Thermal quantum discord in Heisenberg models with Dzyaloshinski–Moriya interaction*

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We study the quantum discord of the bipartite Heisenberg model with the Dzyaloshinski–Moriya (DM) interaction in thermal equilibrium state and discuss the effect of the DM interaction on the quantum discord. The quantum entanglement of the system is also discussed and compared with quantum discord. Our results show that the quantum discord may reveal more properties of the system than quantum entanglement and the DM interaction may play an important role in the Heisenberg model.

Keywords: quantum discord, thermal equilibrium state, Heisenberg model, Dzyaloshinski–Moriya interaction

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1. Introduction

Among the fundamental concepts of the quantum mechanics, the coherent superposition principle, which shows the nonlocal property, is perhaps the most crucial profound rule since it allows the simultaneous existence of the dichotomic orthogonal states determining the qubit which lead to more efficient ways to process information. It also allows for the existence of entangled states when extended to two or more subsystems. Entanglement is a kind of quantum nonlocal correlation and has been deeply studied in the past years,[1−6] nevertheless, the quantum discord measures quantum correlations of a more general type of quantum correlation, and there exists separable mixed state having nonzero quantum discord.[7−9]

The quantum discord, which was investigated first by Ollivier and Zurek,[7] is defined by the difference of two ways of quantum mutual information, i.e.,

$$D(\rho_{AB}) = \mathscr{I}_{\rm q}(\rho_{AB}) - \mathscr{J}_{\rm q}(\rho_{AB}), \tag{1}$$

where

$$\mathscr{I}_{\rm q}(\rho_{AB}) = \mathscr{H}(\rho_A) + \mathscr{H}(\rho_B) - \mathscr{H}(\rho_{AB}) \tag{2}$$

is the quantum mutual information, and

$$\mathscr{J}_{\rm q}(\rho_{AB}) = \max_{\{\Pi_k\}}[\mathscr{H}(\rho_A) - \mathscr{H}(\rho_{AB}|\{\Pi_k\})] \tag{3}$$

is the quantum conditional entropy under the projective measurement $\{\Pi_k\}$. In the above definition, $\mathscr{H}(\rho) = -\mathtt{Tr}[\rho\log_2\rho]$ is the von Neumann entropy of ρ, and $\rho_{A(B)}$ is the reduced density matrix of ρ_{AB}. $\mathscr{I}_{\rm q}(\rho_{AB})$ and $\mathscr{J}_{\rm q}(\rho_{AB})$ are different because in the quantum system the correlation depends on the measurement of the other quantum system. One can introduce a complete set of projectors $\{\Pi_i\}$, corresponding to the outcome i, which makes $\rho_{A|i} = \mathtt{Tr}(\Pi_i\rho_{AB}\Pi_i)/p_i$, with $p_i = \mathtt{Tr}_{AB}(\Pi_i\rho_{AB}\Pi_i)$.

Note that in the classical system, the mutual information measures the correlation between two random variables A and B, which can be expressed as

$$I_{\rm c}(A,B) = \mathscr{H}(A) + \mathscr{H}(B) - \mathscr{H}(A,B),$$

and for the classical probability distributions, by using the Bayes's rule, $\mathscr{H}(A|B) = \mathscr{H}(A,B) - \mathscr{H}(B)$, the mutual information can also be expressed as

$$J_{\rm c}(A,B) = \mathscr{H}(A) - \mathscr{H}(A|B) = I_{\rm c}(A,B).$$

Here, $\mathscr{H}(X) = -\sum_x p_{X=x}\log p_{X=x}$ is the information entropy in a random variable X, which contains state x with the probability $p_{X=x}$, and $\mathscr{H}(X,Y) = -\sum_{x,y} p_{X=x,Y=y}\log p_{X=x,Y=y}$ is the joint entropy, with $p_{X=x,Y=y}$ being the probability in the case of $X=x$ and $Y=y$, which measures the total uncertainty of a pair of random variables X and Y.

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Thus, the quantum discord will show clearly the existence of quantum correlation in quantum system and will also incur a distinction between quantum correlation and classical correlation which will also provide the probability used in quantum information theory,[10] such as the Grover search.[11] Furthermore, the quantum discord has been on an equal footing with the entanglement, dissonance, and classical correlations in using the concept of relative entropy.[12]

The quantum discord has been used to study many kinds of quantum systems[13−16] and investigate the correlations of the systems including the systems with quantum phase transition.[17−20] Recently, the quantum discord of a two-qubit one-dimensional XYZ Heisenberg chain in thermal equilibrium has been studied,[20] where many unexpected ways different from the thermal entanglement have been shown. For the Heisenberg model, many properties have been studied, however, the Dzyaloshinski–Moriya (DM) anisotropic antisymmetric interaction has rarely been considered,[21,22] which arises from the weak intermolecular interactions and describes an interaction of extended superexchange mechanism by considering a term arising naturally from the perturbation theory due to the spin–orbit coupling. It has been shown that the DM interaction may play an important role in the entanglement of the bipartite system and the three-particle system.[23−27] Thus, considering the quantum discord in a two-qubit system with the DM interaction is also interesting. In this paper, we will study the quantum discord in the Heisenberg model with the DM interaction, and discuss how the DM interaction affects the quantum discord in such a system. We will show that the quantum discord can describe more information than quantum entanglement and also indicate more details about the correlation of the system by quantum discord which cannot be shown by the quantum entanglement.

The rest of this paper is organized as follows. We give the analytic solution of the system in Section 2, then discuss the quantum discord in Section 3, and give the summary in Section 4 finally.

2. Solution of thermalized Heisenberg system

We consider the XYZ model in an external magnetic field acting on both qubits and there exits the DM interaction. The DM anisotropic anti-symmetric interaction arises from spin–orbit coupling, which can be described as $\boldsymbol{D}\cdot(\boldsymbol{\sigma}_1\times\boldsymbol{\sigma}_2)$. In our study, we consider only the case of DM interaction along the z direction, i.e., $D_z(\sigma_1^x\sigma_2^y-\sigma_1^y\sigma_2^x)$, then the Hamiltonian of such a model can be expressed as

$$\begin{aligned} H = {} & \frac{\hbar}{2}\omega_1\sigma_1^z+\frac{\hbar}{2}\omega_2\sigma_2^z+J_x\sigma_1^x\sigma_2^x+J_y\sigma_1^y\sigma_2^y \\ & +J_z\sigma_1^z\sigma_2^z+D_z(\sigma_1^x\sigma_2^y-\sigma_1^y\sigma_2^x), \end{aligned} \tag{4}$$

where J_x, J_y and J_z are the coupling constants; σ_j^x, σ_j^y and σ_j^z are the Pauli operators acting on qubit $j=1,2$; ω_1 and ω_2 are the Rabi frequency in the external magnetic field. In the following study, we will mainly consider the case of XXZ model, i.e., $J_x=J_y=J$. In the standard basis $\{|\uparrow\uparrow\rangle,|\uparrow\downarrow\rangle,|\downarrow\uparrow\rangle,|\downarrow\downarrow\rangle\}$, the Hamiltonian can be expressed in the following matrix form:

$$H=\begin{pmatrix} \frac{\hbar}{2}(\omega_1+\omega_2)+J_z & 0 & 0 & J_x-J_y \\ 0 & \frac{\hbar}{2}(\omega_1-\omega_2)-J_z & J_x+J_y+2\mathrm{i}D & 0 \\ 0 & J_x+J_y-2\mathrm{i}D & -\frac{\hbar}{2}(\omega_1-\omega_2)-J_z & 0 \\ J_x-J_y & 0 & 0 & -\frac{\hbar}{2}(\omega_1+\omega_2)+J_z \end{pmatrix}. \tag{5}$$

Then the equilibrium with a thermal reservoir at temperature T (canonical ensemble) is

$$\rho=\exp(-H/kT)/Z,$$

with

$$Z=\mathtt{Tr}[\exp(-H/kT)]$$

being the partition function and k being Boltzmann's constant. This density matrix can be worked out to be

$$\rho=\frac{1}{Z}\begin{pmatrix} A_{11} & 0 & 0 & A_{12} \\ 0 & B_{11} & B_{12} & 0 \\ 0 & B_{21} & B_{22} & 0 \\ A_{21} & 0 & 0 & A_{22} \end{pmatrix}, \tag{6}$$

where the elements of the matrix have been defined as

$$A_{11}=\left(\frac{1-\cos\alpha}{2}\,\mathrm{e}^{M/kT}+\frac{1+\cos\alpha}{2}\,\mathrm{e}^{-M/kT}\right)$$

$$\times\ \mathrm{e}^{-J_z/kT},$$
$$A_{12} = \frac{\sin\alpha}{2}(\mathrm{e}^{-M/kT} - \mathrm{e}^{M/kT})\,\mathrm{e}^{-J_z/kT},$$
$$A_{21} = \frac{\sin\alpha}{2}(\mathrm{e}^{-M/kT} - \mathrm{e}^{M/kT})\,\mathrm{e}^{-J_z/kT},$$
$$A_{22} = \left(\frac{1+\cos\alpha}{2}\,\mathrm{e}^{-M/kT} + \frac{1-\cos\alpha}{2}\,\mathrm{e}^{M/kT}\right) \times\ \mathrm{e}^{-J_z/kT},$$
$$B_{11} = \left(\frac{1-\cos\beta}{2}\,\mathrm{e}^{N/kT} + \frac{1+\cos\beta}{2}\,\mathrm{e}^{-N/kT}\right) \times\ \mathrm{e}^{J_z/kT},$$
$$B_{12} = \frac{\sin\beta}{2}(\mathrm{e}^{-N/kT} - \mathrm{e}^{N/kT})\,\mathrm{e}^{J_z/kT}\,\mathrm{e}^{\mathrm{i}\phi},$$
$$B_{21} = \frac{\sin\beta}{2}(\mathrm{e}^{-N/kT} - \mathrm{e}^{N/kT})\,\mathrm{e}^{J_z/kT}\,\mathrm{e}^{-\mathrm{i}\phi},$$
$$B_{22} = \left(\frac{1+\cos\beta}{2}\,\mathrm{e}^{N/kT} + \frac{1-\cos\beta}{2}\,\mathrm{e}^{-N/kT}\right) \times\ \mathrm{e}^{J_z/kT}, \quad (7)$$

and $Z = 2\cosh\beta M + 2\cosh\beta N$ with

$$M = \sqrt{\left[\frac{\hbar}{2}(\omega_1+\omega_2)\right]^2 + (J_x - J_y)^2},$$
$$N = \sqrt{\left[\frac{\hbar}{2}(\omega_1-\omega_2)\right]^2 + (J_x + J_y)^2 + 4D^2}, \quad (8)$$

α, β and ϕ are defined as

$$\tan\alpha = \frac{J_x - J_y}{\frac{\hbar}{2}(\omega_1+\omega_2)},$$
$$\tan\beta = \frac{\sqrt{(J_x+J_y)^2+4D^2}}{\frac{\hbar}{2}(\omega_1-\omega_2)},$$
$$\tan\phi = \frac{2D}{J_x+J_y}. \quad (9)$$

3. Effects of DM interaction on discord and entanglement

Now we can study the effect of the DM interaction on quantum discord. The complete set of quantum orthogonal projectors can be chosen to be

$$\Pi_j = |\vartheta_j\rangle\langle\vartheta_j|, \quad j = 1, 2 \quad (10)$$

with

$$|\vartheta_1\rangle = \cos\theta|0\rangle + \mathrm{e}^{\mathrm{i}\phi}\sin\theta|1\rangle,$$
$$|\vartheta_2\rangle = \mathrm{e}^{-\mathrm{i}\phi}\sin\theta|0\rangle - \cos\theta|1\rangle, \quad (11)$$

and the projector measuring on subsystem 2 is taken over all possible values $\theta \in [0, \pi]$ and $\phi \in [0, 2\pi]$ when we calculate the maximum classical correlation between the subsystems.

In order to analyse the correlation between the qubits, we will also compare the quantum discord with the quantum entanglement measured by the entanglement of formation (EOF) in the following study. In the standard basis $\{|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle\}$, the Wootter's concurrence[25] is defined by

$$C(\rho) = \max\{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\}, \quad (12)$$

where λ_i $(i = 1, 2, 3, 4)$ is the square root of $\rho\tilde{\rho}$ with $\tilde{\rho} = (\sigma_1^y \otimes \sigma_2^y)\rho^*(\sigma_1^y \otimes \sigma_2^y)$. The EOF between the qubits is a monotonically increasing function of the Wootter's concurrence $C(\rho)$, i.e.,

$$\text{EOF} = -f(C)\log_2 f(C) - [1-f(C)]\log_2[1-f(C)], \quad (13)$$

with $f(C) = (1+\sqrt{1-C^2})/2$.

3.1. In the absence of external magnetic field

First, we consider the case of no external field acting on the qubits, i.e., $\omega_1 = \omega_2 = 0$. Considering the XXZ model $J_x = J_y \neq J_z$, the numerical results are shown in Figs. 1 and 2, where we have set $J_x = J_y = -0.5$, $J_z = -1$. The results show that in the case of $|D| < 0.85$, the quantum discord starts from zero and increases with temperature increasing to a maximum value, then decreases with the temperature (see Fig. 1(b)), showing the existence of quantum correlation in the thermal equilibrium, while the EOF is always zero in this case (see Fig. 1(a)). This result is coincident with the result in Ref. [20], while in our study, the result has been extended to a general case by considering the DM interaction. However, we can find that such a property of the quantum discord with temperature is maintained only in the case of small DM interaction ($|D| < 0.85$); when the DM interaction is larger than a certain value, for example $|D| > 0.85$, the quantum discord will start from 1 at zero temperature and turns into a monotonic decrease with temperature, while in this case the entanglement will decrease with a sudden death.[29] This means that with the increase of the DM interaction, a quantum phase transition will happen to this system. The strength of the DM interaction determines which phase the qubit is in. These properties of the quantum discord are very interesting and exhibit different quantum correlations which cannot be shown by the quantum entanglement.

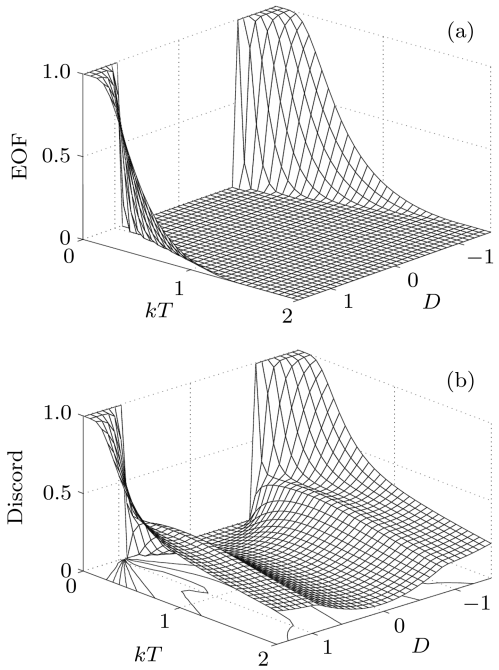


Fig. 1. Entanglement (a) and discord (b) versus temperature and DM interaction in the absence of external magnetic field, with using $J_x = J_y = -0.5$ and $J_z = -1$ for the XXZ model and $D \in [-1.5, 1.5]$ in numerical calculation.

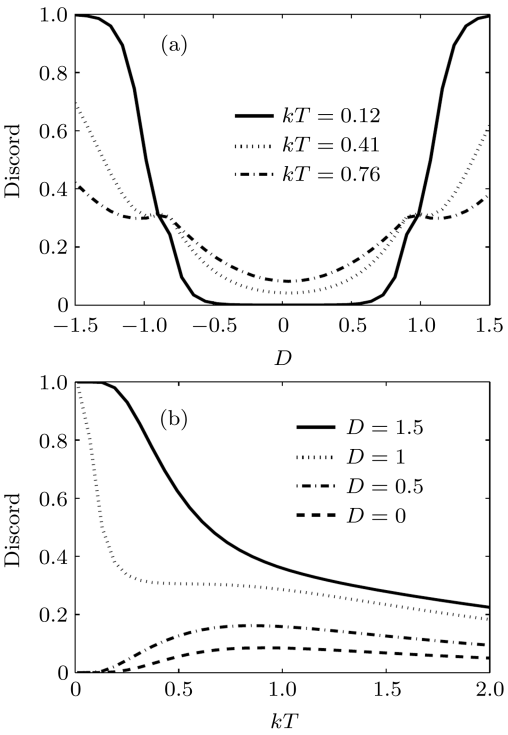


Fig. 2. (a) Curves for discord versus DM interaction for $kT = 0.12, 0.41, 0.76$; (b) Curves for discord versus temperature for $D = 0, 0.5, 1.0, 1.5$.

When we consider the XXX model, the property of the quantum discord is a little different, i.e., $D = 0$ is the critical point, and near the critical point the quantum discord is 1 at zero temperature and with temperature increasing, the discord decreases first, then increases with temperature and reaches a maximum value and decreases again finally. This property cannot be revealed by the quantum entanglement, either. Such a property is a little more complicated than the XXZ model (see Fig. 3), where we have set $J_x = J_y = J_z = -1$. Different from the case of the XXZ model, no clearly critical line can be found in this case, but it is similarly to the case of the XXZ model. So, the quantum discord reveals more information about the quantum correlation than the quantum entanglement.

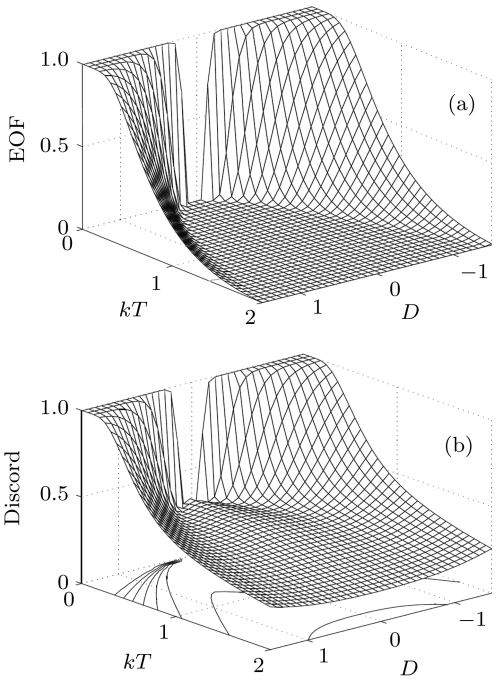


Fig. 3. Entanglement (a) and discord (b) versus temperature and DM interaction in the absence of an external field, with using $J_x = J_y = J_z = -1$ for the XXX model and $D \in [-1.5, 1.5]$ in numerical calculation.

3.2. In the presence of external magnetic field

Now, we consider the case where the magnetic field is added to the qubits system. Figures 4 and 5 show the variations of quantum discord under the influence of the field, where we have set $J_x = J_y = 0.5$, $J_z = -1$, and $D = 0.5$ for Fig. 4(a), $D = 1.5$ for Fig. 4(b). Note that, in the case of $D = 0.5$, and $\omega \in [0, 2]$ in units of $1/2\hbar$, the quantum discord also increases with temperature increasing, reaches a maximum and then decreases with temperature increasing, but the amplitude decreases with the strength of the field. While in this case, the quantum entanglement

EOF is always zero and it is unable to show any correlation property between the qubits. It is interesting to note that in the case of $D = 1.5$, with the increase of the field, the property of quantum discord will also undergo a quantum phase transition, i.e., the discord starts from 1 at zero temperature and monotonically decreases with temperature increasing when the field strength is small, and the discord starts from zero at zero temperature and then increases, with the increase of temperature, to a maximum value (see Fig. 4(b)) where the field is strong enough, showing the same property as that in the case of $D = 0.5$.

The above results imply that more properties of the effect of the DM interaction of the Heisenberg model can be revealed by the quantum discord, while they cannot be described completely by the quantum entanglement.

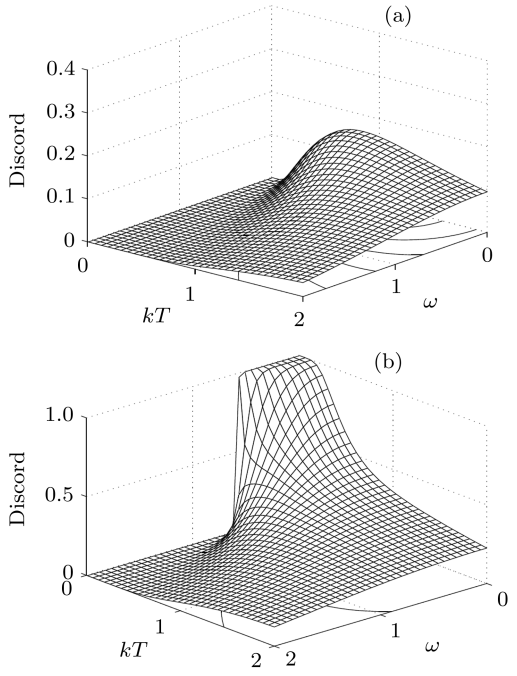


Fig. 4. Curves for discord versus temperature and field strength, with using $J_x = J_y = -0.5$, $J_z = -1$ for the XXZ model, and $\omega_1 = \omega_2 = \omega$, $\omega \in [0, 2]$ (in units of $1/2\hbar$) in numerical calculation. (a) $D = 0.5$; (b) $D = 1.5$.

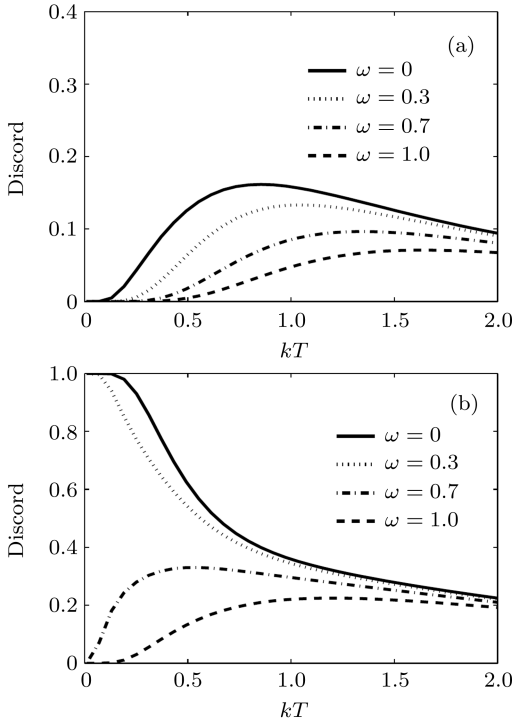


Fig. 5. Curves for discord versus temperature for certain values of the field, $\omega_1 = \omega_2 = \omega = 0, 0.3, 0.7, 1.0$ (in units of $1/2\hbar$), with using parameters with $D = 0.5$ (a) and $D = 1.5$ (b), $J_x = J_y = -0.5$ and $J_z = -1$.

4. Conclusion

We have studied the quantum discord in Heisenberg models with DM interaction and the relation between quantum discord and the DM interaction. Our results show that the quantum discord can describe more information about quantum correlation than quantum entanglement and more properties can be revealed by quantum discord. The DM interaction may also play an important role in the model and the correlation of thermal equilibrium state of the qubits shows different properties for different DM interactions. However, not all properties can be revealed by the quantum entanglement. These results also imply that the quantum discord may serve as a more general tool to study the quantum system than entanglement especially to study the quantum correlations in quantum systems.

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