Quantum thermal discord in a two-spin-1/2 XXZ model*

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We study the quantum discord in a two-spin-1/2 XXZ model in thermal equilibrium at temperature T in the presence of an external magnetic field B. Special attention is paid to the dependence of quantum discord on the temperature T and magnetic field B. It is found that quantum thermal discord is more robust than concurrence against temperature, in the sense that quantum thermal discord does not vanish at finite temperatures, but concurrence vanishes completely at a critical temperature.

Keywords: quantum discord, concurrence, thermal equilibrium
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1. Introduction

It is well known that quantum entanglement is a fundamental quantum-mechanical feature which sets the basic differences between classical and quantum correlations and numerous works have been devoted to the study of quantum entanglement.[1−6] In the studies on the thermal entanglement of the Heisenberg spin model, a lot of interesting works have been done.[7−11] It is shown that there is no entanglement above a critical temperature T_c no matter what the external magnetic field is for a two-spin-1/2 XY model.[7] Also, the entanglement is enhanced by increasing the interaction of z-component J_z in the XXZ model.[8] Furthermore, quantum phase transition appears in the XY model.[10]

Quantum discord, as introduced by Olliver and Zurek,[12] is a measure of the quantumness of correlations. Such a quantum correlation is more general than entanglement in the sense that quantum discord can be nonzero for states that are separable, showing the presence of quantum correlations in non-entangled states. Up to now, numerous works have been devoted to quantum discord in studies of quantum phase transition,[13,14] quantum correlations in two-qubit systems[15,16] as well as in Grover search algorithm,[17] the action of decoherence,[18] non-Markovian effect,[19] the condition for completely positive maps,[20] and the rules of quantum discord to quantum computation[21−23] and quantum teleportation.[24] As seen in Refs. [22] and [23] that states with non-zero discord can lead to an exponential speedup in a model of deterministic quantum computation with one quantum bit,[25] even in the absence of entanglement. Hence, the notion of quantum discord might play a significant role in quantum information protocols.

In the studies of response of quantum discord to noises, some studies[16] have usually been paid to explore only the time evolution of quantum discord. In this paper, we study the temperature-dependence of quantum discord for a two-spin-1/2 XXZ model in thermal equilibrium in the presence of an external magnetic field. It is found that quantum thermal discord has many similar traits compared with quantum thermal entanglement. In the ground state, they are always equal no matter what the magnetic field is. When temperature goes up from zero, the overall behaviours are also similar. However, quantum discord is more robust than concurrence against temperature, since quantum thermal discord vanishes asymptotically with the increasing of temperature, but concurrence behaves sudden death at a critical temperature T_c.

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2. Two-spin-1/2 XXZ model

Let us start by introducing a two-spin-1/2 XXZ model in an external magnetic field B, which is described by the following Hamiltonian (with $\hbar = 1$)

$$H_{\rm S} = \frac{1}{2}[J\sigma_x^{(1)}\sigma_x^{(2)} + J\sigma_y^{(1)}\sigma_y^{(2)} + J_z\sigma_z^{(1)}\sigma_z^{(2)} + B(\sigma_z^{(1)} + \sigma_z^{(2)})]. \quad (1)$$

Here J and J_z are the coupling constants between the two spins, and the Pauli operators are defined as $\sigma_x^{(i)} = |1\rangle_{ii}\langle 0| + |0\rangle_{ii}\langle 1|$, $\sigma_y^{(i)} = i(|0\rangle_{ii}\langle 1| - |1\rangle_{ii}\langle 0|)$ and $\sigma_z^{(i)} = |1\rangle_{ii}\langle 1| - |0\rangle_{ii}\langle 0|$, with $|1\rangle_i$ and $|0\rangle_i$ standing for spin up and spin down for the i-th ($i = 1, 2$) spin respectively. The coupling constants J, J_z may be positive or negative, which correspond respectively to the anti-ferromagnetic or ferromagnetic cases. The four eigenstates of the Hamiltonian (1) read

$$\begin{aligned} |\phi_1\rangle &= |0,0\rangle, \quad |\phi_2\rangle = |1,1\rangle, \\ |\phi_3\rangle &= \frac{1}{\sqrt{2}}\left(-\frac{|J|}{J}|1,0\rangle + |0,1\rangle\right), \\ |\phi_4\rangle &= \frac{1}{\sqrt{2}}\left(\frac{|J|}{J}|1,0\rangle + |0,1\rangle\right), \end{aligned} \quad (2)$$

which have eigenenergies

$$\begin{aligned} E_1 &= \frac{1}{2}(J_z - 2B), \\ E_2 &= \frac{1}{2}(J_z + 2B), \\ E_3 &= -\frac{J_z}{2} - |J|, \\ E_4 &= -\frac{J_z}{2} + |J|. \end{aligned} \quad (3)$$

At thermal equilibrium of temperature T, the density matrix of the system reads

$$\rho(T) = Z^{-1}\exp(-\beta H_{\rm S}), \quad (4)$$

where $Z = {\rm Tr}\,[\exp(-\beta H_{\rm S})]$ is the partition function and $\beta = 1/T$ (with $k_B = 1$) is the inverse temperature. In the representation with basis states $\{|1,1\rangle, |1,0\rangle, |0,1\rangle, |0,0\rangle\}$, the thermal equilibrium state can be expressed as

$$\rho(T) = \frac{1}{Z}\begin{pmatrix} {\rm e}^{-\beta E_2} & 0 & 0 & 0 \\ 0 & c & -s & 0 \\ 0 & -s & c & 0 \\ 0 & 0 & 0 & e^{-\beta E_1} \end{pmatrix}, \quad (5)$$

where the partition function $Z = [\exp(2\beta B) + 1]\exp(-\beta E_2) + 2\cosh(\beta|J|)\exp(2\beta J_z)$ and the parameters $s = 2\beta J\sinh(\beta|J|)\exp(J_z)/|J|$, $c = \cosh(\beta|J|)\exp(2\beta J_z)$.

3. Quantum thermal discord and entanglement

In this section, we mainly study the dependence of quantum discord on temperature and external magnetic field for the thermal equilibrium system mentioned above. Let us first review briefly the notion of quantum discord. For a bipartite quantum system, the quantum mutual information between the two subsystems $\mathscr{A}$ and $\mathscr{B}$ is given by

$$\mathscr{I}(\rho_{\mathscr{A}\mathscr{B}}) = S(\rho_{\mathscr{A}}) + S(\rho_{\mathscr{B}}) - S(\rho_{\mathscr{A}\mathscr{B}}), \quad (6)$$

where $S(\rho) = -{\rm Tr}\,(\rho\log\rho)$ is the von Neumann entropy of the density matrix ρ. The quantum mutual information has fundamental physical significance, and is usually used as a measure of total correlations that include quantum and classical ones. The classical correlation may be defined in terms of projective measurement. Suppose we perform a set of projective measurements $\{\Pi_k^{\mathscr{B}}\}$ on the subsystem $\mathscr{B}$, then the probability of measurement outcome k may read $p_k = {\tt Tr}_{\mathscr{A}\mathscr{B}}[(I^{\mathscr{A}} \otimes \Pi_k^{\mathscr{B}})\rho_{\mathscr{A}\mathscr{B}}(I^{\mathscr{A}} \otimes \Pi_k^{\mathscr{B}})]$ with $I^{\mathscr{A}}$ the identity operator for subsystem $\mathscr{A}$. After this measurement, the state of subsystem $\mathscr{A}$ is described by the conditional density operator $\rho_{\mathscr{A}|k} = {\tt Tr}_{\mathscr{B}}[(I^{\mathscr{A}}\otimes\Pi_k^{\mathscr{B}})\rho_{\mathscr{A}\mathscr{B}}(I^{\mathscr{A}}\otimes\Pi_k^{\mathscr{B}})]/p_k$. We define the upper limit of the difference between the von Neumann entropy $S(\rho_{\mathscr{A}})$ and the based-on-measurement quantum conditional entropy $\sum_k p_k S(\rho_{\mathscr{A}|k})$ of subsystem $\mathscr{A}$, i.e.,

$$\mathscr{Q}(\rho_{\mathscr{A}\mathscr{B}}) = \sup_{\{\Pi_k^{\mathscr{B}}\}}\left[S(\rho_{\mathscr{A}}) - \sum_k p_k S(\rho_{\mathscr{A}|k})\right], \quad (7)$$

as the classical correlation of the two subsystems. The maximum is taken for all possible kinds of projective measurements. In the end, the quantum discord is defined as the difference between the total and classical correlations,[12]

$$D(\rho_{\mathscr{A}\mathscr{B}}) = \mathscr{I}(\rho_{\mathscr{A}\mathscr{B}}) - \mathscr{Q}(\rho_{\mathscr{A}\mathscr{B}}). \quad (8)$$

It should be noted that the phenomenon of nonzero quantum discord is a manifestation of quantum correlations due to noncommutativity rather than due to entanglement.[15]

It is also noted that the definition of classical correlation of Eq. (7) is related to the optimal choice of projective measurement $\{\Pi_k^{\mathscr{B}}\}$. This sets a severe handicap for the evaluation of classical correlation.

Fortunately, for a single qubit system, this problem can be solved in principle. For qubit subsystem $\mathscr{B}$, a general set of projective measurements may be denoted as $\Pi_k^{\mathscr{B}} = V|k\rangle_{\mathscr{B}\mathscr{B}}\langle k|V^+$, where $k = 0, 1$ and V is a unitary transformation on subsystem $\mathscr{B}$,

$$V = \begin{pmatrix} \cos\dfrac{\theta}{2} & \sin\dfrac{\theta}{2}\mathrm{e}^{-\mathrm{i}\,\phi} \\ \sin\dfrac{\theta}{2}\mathrm{e}^{\mathrm{i}\,\phi} & -\cos\dfrac{\theta}{2} \end{pmatrix} \tag{9}$$

with $0 \leq \theta < \pi$ and $0 \leq \phi < 2\pi$. For given temperature T and magnetic field B, it suffices to evaluate only the maximum of Eq. (7) with respect to parameters θ and ϕ.

We will also calculate the quantum entanglement of the system and make a comparison with quantum discord. For a two-qubit system with density matrix ρ, the concurrence C is defined as[26]

$$C = \max\{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\}. \tag{10}$$

Here $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4$ are the square roots of the eigenvalues of the matrix $R = \rho\widetilde{\rho}$, with $\widetilde{\rho} = \sigma_y^{(1)} \otimes \sigma_y^{(2)} \rho^* \sigma_y^{(1)} \otimes \sigma_y^{(2)}$ and the sign "$*$" standing for complex conjugate.

For simplicity, we in the following only consider the anti-ferromagnetic system, i.e., $J, J_z > 0$. (Note that ferromagnetic system may be studied in a similar way and we have found the behaviours are similar to that of anti-ferromagnetic case). The discussion is divided into three cases: (i) XXX model ($J_z = J$); (ii) XX model ($J_z = 0$); (iii) XXZ model ($J \neq J_z \neq 0$).

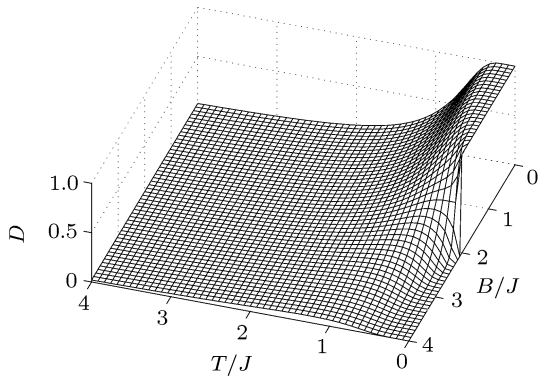


Fig. 1. Quantum discord D of the thermal state of XXX model plotted as a function of temperature T and external magnetic field B, where T and B are scaled by J.

For the XXX model, the quantum discord and concurrence of the thermal state (5) as functions of temperature T and external magnetic field B are plotted in Figs. 1 and 2. One can see that the overall behaviours of discord and concurrence are similar. For $0 < B/J < 2$, both D and C decay from 1 monotonically when temperature T increases from zero. For $B/J > 2$, they increase from zero to some peak values (note that the peak values depend on B) in the beginning and then decay with temperature increasing. The distinct difference between discord and concurrence is: D vanishes in an asymptotic way, but C behaves as sudden death at a finite critical temperature T_c (T_c/J is about 1.82 in Fig. 2)

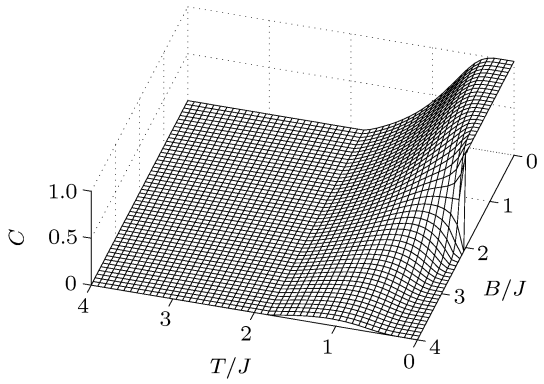


Fig. 2. Concurrence C of the thermal state of XXX model plotted as a function of the scaled temperature T/J and external magnetic field B/J.

As stated by Boltzmann distribution, when $T \to 0$, the system should be in the ground state with minimum energy. According to Eq. (3), for $B > |J| + J_z$, $E_1 < E_3$ and the ground state of the system is $|\phi_1\rangle = |0, 0\rangle$ which is a separable state with $D = C = 0$. For $B < |J| + J_z$, $E_1 > E_3$ and the ground state becomes $|\phi_3\rangle = (|0, 1\rangle - |1, 0\rangle)/\sqrt{2}$ which has $D = C = 1$. Thus

$$B_\mathrm{c} = |J| + J_z \tag{11}$$

is a critical magnetic field for the phase transition of ground state. For XXX anti-ferromagnetic model, the critical magnetic field for phase transition of ground state is $B_\mathrm{c} = 2J$. This character is described by the rectangular lines in Figs. 1 and 2.

For the XX model, the behaviours of quantum discord and concurrence versus temperature and external magnetic field are similar to that of the XXX model (see Figs. 3 and 4). The differences are that the critical magnetic field for phase transition of ground state now becomes $B_\mathrm{c} = J$. For $B < J$, both D and C decay more rapidly as temperature goes up. For $B > J$, the peak values of D and C fall. The critical temperature for entanglement death also decreases to

$T_c/J = 1.13$.

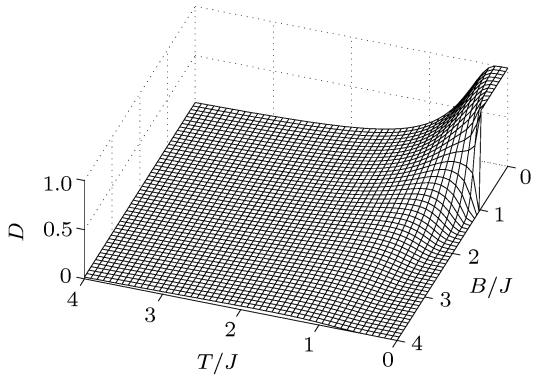


Fig. 3. Quantum discord D of the thermal state of XX model versus scaled temperature and external magnetic field.

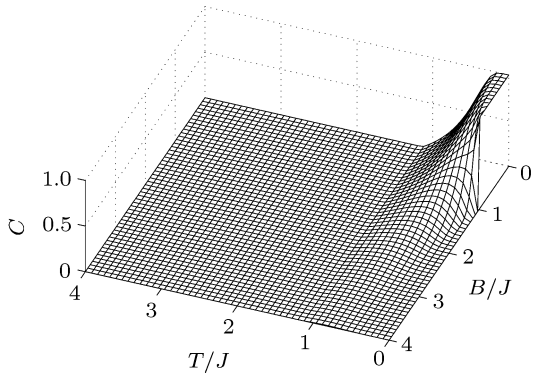


Fig. 4. Concurrence C of thermal state of XX model versus scaled temperature and external magnetic field.

Finally, for the more general XXZ model, we plot quantum discord and concurrence as functions of T and B for $J_z = 2J$ in Figs. 5 and 6 respectively. One can see obviously that, for $B < B_c$ ($B_c = 3J$ in this case), both D and C decay more slowly compared with Figs. 1–4. For $B > B_c$, the peak values of D and C move up. The critical temperature for entanglement death increases to $T_c/J = 2.38$.

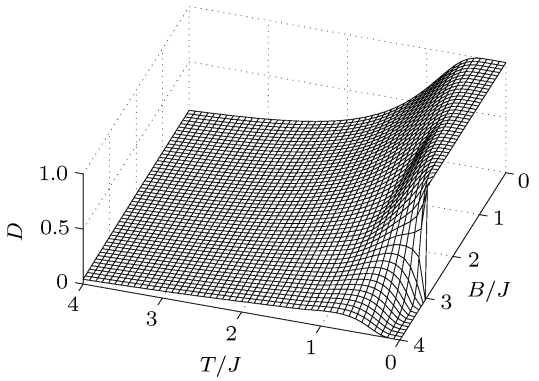


Fig. 5. Quantum discord D of the thermal state of XXZ model with $J_z = 2J$ versus scaled external magnetic field and temperature.

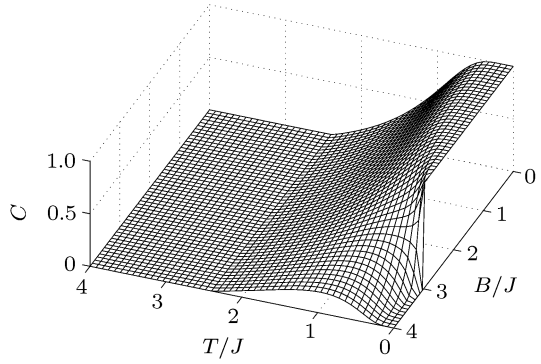


Fig. 6. Concurrence C of the thermal state of XXZ model with $J_z = 2J$ versus scaled external magnetic field and temperature.

From the above analyses, we conclude: i) There is a critical magnetic field for the phase transition of ground state $B_c = |J| + J_z$. Below B_c, the ground state has maximum quantum correlation and entanglement $D = C = 1$. Above B_c, the ground state is a separable state with $D = C = 0$. ii) When the temperature goes up from zero, D and C either decay monotonically from 1 (for $B < B_c$), or increase from zero to some peaks first and then decrease (for $B > B_c$). iii) D does not vanish up to infinite temperature, but C vanishes completely at a finite critical temperature T_c. iv) For larger J_z/J, as temperature goes up from zero, D and C either decay more slowly (for $B < B_c$) or have higher peak values (for $B > B_c$). Further, the critical temperature for entanglement death rises with J_z/J increasing.

Indeed, for thermal equilibrium state (5), the concurrence can be evaluated as

$$C = \frac{2}{Z}\max\left\{0, \mathrm{e}^{-J_z/2T}\left(\mathrm{e}^{J_z/T}\sinh\left(\frac{J}{T}\right) - 1\right)\right\}. \tag{12}$$

The critical temperature T_c for entanglement death should satisfy

$$\mathrm{e}^{J_z/T_c}\sinh(J/T_c) = 1. \tag{13}$$

When $J_z = 0$, it reduces to the result of Ref. [10]. Obviously, T_c is independent of magnetic field B. The relation that T_c rises with the increase of J_z/J is listed in Table 1.

Table 1. The scaled critical temperature T_c/J for different J_z/J of XXZ model.

J_z/J	0	0.1	0.2	0.3	0.4	0.5	1	2	5
T_c/J	1.13	1.21	1.29	1.36	1.43	1.50	1.82	2.38	3.79

In the end of this section, we point out that quantum discord and concurrence depict different types of quantum correlations between two subsystems. Their values are in general not the same. As an explanation, we plot quantum discord and concurrence of the thermal state of XXZ model with $J_z = 2J$ versus scaled temperature in Fig. 7.

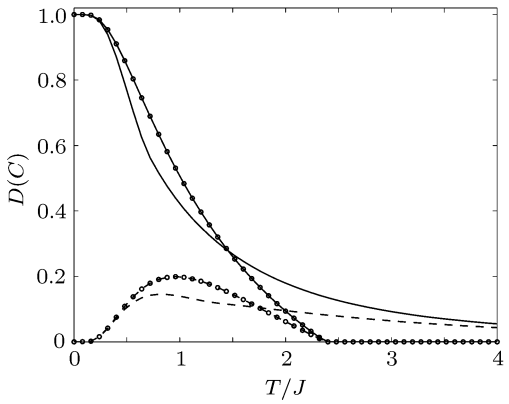


Fig. 7. Quantum discord D and concurrence C of the thermal state of XXZ model versus scaled temperature, where $J_z = 2J$. The solid and circle-solid lines denote respectively the D and C with $B/J = 2$, while dashed and circle-dashed lines denote respectively the D and C with $B/J = 4$.

The solid and circle-solid lines denote respectively the discord and concurrence for $B/J = 2$, while dashed and circle-dashed lines for $B/J = 4$. It is shown that in the beginning parts of temperature increasing, the quantum concurrence is larger than quantum discord. But when temperature exceeds some values, the quantum discord becomes dominant.

4. Conclusion

In conclusion, we have investigated the quantum discord in a two-spin-1/2 XXZ model in thermal equilibrium at temperature T in the presence of an external magnetic field B. For the ground state of the system, there is a critical magnetic field of phase transition $B_c = |J| + J_z$. Below B_c, the ground state has both maximum quantum discord and maximum entanglement. Then they decay monotonically from this maximum as temperature goes up. Quantum discord decays asymptotically, but entanglement vanishes completely at a finite critical temperature T_c. When the magnetic field is above B_c, the ground state is a product state with neither quantum discord nor entanglement. Then they increase from zero to some peak values in the beginning of temperature and immediately lessen when temperature moves up from zero. In addition, larger J_z/J can either slow down the decaying speed of both quantum discord and entanglement for $B < B_c$, or raise their peak values for $B > B_c$. The critical temperature T_c for entanglement death also rises as J_z/J increases. In the end, quantum discord and concurrence depict not the same quantum correlation, there are some dominant regions of discord or concurrence in the XXZ model.

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