Thermal quantum and classical correlations in a two-qubit XX model in a nonuniform external magnetic field

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Abstract
We investigate how thermal quantum discord (QD) and classical correlations (CC) of a two-qubit one-dimensional XX Heisenberg chain in thermal equilibrium depend on the temperature of the bath as well as on nonuniform external magnetic fields applied to two qubits and varied separately. We show that the behavior of QD differs in many unexpected ways from the thermal entanglement (EOF). For the nonuniform case \(B_1=-B_2\), we find that QD and CC are equal for all values of \(B_1=-B_2\) and for different temperatures. We show that, in this case, the thermal states of the system belong to a class of mixed states and satisfy certain conditions under which QD and CC are equal. The specification of this class and the corresponding conditions are completely general and apply to any quantum system in a state in this class satisfying these conditions. We further find that the relative contributions of QD and CC can be controlled easily by changing the relative magnitudes of \(B_1\) and \(B_2\). Finally, we connect our results with the monogamy relations between the EOF, CC and the QD of two qubits and the environment.

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1. Introduction

It is now quite well known that composite quantum systems can be in a class of states, called entangled states, in which the correlations between the constituents of the system cannot be achieved in a classical world [1, 2]. Although all pure entangled states possess such nonlocal quantum correlations, there are mixed entangled states which do not, in the sense of violating Bell inequalities [3]. The entanglement in quantum states and the resulting nonlocal quantum correlations form an area of intense research, due to their huge technological promise, especially in the areas of quantum communication and cryptography [4]. However, quantum correlations breaking Bell inequalities need not account for all quantum correlations in a
composite quantum system in a given state. In order to account for the quantum correlation in a given state, we must find some means to divide the total correlation into a classical part and a purely quantum part. This is particularly important for mixed states, since their quantum correlations are often hidden by their classical correlations (CC). An answer to this requirement is given by quantum discord (QD) [5], a measure of the quantumness of correlations. QD is built on the fact that two classically equivalent ways of defining the mutual information (MI) turn out to be inequivalent in the quantum domain. In addition to its conceptual role, some recent results, [6], suggest that QD and not entanglement may be responsible for the efficiency of a mixed-state-based quantum computer. The present authors believe that QD will turn out to be a very useful tool to analyze mixed state quantum correlations and their consequences, as mixed state entanglement is very difficult and eluding to deal with [7]. To realize this hope we need a viable relation between mixed state entanglement and QD [8]. Pointers toward such a relation may be obtained by studying these properties for various quantum systems.

Motivated by these considerations, we present here the results of our investigation of the amount of QD and CC in a two-qubit Heisenberg XX chain at finite temperature subjected to the nonuniform external magnetic fields $B_1$ and $B_2$ acting separately on each qubit. We study two distinct cases, namely $B_1 = -B_2$ (nonuniform field) and $B_1 = B_2$ (uniform field). In each case, we obtain the dependence of QD, CC and the entanglement of formation (EOF) [17] in the system on the external magnetic field and temperature. Such a model is realized, for example, by a pair of qubits (spin 1/2) within a solid at finite temperature experiencing a spatially varying magnetic field. Such Heisenberg models can describe fairly well the magnetic properties of real solids [9] and are well adapted to the study of the interplay of disorder and entanglement as well as of entanglement and quantum phase transitions [10, 11]. The variation of entanglement [12] and QD [13, 14] in a two-qubit Heisenberg XX chain with an external magnetic field has already been reported.

In order to quantify entanglement in a thermally mixed two-qubit state, we use the EOF derived using concurrence given by [15]

$$ C = \max\{\lambda_1 - \lambda_2 - \lambda_3 - \lambda_4, 0\}, \quad (1) $$

where $\lambda_i (i = 1, 2, 3, 4)$ are the square roots of the eigenvalues of the operator $\rho \hat{\rho}$ in descending order

$$ \hat{\rho} = (\sigma_1^y \otimes \sigma_2^y) \rho^* (\sigma_1^y \otimes \sigma_2^y), \quad (2) $$

with $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4$ and $\rho$ is the density matrix of the pair qubits; $\sigma_1^y$ and $\sigma_2^y$ are the normal Pauli operators. The EOF is related to the concurrence by

$$ EN = b \left( 1 + \sqrt{1 - C^2} \right), $$

where $b(x) = -x \log_2 x - (1 - x) \log_2 (1 - x)$. Henceforth, we denote the EOF by EN. The concurrence $C = 0$ corresponds to an unentangled state and $C = 1$ corresponds to a maximally entangled state.

2. The thermalized Heisenberg system

The model Hamiltonian we study is given by

$$ H = J ( S_1^x S_2^x + S_1^y S_2^y ) + B_1 S_1^z + B_2 S_2^z, \quad (3) $$

where $S^\alpha = \sigma^\alpha/2 (\alpha = x, y, z)$ are the spin-1/2 operators, $\sigma^\alpha$ are the Pauli operators and $J$ is the strength of Heisenberg interaction. $B_1$ and $B_2$ are external magnetic fields. As stated in
the introduction, by changing $B_1$ and $B_2$ separately, we study the effects of magnetic field on the thermal QD, CC and EN in a very general way. The eigenvalues and eigenvectors of $H$ are

$$
H\langle 00 \rangle = -(B_1 + B_2)|00\rangle , \\
H\langle 11 \rangle = (B_1 + B_2)|11\rangle , \\
H|\psi^\pm\rangle = \pm D|\psi^\pm\rangle ,
$$

where $D^2 = (B_1 - B_2)^2 + J^2$ and $|\psi^\pm\rangle = \frac{1}{\sqrt{2}}[(01) + \frac{(B_1-B_2)J}{D}|10\rangle]$. We denote the eigenvalues corresponding to $|00\rangle$, $|11\rangle$, $|\psi^\pm\rangle$ by $E_{00}$, $E_{11}$, $E_{\pm}$, respectively. In the standard basis $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$, the density matrix $\rho(T)$ is given by

$$
\rho(T) = \frac{1}{Z} \begin{bmatrix}
    u_1 & 0 & 0 & 0 \\
    0 & w_1 & v & 0 \\
    0 & v & w_2 & 0 \\
    0 & 0 & 0 & u_2
\end{bmatrix},
$$

where

$$
u_1 = e^{(B_1 + B_2)/kT}, \\
u_2 = e^{-(B_1 + B_2)/kT}, \\
w_1 = \cosh\left(\frac{D}{kT}\right) + \frac{(B_1 - B_2)}{D} \sinh\left(\frac{D}{kT}\right), \\
w_2 = \cosh\left(\frac{D}{kT}\right) - \frac{(B_1 - B_2)}{D} \sinh\left(\frac{D}{kT}\right),
$$

and $Z = \text{Tr}\left[\exp\left(\frac{-H}{kT}\right)\right]$ is the partition function. In the following we select $|J|$ as the energy unit and set $k = 1$.

3. Quantum discord

In classical information theory (CIT) [5, 13], the total correlation between the two systems (two sets of random variables) A and B described by a joint distribution probability $p(A, B)$ is given by the MI,

$$
I(A, B) = H(A) + H(B) - H(A, B),
$$

with the Shannon entropy $H(\cdot) = -\sum_j p_j \log_2 p_j$. Here $p_j$ represents the probability of an event $j$ associated with the systems $A, B$, or to the joint system $AB$. Using Bayes’s rule we may write MI as

$$
I(A, B) = H(A) - H(A|B),
$$

where $H(A|B)$ is the classical conditional entropy. In CIT these two expressions are equivalent but in the quantum domain this is no longer true [5, 16]. The first quantum extension of MI, denoted by $I(\rho)$, is obtained by directly replacing the Shannon entropy in equation (7) with the von Neumann entropy, $S(\rho) = -\text{Tr}(\rho \log_2 \rho)$, with $\rho$ a density matrix, replacing probability distributions. To obtain a quantum version of equation (8), it is necessary to generalize the classical conditional entropy. This is done recognizing $H(A|B)$ as a measure of our ignorance about system $A$ after we make a set of measurements on $B$. When $B$ is a quantum system, the choice of measurements determines the amount of information we can extract from it.
We restrict ourselves to von Neumann measurements on $B$ described by a complete set of orthogonal projectors, $\Pi_j$, corresponding to the outcomes $j$.

After a measurement, the quantum state $\rho$ changes to $\rho_j = [(I \otimes \Pi_j)\rho(I \otimes \Pi_j)]/p_j$, with $I$ the identity operator for system $A$ and $p_j = \text{Tr}[(I \otimes \Pi_j)\rho(I \otimes \Pi_j)]$. Thus, one defines the quantum analog of the conditional entropy as $S(\rho\{\Pi_j\}) = \sum_j p_j S(\rho_j)$ and, consequently, the second quantum extension of the classical MI as $J(\rho\{\Pi_j\}) = S(\rho^A) - S(\rho\{\Pi_j\})$. The value of $J(\rho\{\Pi_j\})$ depends on the choice of $\{\Pi_j\}$.

Henderson and Vedral [5] have shown that the maximum of $J(\rho\{\Pi_j\})$ with respect to $\{\Pi_j\}$ can be interpreted as a measure of CC. Therefore, the difference between the total correlations $I(\rho)$ and the CC $Q(\rho) = \sup_{\{\Pi_j\}} J(\rho\{\Pi_j\})$ is defined as

$$D(\rho) = I(\rho) - Q(\rho),$$

(9)
giving, finally, a measure of quantum correlations [5] called quantum discord. For pure states, QD reduces to the entropy of entanglement [17], highlighting that in this case all correlations come from entanglement. However, it is possible to find separable (not-entangled) mixed states with nonzero QD [5, 16], meaning that entanglement does not cause all nonclassical correlations contained in a composite quantum system. Also, QD can be operationally seen as the difference of work that can be extracted from a heat bath using a bipartite system acting either globally or locally [18].

4. Results and discussion

Case I: $B_1 = -B_2$ and $J > 0$.

In this case, $|\psi^{-}\rangle$ is the ground state with eigenvalue $E_{-} = -\sqrt{4B_1^2 + J^2}$. Other eigenvalues are $0, 0, \sqrt{4B_1^2 + J^2}$ for the eigenvectors $\{|00\rangle, |11\rangle, |\psi^{+}\rangle\}$, respectively.

In this case the variation of QD, CC and EN with $B_1$ at different temperatures ($T = 0.2, 0.9, 1.5$) is depicted in figures 1, 2, 3, respectively. We observe that QD and CC in the thermal state coincide for all values of $B_1$ for different temperatures ($T = 0.2, 0.9, 1.5$).
In order to understand this observation, we take a close look at the thermal state. At temperature $T$, the thermal state is given by

$$\rho = \frac{1}{Z} \left[ |00\rangle\langle 00| + |11\rangle\langle 11| + e^{\sqrt{A_1+B^2/T}} |\psi^-\rangle\langle \psi^-| + e^{-\sqrt{A_1+B^2/T}} |\psi^+\rangle\langle \psi^+| \right].$$

This $\rho$ has the Bloch representation [21]

$$\rho = \frac{1}{4} \left[ I \otimes I + \sum_{i=1}^{3} c_i \sigma_i \otimes \sigma_i \right],$$

where $\sigma_i (i = 1, 2, 3)$ are the one-qubit Pauli operators. In the appendix, we prove that the class of mixed states as in equation (11) has equal classical and quantum correlations (like bipartite pure states [19]) provided

$c_i = c_j > c_k$

and

$c_k = -c_i^2.$
where \( i \neq j \neq k \in \{1, 2, 3\} \). Here \( c_i, c_j \) are the diagonal elements of the correlation matrix defined by \( c_{ij} = \text{Tr}(\rho \sigma_i \otimes \sigma_j) \). It is straightforward to check that the thermal state \( \rho \) in equation (10) which has the form of equation (11) satisfies conditions (12). This explains the observations in figures 1–3 that the two-qubit thermal state \( \rho \) for \( B_1 = -B_2 \) in equation (10) gives rise to equal QD and CC for all values of \( B_1 \) and temperature. In order to see why the common curve for QD and CC peaks at \( B_1 = 0 \), we can maximize the expression for QD = CC with respect to \( B_1 \) and check that the maximum occurs at \( B_1 = 0 \).

From figures 1–3, we also see that EN as a function of \( B_1 \) has a peak at \( B_1 = 0 \) for \( T = 0.2 \), a dip for \( T = 0.9 \) and goes to zero over an interval symmetric about \( B_1 = 0 \) for \( T = 1.5 \) [12]. From equation (10) we see that the concurrence of the thermal state is governed by the admixture of the \( |\psi^+ \rangle \) and \( |\psi^- \rangle \) states. We expect concurrence to fall as the state \( |\psi^+ \rangle \) classically mixes more and more with the ground state \( |\psi^- \rangle \). For fixed \( J = 1 \) and a fixed temperature \( T \), this happens for \( B_1 = 0 \). That is why we observed a dip in the EN curve at \( B_1 = 0 \). The size of this dip increases with temperature. In fact, the dip touches the \( B_1 \) axis when, at \( B_1 = 0 \), the concurrence is zero. To see this, we note that the concurrence for \( \rho \) in equation (10) is given by [20]

\[
C = \frac{2}{Z} \max \{|v| - \sqrt{u_1u_2}, 0\},
\]

where \( v, u_1 \) and \( u_2 \) are given in equation (6). Therefore, for \( B_1 = 0 \) and \( J = 1 \), \( C > 0 \), provided \( \sinh \frac{1}{T} \geq 1 \) or \( T \leq 1.1346 \). For \( T = 1.5 \) and \( J = 1 \), using the requirement \( \sinh \frac{1}{T} = D \), we can find the range of \( B_1 \) around \( B_1 = 0 \) in which \( C = 0 \). This is \(-1.1456 \leq B_1 \leq 1.1456 \). Figures 1–3 confirm the corresponding behavior of EN.

Figure 4 shows the variation of EN, QD and CC with temperature at fixed values of \( B_1 = -B_2 \). As expected we have QD ≈ CC for all temperatures. Both EN and QD(CC) curves have plateau at low temperatures corresponding to their ground state values, as at these temperatures, the ground state is not thermally connected to other exited states. Another interesting observation is the vanishing of concurrence at a finite critical temperature \( T_c \), which increases with \( B_1 \) value, while QD and CC asymptotically go to zero with temperature. The increase in \( T_c \) with \( B_1 \) [12] can be understood from the thermal state equation (10), which says that higher temperatures are required to obtain a given admixture of \( |\psi^- \rangle \) and \( |\psi^+ \rangle \) for higher \( B_1 \) values.

We now deal with the case \( B_2 = -aB_1, a \neq 1 \) and positive. \( B_1 = 0 \) satisfies both \( B_2 = -aB_1 \) and \( B_2 = -B_1 \), so that QD = CC at \( B_1 = 0 \), for all temperatures \( T \). For a fixed temperature \( T \), it turns out that QD > CC for \( B_1 \neq 0 \) if \( a > 1 \) and CC > QD for \( B_1 \neq 0 \) if \( 0 < a < 1 \). This is depicted in figure 5, for \( a = 2 \) and \( a = 1/2 \) for \( T = 1.5 \). The dominance of QD over CC (or vice versa) varies continuously with \( a \). This observation gives us the key to controlling the contributions of QD and CC to a two-qubit thermal state in the Heisenberg model via the continuous variation of the applied magnetic field. The behavior of concurrence in this case can be analyzed in a way similar to the case \( B_2 = -B_1(a = 1) \). From figure 5, we see that for the same temperature, the range over which concurrence vanishes depends on \( a \); this range decreases monotonically with \( a \). Also, the peak position of concurrence (or EN) on the \( B_1 \) axis shifts monotonically toward \( B_1 = 0 \) as \( a \) increases. Thus, the main entanglement features can be controlled by varying external magnetic fields.

Case II: \( B_1 = B_2 \).

For a uniform external magnetic field \( B_1 = B_2 \), figures 6, 7 and 8 show the variation of QD, CC and EN with \( B_1 \) for temperatures \( T = 0.2, 0.9 \) and 1.5, respectively. We see that all three quantities are symmetric about \( B_1 = 0 \) where they have their maxima. Further, QD > CC, except at \( B_1 = 0 \), where QD = CC. For higher temperatures, the qualitative
behavior of QD and CC remains the same, while EN curve drops down below those of QD and CC. This can be qualitatively understood by looking at the thermal state given by

\[ \rho = \frac{1}{Z} \left[ e^{2B_1 T} |00\rangle \langle 00| + e^{-2B_1 T} |11\rangle \langle 11| + e^{J/T} |\psi^-\rangle \langle \psi^-| + e^{-J/T} |\psi^+\rangle \langle \psi^+| \right]. \quad (14) \]

For small temperatures, the entanglement of the thermal state is largely dictated by that of $|\psi^-\rangle$ and becomes dominant. At higher temperatures, admixture due to other states reduces the entanglement, so that QD and CC dominate. Such complementary behavior of entanglement and discord can serve as a pointer towards a possible connection between them.

Figure 9 shows the variation of QD, CC and EN with temperature for $B_1 = B_2 = 1$ and $B_1 = B_2 = 2$. We see that for high temperatures, QD hugely dominates EN, showing the robustness of QD with temperature. As temperature becomes large, QD and CC converge toward each other. For larger values of $B_1$, this happens at higher temperatures. As the temperature increases, all the coefficients in the thermal mixture (equation (14)) tend to be equal and the thermal state approaches random mixture. Thus, it seems that QD and CC approach each other as an arbitrary thermal state approaches a random mixture. Obviously, for random mixture $\rho = \frac{1}{2}(I \otimes I)$, QD $= CC = 0$. A quantitative analysis of the relative
behaviors of QD and CC with temperature will be very interesting, but possibly have to wait for further developments in the theory.
It will be interesting to connect our results with the monogamy relations between the EN and the CC [22] of two subsystems (qubits) and the environment

\[ EN_{AB} + CC_{AE} = S_A, \]
\[ EN_{AE} + CC_{AB} = S_A, \]  
and the relation between EN and QD [23],

\[ EN_{AB} + EN_{AE} = QD_{AE} + QD_{AB}, \]  
showing us that EN and QD always exist in pairs. Here \( A \) and \( B \) label the qubits and \( E \) stands for the environment. We assume that environment (heat bath) comprises the universe minus the qubits \( A \) and \( B \) so that the state \( \rho_{ABE} \) is a pure state. Since the variation of all the quantities pertaining to the system \( AB \) with \( B_1 \) and \( T \) are obtained from the XX model, we can use equations (15) and (16) to find the corresponding dependence of \( EN_{AE} \) and \( QD_{AE} \) on \( B_1 \) and \( T \). Figures 10 and 11 (for \( B_1 = -B_2 \)) show the variation of \( EN_{AE} \) and \( QD_{AE} \) with \( B_1 \) and \( T \).
Figure 9. QD (dashed line), CC (dash-dotted line) and EN (solid line) as a function of the absolute temperature $T$ for (a) $B_1 = B_2 = 1$ (b) $B_1 = B_2 = 2$.

Figure 10. $\text{EN}_{\text{AB}}$ (solid line), $\text{QD}_{\text{TT}}$ (dashed line), $\text{EN}_{\text{AE}}$ (dotted line) and $\text{QD}_{\text{TE}}$ (dash-dotted line), as a function of the external magnetic field $B_1 = -B_2$ at $T = 0.9$. 
The monogamic relations also help us establish a necessary and sufficient condition for $\text{QD}_{\chi B} = \text{CC}_{\chi B}$ when the environment is present. This is $\text{QD}_{\chi B} = \text{CC}_{\chi B}$ if and only if $\frac{1}{2} I_{AB} = \text{EN}_{AE} + \text{EN}_{AB} - \text{QD}_{\chi E}$. To prove the necessity we note that when $\text{QD}_{\chi B} = \text{CC}_{\chi B}$ (that is, $\text{QD}_{\chi B} = \frac{1}{2} I_{AB}$), equation (16) can be written as

$$\frac{1}{2} I_{AB} = \text{EN}_{AE} + \text{EN}_{AB} - \text{QD}_{\chi E}. \quad (17)$$

Now suppose that equation (17) is true. Then using equation (16) we have

$$\text{QD}_{\chi B} = \frac{1}{2} I_{AB},$$

which implies $\text{QD}_{\chi B} = \text{CC}_{\chi B}$. Figures 12 and 13 show the variation of both sides of equation (17) with $B_1$ and $T$, which establishes equation (17) for the XX model.
5. Summary

In this paper we have studied the variation of QD, CC and EN in a two-qubit XX Heisenberg chain as functions of the independently varied magnetic fields $B_1$ and $B_2$ on each qubit and also with temperature. We deal with two cases $B_1 = -B_2$ (nonuniform field) and $B_1 = B_2$ (uniform field). Our first observation is the complementary behavior of entanglement and QD/CC. For the nonuniform magnetic field, we find the interesting observation that QD and CC are equal for all $B_1 = -B_2$ values as well as all temperatures. Surprisingly, this observation is explained quite simply, using the symmetric form of the thermal state. A very interesting observation is that the relative contributions of QD and CC can be tunably controlled by varying the applied magnetic field. Another interesting finding is that the equality of QD and CC of the subsystem (qubits) imposes a constraint on the distribution of QD and EN over the subsystem and its environment. Further investigation of general Heisenberg models such as XXZ along these lines may turn out to be interesting and fruitful.

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Appendix

We prove the following statement.

If the quantum state has the Bloch representation [21]

$$\rho = \frac{1}{4} \left[ I \otimes I + \sum_{i=1}^{3} c_i \sigma_i \otimes \sigma_i \right],$$  \hspace{1cm} (A.1)

Figure 13. $\frac{1}{4} \langle I_A \rangle$ (solid line), $\Delta N_{AE} + \Delta N_{AB} - \Delta N_{EX}$ (dashed line), as a function of the temperature $T$ for $B_2 = -B_1 = -1$. 

and $c_i = c_j > c_k$ and $c_k = -c_i^2$ where $i \neq j \neq k \in \{1, 2, 3\}$, then this state contains the same amount of quantum and classical correlation (QD = CC).

**Proof.** In [24] Luo evaluated analytically the QD for a large family of two-qubit states, which have the maximally mixed marginal, and their Bloch representation is

$$
\rho = \frac{1}{4} \left[ 1 \otimes I + \sum_{i=1}^{3} c_i \sigma_i \otimes \sigma_i \right].
$$

For this class of quantum states, the quantum MI is

$$
\mathcal{I}(\rho) = \frac{1}{4} \left[ (1 - c_1 - c_2 - c_3) \log_2(1 - c_1 - c_2 - c_3) + (1 - c_1 + c_2 + c_3) \log_2(1 - c_1 + c_2 + c_3) + (1 + c_1 - c_2 + c_3) \log_2(1 + c_1 - c_2 + c_3) + (1 + c_1 + c_2 - c_3) \log_2(1 + c_1 + c_2 - c_3) \right].
$$

We substitute the conditions above into the quantum MI. Putting $c = c_1 = c_2 > c_3$ and $c_3 = -c_i^2$, we get

$$
\mathcal{I}(\rho) = \frac{1}{4} \left[ (1 - 2c + c^2) \log_2(1 - 2c + c^2) + (1 - c^2) \log_2(1 - c^2) + (1 - c^2) \log_2(1 - c^2) + (1 + 2c + c^2) \log_2(1 + 2c + c^2) \right].
$$

After some algebraic simplification, we get

$$
\mathcal{I}(\rho) = (1 - c) \log_2(1 - c) + (1 + c) \log_2(1 + c),
$$

which equals 2CC as in [24]. It is also easy to check that the above argument goes through when $c = c_1 = c_3 > c_2$ and $c_2 = -c^2$ and when $c = c_3 = c_2 > c_1$ and $c_1 = -c^2$, to get

$$
\mathcal{I}(\rho) = 2CC.
$$

Thus,

$$
\text{QD}(\rho) = \mathcal{I}(\rho) - \text{CC}(\rho) = \text{CC}(\rho).
$$

□

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