Quantum Correlations in Ising-XYZ Diamond Chain Structure under an External Magnetic Field *

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We consider an entangled Ising-XYZ diamond chain structure. Quantum correlations for this model are investigated by using quantum discord and trace distance discord. Quantum correlations are obtained for different values of the anisotropy parameter, magnetic field and temperature. By comparison between quantum correlations, we show that the trace distance discord is always larger than quantum discord. Finally, some novel effects such as increasing the quantum correlations with temperature and constructive role of anisotropy parameter, which may play to the quantum correlations, are observed.

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A very fertile interaction between the theories of quantum information and condensed matter has expanded during the last decade. Condensed matter theory has proposed a wide range of possibilities for the implementation of quantum communication and computational tasks. On the other hand, quantum information theory has provided deep insights into the physics of condensed matter systems. Since the capability of entanglement to mark quantum phase transitions, the concept of quantum correlations has become necessary in characterizing quantum critical phenomena. In this context, quantum correlations and entanglement have been usually granted as one concept. We now recognize that the notion of entanglement cannot capture the whole amount of quantum correlations in a system. The introduction of quantum discord (QD) indicated that a system can exhibit quantum correlations even in the absence of entanglement. Also, QD allows us to distinguish the total correlations between two subsystems in terms of quantum and classical theories. QD was first used in the realm of quantum measurement theory while it has been used in many physical systems. In a quantum information domain, it has been shown that QD may be the most basic resource allowing for the speeding up of quantum over classical computation, and it has an important role in quantum communication protocols. Analytical solutions for QD are known only for some certain cases. Dakic et al. introduced a geometric measure of QD, which is obtainable analytically for two-qubit states and for arbitrary bipartite states. Such a distance is not too contractive under trace-preserving quantum channels. This leads to a re-definition of the geometric discord in terms of a metric that fulfills the contractivity property. Such a metric is the trace distance, which uses the trace norm. Here we refer to this particular measure as the trace distance discord (TDD).

In recent years, spin systems have an extensive application in the field of quantum information. The Heisenberg model has been researched in many fields of quantum information and computation. It can be implemented in many physical systems such as quantum dot system, nucleus system, electronic spin system and optical lattices system. Quantum correlation in the Heisenberg model makes a bridge between quantum information and condensed matter physics.

We are motivated by real materials like Cu3(CO3)2(OH)2 known as azurite, which is an exciting quantum anti-ferromagnetic model characterized by the Heisenberg model on a generalized diamond chain. Honecker et al. investigated the dynamic and thermodynamic properties for this model. Moreover, the thermodynamics of the Ising-Heisenberg model on a diamond-like chain was also vastly discussed. The motivation to research the Ising-XYZ diamond chain model is based on some recent works. Lately, thermal entanglement has been studied in the Ising-XXZ model on a diamond chain, and in the Ising-XYZ model on a diamond chain. In this Letter, we study the QD of the Ising-XYZ model on a diamond chain. Also, only a few studies are directed to the relation between QD and TDD in the quantum channels. Thus we compare the QD and TDD and show their different characteristics.

We first review the definitions of QD and TDD. In classical information theory, the total correlation between two arbitrary parts can be expressed as two kinds of equivalent expressions of mutual information. In the quantum domain, one of quantum extension of mutual information is equal to total correlation. It can be expressed as

\[ I(\rho_{AB}) = S(\rho_A) + S(\rho_B) - S(\rho_{AB}), \]

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where $S(\cdot)$ is the von Neumann entropy, and $\rho_A$ ($\rho_B$) is the reduced density operator of the part A (B). The other quantum version of mutual information can be written after a complete set of projection measurements $\{B_k\}$. Since the systems have quantum correlation, the quantum correlation will unavoidably cause another system to be disturbed when we measure one quantum system. Therefore, the two quantum extensions of mutual information are not equal to each other. However the maximum of the second extension can be interpreted as a measure of classical correlations $C(\rho_{AB})$. It can be written as\cite{14}

$$C(\rho_{AB}) \equiv S(\rho_A) - \min_{\{B_k\}} \tilde{S}(\rho_{AB}|\{B_k\}),$$ \hspace{1cm} (2)

where $\tilde{S}(\rho_{AB}|\{B_k\}) = \sum_k p_k S(\rho_{AB}^k)$ is the conditional entropy of part A, $\rho_{AB}^k = (I \otimes B_k)\rho_{AB}(I \otimes B_k)/p_k$ and $p_k = \text{Tr}[I \otimes B_k] \rho_{AB}(I \otimes B_k)$. The minimum value in Eq. (2) is due to the complete set of projection measurements $\{B_k\}$. The minimum difference between the two quantum versions of mutual information is equal to QD. It can be written as\cite{10}

$$D(\rho_{AB}) = I(\rho_{AB}) - C(\rho_{AB}).$$ \hspace{1cm} (3)

For any bipartite system AB described by the density operator $\rho$, the TDD is defined as the minimal trace distance between $\rho$ and all of the classical-quantum states $\rho_{CQ}$,\cite{35} that is,

$$D_T(\rho) = \min_{\chi \in \rho_{CQ}} \|\rho - \chi\|_1,$$ \hspace{1cm} (4)

where $\|\chi\|_1 = \text{Tr} \sqrt{\chi^\dagger \chi}$ shows the trace norm, and $\rho_{CQ}$ is

$$\rho_{CQ} = \sum_i p_i \Pi_i^A \otimes \rho_i^B,$$ \hspace{1cm} (5)

which is a linear combination of the tensor products of $\Pi_i^A$ (the orthogonal projection in the Hilbert space $H_A$) and $\rho_i^B$ (an arbitrary density operator in $H_B$), with $\{p_i\}$ being a probability distribution. For the certain case of the two-qubit X states\cite{36} the TDD with $\rho_X$ can be expressed analytically as\cite{37}

$$D_T(\rho_X) = \sqrt{\gamma_1^2 \gamma_2^2 - \gamma_2^2 \gamma_3^2 - \gamma_3^2 \gamma_4^2},$$ \hspace{1cm} (6)

where $\gamma_{1-4} = 2|\langle \rho_{23} | \pm | x_{14} \rangle|$. $\gamma_2 = 1 - 2(\rho_{22} + \rho_{33})$, $\gamma_3 = \max\{\gamma_2 \gamma_3, \gamma_2 x_{A3} \}$ and $\gamma_4 = \min\{\gamma_2^2, \gamma_3^2 \}$, with $x_{A3} = 2(\rho_{11} + \rho_{22}) - 1$.

Pairwise thermal entanglement in the Ising-XYZ diamond chain structure was discussed in Ref.\cite{33}. Here we discuss the pairwise QD and TDD for this model. An Ising-XYZ diamond chain structure is shown schematically in Fig.1.\cite{32} The Ising-XYZ Hamiltonian can be written as\cite{36}

$$H = \sum_{i=1}^{N} H_i = - \sum_{i=1}^{N} [J(1 + \gamma)\sigma_{a,i}^z\sigma_{b,i}^z + J(1 - \gamma)\sigma_{a,i}^z\sigma_{b,i}^z + J_2\sigma_{a,i}^z\sigma_{b,i}^z + J_0(\sigma_{a,i}^+ + \sigma_{a,i}^-)](S_i + S_{i+1}) + h(\sigma_{a,i}^z + \sigma_{b,i}^z) + \frac{1}{2}(S_i + S_{i+1})],$$ \hspace{1cm} (7)

where the summations run over clusters (Fig.1). $H_i$ shows the Hamiltonian of the ith clusters, $\sigma_{a(b)}$ are the Pauli matrix with $\alpha = \{x, y, z\}$, $S$ corresponds to the Ising spins, $\gamma$ is the XY-anisotropy parameter, and $h$ shows the magnetic field.

Since we consider pairwise quantum correlations, we should use the reduced density matrix, by tracing out two (of four) spins of the cluster. We would like to point out that the only entangled pair is formed by the Heisenberg spins. Other pairs are disentangled (separable) due to the classical (diagonal) character of the Ising-type interaction between them. Hence we are interested in the reduced density matrix, constructed by tracing out two Ising-type spins $S_i$ and $S_{i+1}$. The reduced density matrix in terms of the correlation function between two entangled particles, i.e., ab-dimer, has the following form\cite{38}

$$\rho_X = \begin{pmatrix}
\rho_{11} & 0 & 0 & \rho_{14} \\
0 & \rho_{22} & \rho_{23} & 0 \\
0 & \rho_{23} & \rho_{33} & 0 \\
\rho_{14} & 0 & 0 & \rho_{44}
\end{pmatrix},$$ \hspace{1cm} (8)

where the elements of density matrix are given by

$$\rho_{11} = \frac{1}{4} + \langle \sigma_a^z \sigma_b^z \rangle, \langle \sigma_a^z \rangle,$$
$$\rho_{22} = \frac{1}{4} - \langle \sigma_a^z \sigma_b^z \rangle,$$
$$\rho_{23} = \frac{1}{4} + \langle \sigma_a^z \sigma_b^z \rangle,$$
$$\rho_{44} = \frac{1}{4} + \langle \sigma_a^z \sigma_b^z \rangle - \langle \sigma_a^z \rangle,$$
$$\rho_{14} = \langle \sigma_a^+ \sigma_b^z \rangle - \langle \sigma_a^z \sigma_b^+ \rangle,$$
$$\rho_{23} = \langle \sigma_a^+ \sigma_b^z \rangle + \langle \sigma_a^z \sigma_b^+ \rangle.$$ \hspace{1cm} (9)

At finite temperature, all the expected values are
temperature-dependent quantities expressed as[33]

\[
\langle \sigma_\alpha^x \sigma_\beta^x \rangle = e^{\beta \Delta(2)} e^{-\frac{\beta^2 e^{\beta \Delta(2)} \sinh(\beta \Delta(2))}{\Delta(1)\lambda_+}} 
\]

\[
\langle \sigma_\alpha^y \sigma_\beta^y \rangle = e^{\beta \Delta(2)} e^{-\frac{\beta^2 e^{\beta \Delta(2)} \sinh(\beta \Delta(2))}{\Delta(1)\lambda_+}} 
\]

\[
\langle \sigma_\alpha^z \sigma_\beta^z \rangle = e^{\beta \Delta(2)} \frac{e^{\frac{\beta J \gamma}{2}} \sinh(\beta \frac{J \gamma}{2}) - e^{-\frac{\beta J \gamma}{2}} \sinh(\beta \Delta(1))}{\Delta(1)\lambda_+} 
\]

\[
\langle \sigma_\alpha^z \sigma_\beta^x \rangle = e^{\beta \Delta(2)} \frac{e^{\frac{\beta J \gamma}{2}} \sinh(\beta \frac{J \gamma}{2}) - e^{-\frac{\beta J \gamma}{2}} \sinh(\beta \Delta(1))}{\Delta(1)\lambda_+} 
\]

where

\[
\Delta(\mu) = \sqrt{(h + \mu J_0)^2 + \frac{1}{4} J^2 \gamma^2}, 
\]

\[
\lambda_+ = \omega(2) + \omega(-2) + \sqrt{(\omega(2) - \omega(-2))^2 + 4 \omega(0)^2}. 
\]

Here

\[
\omega(\mu) = 2 e^{\frac{\beta h}{2}} [e^{-\frac{\beta J}{2}} \cosh(\frac{\beta J}{2}) + e^{\frac{\beta J}{2}} \cosh(\beta\Delta(\mu))]. 
\]

where \(\beta = 1/k_B T\) with \(k_B\) being the Boltzmann constant, and \(T\) is the absolute temperature. For simplicity, we can write \(k_B = 1\).

For the \(X\) states described by the density matrix Eq. (8), the explicit expression of QD is given as[39]

\[
D(\rho) = \min\{D_1, D_2\}, 
\]

where

\[
D_1 = S(\rho^A) - S(\rho^{AB}) - \rho_{11} \log_2 \left( \frac{\rho_{11} + \rho_{22}}{\rho_{11} + \rho_{22} + \rho_{44}} \right) 
\]

\[
- \rho_{22} \log_2 \left( \frac{\rho_{22}}{\rho_{11} + \rho_{22} + \rho_{44}} \right) 
\]

\[
- \rho_{44} \log_2 \left( \frac{\rho_{44}}{\rho_{22} + \rho_{44}} \right), 
\]

and

\[
D_2 = S(\rho^A) - S(\rho^{AB}) + \Delta_+ \log_2 \Delta_+ - \Delta_- \log_2 \Delta_-, 
\]

with \(\Delta_+ = \frac{1}{2} (1 + I)\) and \(I^2 = (\rho_{11} - \rho_{44})^2 + 4(|\rho_{14}| + |\rho_{23}|)^2\).

According to Eqs. (6) and (17), QD and TDD can be worked out by numerical calculation. We now discuss them with the corresponding plots. Both QD and TDD are known to vary with parameters \(J_0, h, \gamma, J_z\) and \(T\). By fixing some of the parameters we can analyze the roles that the others play in QD and TDD.

In Fig. 2 quantum correlations are plotted versus \(J_0/J\) and \(T/J\), for fixed parameters \(J_0/J = 0, \gamma = 0.95, h/J = 0.27\) in Figs. 2(a) and 2(b) and for fixed parameters \(J_0/J = 0.3, \gamma = 0.6, h/J = 0.35\) in Figs. 2(c) and 2(d). We can see from Fig. 2, both QD and TDD increase from zero to some peak values in the beginning and then decrease with increasing the temperature. Note that the peak value depends on \(J_0/J\), so that smaller \(J_0/J\) has a higher peak value. Moreover, after reaching the peak values, QD and TDD decrease more slowly for larger values of \(J_0/J\), as temperature goes up, then a smaller value of \(J_0/J\). The distinct difference between QD and TDD is that TDD has a value larger than QD. The fact that the QD and TDD do not monotonically decline with increasing temperature shows the more correlated low-lying excited states in some regions.[40] Pairwise thermal entanglement of the Ising-XYZ diamond chain model has been considered in Ref.[33]. The authors found that thermal entanglement vanishes as the temperature increases, while we find from Fig. 2 that QD and TDD do not vanish up to infinite temperature. It is indicated that both the QD and TDD are more general quantum correlations than entanglement.

Fig. 2. Quantum correlations as functions of \(J_0/J\) and \(T/J\), with \(J_0/J = 0, \gamma = 0.95, h/J = 0.27\) (a) and (b); \(J_0/J = 0.3, \gamma = 0.6, h/J = 0.35\) (c) and (d).

Fig. 3. Quantum correlations as functions of \(\gamma\) and \(h/J\) in the low temperature \((T/J = 0.02)\) and fixed \(J_0/J = -0.3\) and \(J_z/J = 0.3\).

In Fig. 3, quantum correlations as functions of \(\gamma\) and \(h/J\) are illustrated in the low temperature
(T/J = 0.02) at fixed J₀/J = −0.3 and Jₓ/J = 0.3. The phase diagram at zero temperature for this model has been considered in Ref. [36]. The authors found that a density-plot concurrence in the low temperature limit (T/J = 0.01) follows the pattern of the phase diagram. By looking at Fig. 3 we can see that QD and TDD follow the pattern of the phase diagram. Moreover, Fig. 4 illustrates quantum correlations versus h/J and J₀/J for the Ising-XY diamond chain (Jₓ/J = 0) with fixed values of T/J = 0.1 and γ = 0.95. This plot also follows the pattern of the phase diagram. It is worth mentioning that the disentangled region of QD in Fig. 4(a) is similar to the concurrence found in Ref. [33]. However, we can see from Fig. 4(b) that there is an area in which TDD is not zero while QD is. Thus TDD may be more practical than the QD for a resource of information.

![Fig. 4. Quantum correlations as functions of J₀/J and h/J with Jₓ/J = 0 and γ = 0.95 and T/J = 0.1.](image)

We now investigate the dependence of QD and TDD on the magnetic field. Figure 5 shows the behavior of QD and TDD versus the magnetic field and different temperatures at fixed values of γ = 0.5 and J₀/J = −0.3, Jₓ/J = 0.3. For the QD case, as the temperature is low (T/J = 0.2) there are three sharp peaks appearing (Fig. 5(a)). As we increase temperature, the middle peak becomes shorter. Compared with QD, we can see from Fig. 5(b) that the behavior of TDD is different from QD to some extent. As the temperature is low, we can see only one peak. As we increase temperature (T/J = 0.5), one can see that the one peak evolves into three peaks. That is, the left and right peaks appear. When T/J = 0.7 the middle peak becomes shorter. As the temperature is further increased (T/J = 1.5) the middle peak disappears and we can see two sharp peaks.

![Fig. 5. QD (a), TDD (b) as a function of h/J with γ = 0.5, J₀/J = −0.3, Jₓ/J = 0.3 and different values of temperature T/J: T/J = 0.2 (dashed line), T/J = 0.5 (dashed-dotted line), T/J = 0.7 (solid line), and T/J = 1.5 (circle line).](image)

We now move to investigate how the quantum correlations behave as we change the anisotropy parameter at finite temperature. QD and TDD as functions of γ and T/J for fixed values of h/J = 0.5, J₀/J = −0.3 and Jₓ/J = 0.3 are shown in Fig. 7. It is seen that QD and TDD are not symmetric functions about zero anisotropy parameter γ. We can see from Fig. 7 that QD and TDD evolve similarly but not the same. With increasing the absolute value of anisotropy parameter γ, quantum correlations decrease to a minimum value first and then increase to maxima. Moreover, the values of QD and TDD are nearly a constant when γ is large enough. The constant is not the same for differ-

![Fig. 7. Quantum correlations as functions of γ and T/J with J₀/J = −0.3, Jₓ/J = 0.3 and h/J = 0.5.](image)
ent temperatures.

In summary, we have studied the quantum correlations of the spin-\( \frac{1}{2} \) Ising-XYZ chain on the diamond structure. By changing the magnetic field, anisotropy parameter, coupling constant and temperature we observe that the overall behavior of QD and TDD is alike to a large extent. We find that the anisotropy parameter can decrease or increase quantum correlation. Moreover, we observe regimes where QD and TDD increase by increasing temperature \( T \), while concurrence decreases with \( T \). Finally, we observe that a strong magnetic field suppresses quantum correlations, while a weak magnetic field can increase or decrease QD and TDD. By comparison between QD and TDD versus the magnetic field we show that TDD is always greater than QD.

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