. \tag{28}$$

The square roots of the eigenvalues of the matrix (28) are given by

$$\lambda_1 = \frac{2}{Z}\left(u + |v|\right), \quad \lambda_2 = \frac{2}{Z}|u - |v||,$$
$$\lambda_3 = \frac{1}{Z}(w + u), \quad \lambda_4 = \frac{1}{Z}(w + u). \tag{29}$$

From Eqs. (26) and (29), one can straightforwardly evaluate the concurrence of the system.

3. Results and discussion

We calculate the concurrence of the triangular molecular spin ring based on Eqs. (29)–(29) and also numerically evaluate the concurrences of the spin rings with $N = 4, 5, 6, 7, 8$ spins. All the results are shown in figures. Figure 2 shows the concurrence of the triangular molecular spin ring as a function of the Dzyaloshinskii–Moriya interaction D_z and the temperature T. Figure 3 shows the concurrences of the triangular molecular spin ring as a function of the Dzyaloshinskii–Moriya interaction D_z for different ratios J_z/J. Figure 4 shows the concurrence of the molecular spin rings with N spins as a function of the Dzyaloshinskii–Moriya interaction D_z.

For the triangular spin ring, we note that the concurrence of the system has the inverse symmetry about D_z, i.e. $C(D_z) = C(-D_z)$. The concurrence has its maximum 1/3 in the regime with large $|D_z|$ and low temperature. The concurrence gradually approaches to zero from its maximum with the increase of temperature. These features can be seen from Figs. 2 and 3.

For the ferromagnetic case, there exists a special value of the Dzyaloshinskii–Moriya interaction D_z^0. At $\pm D_z^0$, there exist two valleys where the concurrence vanishes for any temperature. For small J_z/J, there is a peak with a plain top between $-D_z^0$ and D_z^0 in low temperature. On the plain top, the concurrence arrives at its maximum 1/3. We can see this feature in Figs. 2(a) and 3(a). There exist a critical value λ for the ratio J_z/J. When the ratio J_z/J is more than the critical value λ, the peak vanishes and two valleys combine into one valley with a plain bottom as shown in Figs. 2(b) and 3(b). At the bottom of the valley, the concurrence is zero. The width of the valley becomes large with the increase of J_z/J after the peak vanishes in the centre.

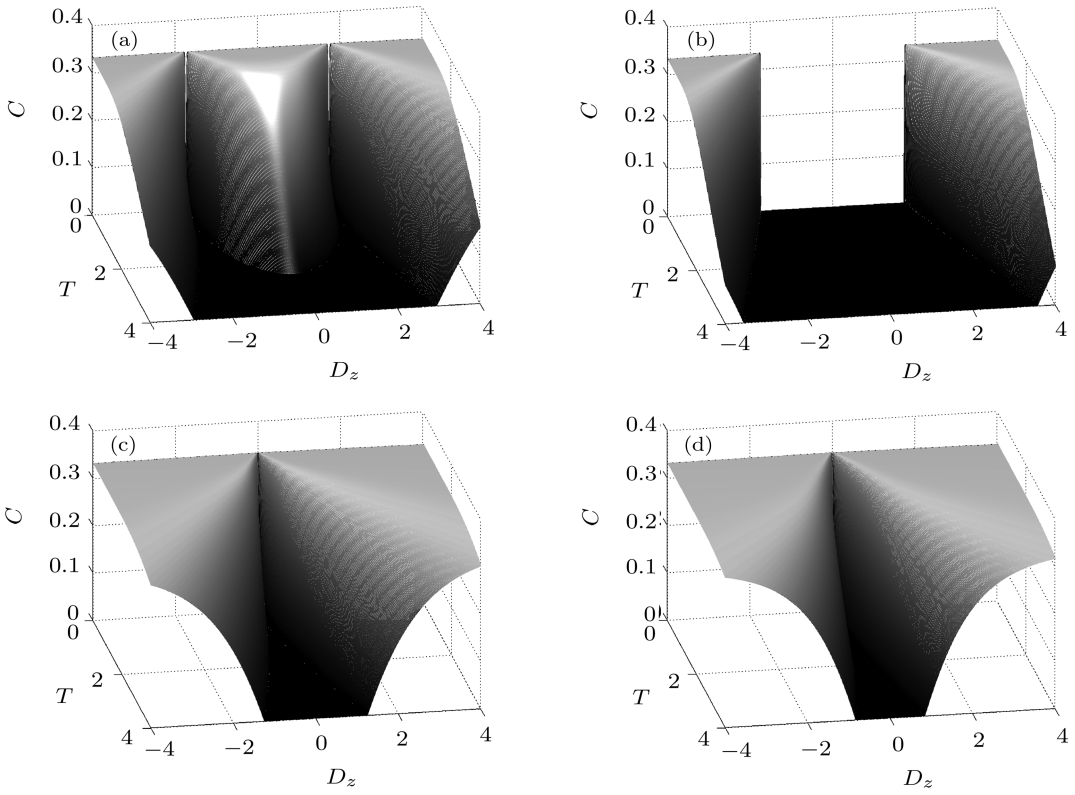


Fig. 2. Concurrences of the triangular molecular spin ring as a function of the Dzyaloshinskii–Moriya interaction parameter D_z and the temperature T for the cases with (a) $J = -1, J_z = 0$; (b) $J = -1, J_z = -1$; (c) $J = 1, J_z = 0$; (d) $J = 1, J_z = 1$.

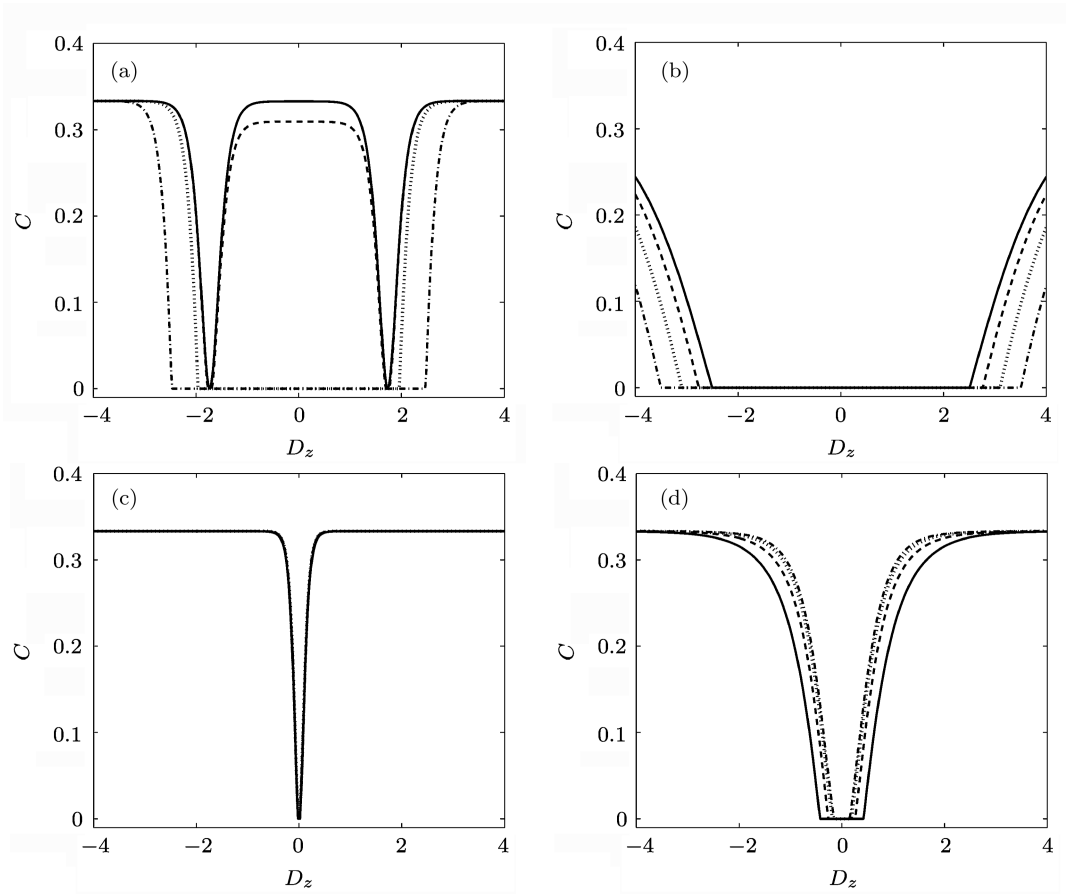
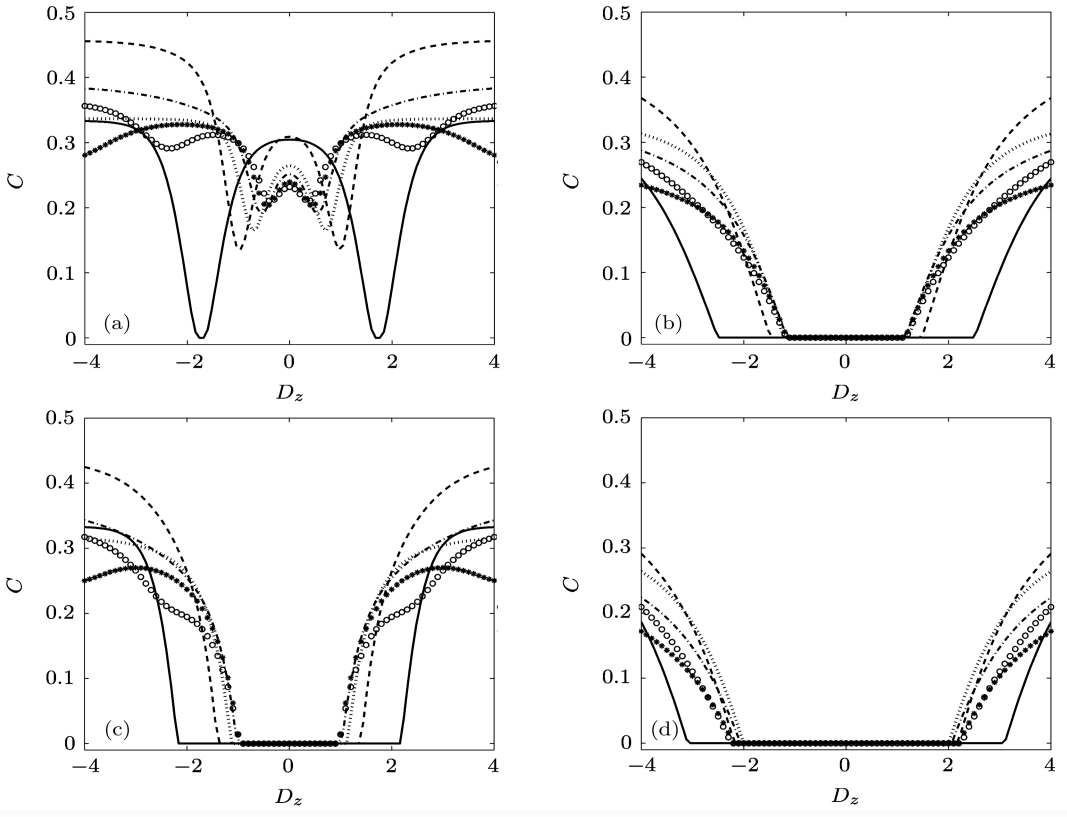


Fig. 3. Concurrences of triangular molecular spin ring as a function of D_z with the values of ratio $J_z/J = 0, 0.5, 1.0, 1.5$ for (a) $J = -1, T = 0.5$; (b)$J = -1, T = 2.0$; (c) $J = 1, T = 0.5$; (d) $J = 1, T = 2.0$. Here solid lines, dash lines, dot lines and dot-dash lines denote $J_z/J = 0, 0.5, 1.0, 1.5$, respectively. In (c), the four lines are almost identical so that we cannot distinguish them.



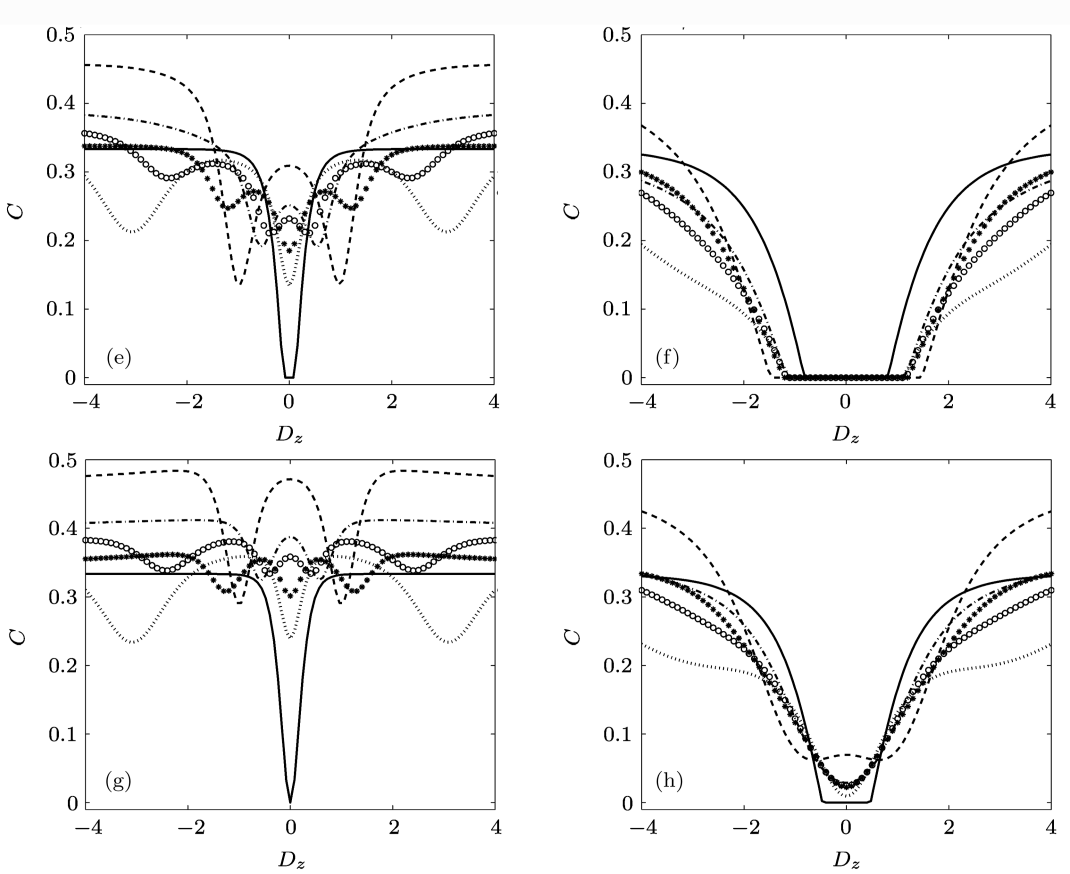


Fig. 4. Concurrence of molecular spin ring as a function of ratio D_z with N spins for (a) $J=-1, J_z=0, T=1$; (b) $J=-1, J_z=0, T=3$; (c)$J=-1, J_z=-1, T=1$; (d)$J=-1, J_z=-1, T=3$; (e) $J=1, J_z=0, T=1$; (f) $J=1, J_z=0, T=3$; (g)$J=1, J_z=1, T=1$; (h)$J=1, J_z=1, T=3$. Here solid lines, dash lines, dot lines, dot-dash lines, stars and cycles denote $N=3,4,5,6,7,8$, respectively.

For the antiferromagnetic case, there exists a valley with its centre at $D_z=0$ as shown in Figs. 2(c) and 2(d) and Figs. 3(c) and 3(d). For low temperatures, the concurrences are almost identical for the different values of ratio J_z/J and the concurrence arrives at its maximum far from the vicinity of $D_z=0$. However, for high temperatures, the width of the valley is related to the ratio J_z/J, and the smaller the value of J_z/J is, the larger will the width of the valley be. That is to say, the the concurrence decays faster with the temperature for the smaller ratio J_z/J.

In addition, we also numerically calculate the concurrences of spin rings for $N=4,5,6,7,8$. The results are shown in Fig. 4. We note that for $N>3$ spin rings the concurrences have similar behaviours to that when the $N=3$ spin ring. The concurrence has the inverse symmetry about D_z. The concurrence has its maximum in the regime with large $|D_z|$ and low temperature. The concurrence gradually approaches to zero from its maximum with temperature increasing. However, the concurrences have some differences for $N>3$ spin rings from that for $N=3$ spin ring. For $N>3$ spin rings, the concurrence has more oscillations along D_z at low temperature. At high temperature, the width of valley for zero-concurrence is a little different from that at low temperature and for larger N their widths approach the same value.

4. Conclusion

We have investigated the thermal entanglement of the triangular molecular spin ring with the Dzyaloshinskii–Moriya interaction. We have given the Hamiltonian and derived the thermal density matrix for the triangular molecular spin ring. Without loss of generality, we trace out one of three spins and obtain the two-qubit thermal density matrix. We evaluate the concurrences of the triangular molecular spin ring for various cases. We also analyse and discuss the features and tendencies of the concurrences for different cases. For the sake of completeness, we also evaluate numerically the concurrence for $N>3$ spin rings and discuss their behaviours.

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