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ORIGINAL ARTICLE

Pairwise correlations via quantum discord and its geometric measure in a four-qubit spin chain

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Abstract The dynamic of pairwise correlations, including quantum entanglement (QE) and discord (QD) with geometric measure of quantum discord (GMQD), are shown in the four-qubit Heisenberg XX spin chain. The results show that the effect of the entanglement degree of the initial state on the pairwise correlations is stronger for alternate qubits than it is for nearest-neighbor qubits. This parameter results in sudden death for QE, but it cannot do so for QD and GMQD. With different values for this entanglement parameter of the initial state, QD and GMQD differ and are sensitive for any change in this parameter. It is found that GMQD is more robust than both QD and QE to describe correlations with nonzero values, which offers a valuable resource for quantum computation.

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1. Introduction

An interacting quantum system is characterized by the presence of correlations amongst its different constituents. The correlations have, in general, both classical and quantum components. The most prominent example of quantum correlations is that of entanglement which serves as the fundamental resource in several quantum information processing tasks such as quantum computation, teleportation and

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ELSEVIER **Production and hosting by Elsevier** dense coding [\[1\].](#page-5-0) It is well known that the total correlation in a bipartite quantum system can be measured by quantum mutual information [\[2\]](#page-5-0), which may be divided into classical and quantum parts [\[3–6\].](#page-5-0) The quantum part is called quantum discord (QD) which is originally introduced in Ref. [\[5\].](#page-5-0) Recently, there has been awareness of the fact that quantum discord is a more general concept to measure quantum correlation than quantum entanglement (QE) since there is a nonzero quantum discord in some separable mixed states [\[5\]](#page-5-0). Interestingly, it has been proven both theoretically and experimentally that such states provide computational speedup compared to classical states in some quantum computation models [\[17,18\].](#page-5-0) In these contexts, quantum discord could be a new resource for quantum computation. The dynamics of quantum discord and entanglement has been recently compared under the same conditions when entanglement dynamic undergoes a sudden death [\[7–12\].](#page-5-0) The entanglement sudden

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death, in which the entanglement can decrease to zero abruptly and remains zero for a finite time [\[13,14\]](#page-5-0), has been experimentally observed in an implementation using twin photons [\[15\]](#page-5-0), and atomic ensembles [\[16\]](#page-5-0).

The calculation of quantum discord is based on numerical maximization procedure, it does not guarantee exact results and there are few analytical expressions including special cases [\[19,20\].](#page-6-0) Therefore, to avoid this difficulty, geometric quantum discord (GMQD), introduced in Ref. [\[21\],](#page-6-0) measures the quantum correlations through the minimum Hilbert–Schmidt distance between the given state and zero discord state.

On the other hand, there are an effort to characterize the entanglement properties in solid state systems such as spin chains [\[22–24\].](#page-6-0) Where the spin chains, as the natural candidates, not only have been used to simulate a quantum computer, as well as quantum dots [\[25\]](#page-6-0), nuclear spins [\[26\],](#page-6-0) electronic spins [\[27\]](#page-6-0), and optical lattice [\[28\]](#page-6-0), but also display useful applications such as quantum state transfer [\[29\].](#page-6-0)

In previous studies only the correlations of the nearest neighbor spin–spin interactions in the spin chain are considered [\[30–34\]](#page-6-0). But from the practical point of views, more attention should be paid to study the correlations of spin models with not only nearest neighbor spin–spin interactions, but also with next-to-nearest neighbor, since those models are closer to real quasi-one-dimensionalmagnets comparing to standard ones with only nearest neighbor couplings. Therefore, a lot of interesting work about pairwise entanglement has been done [\[35–37\].](#page-6-0) But pairwise correlations, via quantum discord and its geometric measure, in spin chains seems to have been seldom exploited before [\[38\].](#page-6-0) It is very interesting and necessary to study the relation between quantum entanglement and various quantum correlations in such systems.

Motivated by the previous topics, in this paper, one will be concerned with the dynamic properties of pairwise correlations in a four-qubit Heisenberg XX spin chain. Different from the previous work, the dynamics of pairwise correlations via quantum discord and its geometric measure as other types for quantum correlations, further to entanglement, are presented. In addition, one also discusses the effects of the degree of entanglement of the initial state on the behavior of pairwise correlations.

2. Measures of correlations

Here, one uses the quantum discord and its geometric measure and entanglement as the measures of quantum correlations.

To quantify the quantum correlations of a bipartite system, no matter whether it is separable or entangled, one can use the quantum discord measure [\[3,5\]](#page-5-0). Quantum discord measures all nonclassical correlations and defined as the difference between total correlation and the classical correlation with the following expression

$$
D(\rho^{AB}) = \mathcal{I}(\rho^{AB}) - \mathcal{Q}(\rho^{AB}),\tag{1}
$$

which quantifies the quantum correlations in ρ^{AB} and can be further distributed into entanglement and quantum dissonance (quantum correlations excluding entanglement) [\[39\]](#page-6-0). Here the total correlation between two subsystems A and B of a bipartite quantum system ρ^{AB} is measured by quantum mutual information,

$$
\mathcal{I}(\rho^{AB}) = \mathcal{S}(\rho^A) + \mathcal{S}(\rho^B) - \mathcal{S}(\rho^{AB}),
$$
\n(2)

where $S(\rho^{AB}) = Tr(\rho^{AB} \log \rho^{AB})$ is the von Neumann entropy, $\rho^A = Tr_B(\rho^{AB})$ and $\rho^B = Tr_A(\rho^{AB})$ are the reduced density operators of the subsystems A and B , respectively. The measure of classical correlation is introduced implicitly in the Ref. [\[5\]](#page-5-0) and interpreted explicitly in the Ref. [\[3\]](#page-5-0). The classical correlation between the two subsystems A and B is given by

$$
\mathcal{Q}(\rho^{AB}) = \max_{\{H_k\}} \left[\mathcal{S}(\rho^A) - \sum_k p_k \mathcal{S}(\rho_k) \right],\tag{3}
$$

where $\{H_k\}$ is a complete set of projectors to measure the subsystem B, and $\rho_k = Tr_B[(I^A \otimes \Pi_k)\rho^{AB}(I^A \otimes \Pi_k)]/p_k$ is the state of the subsystem A after the measurement resulting in outcome k with the probability $p_k = Tr_{AB}[(I^A \otimes \Pi_k)\rho^{AB}(I^A \otimes \Pi_k)],$ and I^A denotes the identity operator for the subsystem A. Here, maximizing the quantity represents the most gained information about the system A as a result of the perfect measurement ${T_k}$. It can be shown that quantum discord is zero for states with only classical correlations and nonzero for states with quantum correlations. Note that discord is not a symmetric quantity, i.e., its amount depends on the measurement performed on the subsytem A or B [\[21\]](#page-6-0). However the density matrix that one will consider provides equal values of measurement of classical correlations, irrespective of whether the measurement is performed on the subsytem \vec{A} or \vec{B} [\[8,19\]](#page-5-0).

The geometric measure of quantum discord quantifies the quantum correlation through the nearest Hilbert–Schmidt distance between the given state and the zero discord state [\[21\]](#page-6-0), which is given by

$$
D_A^g = \min_{\chi \in S} ||\rho^{AB} - \chi||^2,
$$
\n(4)

where S denotes the set of zero discord states and $||A||^2 = Tr(A^{\dagger}A)$ is the square of Hilbert-Schmidt norm of Hermitian operators. The subscript A of D_A^g implies that the measurement is taken on the system A. A state χ on $H^A \otimes H^B$ is of zero discord if and only if it is a classical-quantum state [\[40\],](#page-6-0) which can be represented as

$$
\chi=\sum_{k=1}^2p_k|k\rangle\langle k|\otimes\rho_k,
$$

where $\{p_k\}$ is a probability distribution, $|k\rangle$ is an arbitrary orthonormal basis for H^4 and ρ_k is a set of arbitrary states (density operators) on H^B . An easily computable exact expression for the geometric measure of quantum discord is obtained [\[21\]](#page-6-0) for a two qubit system, which can be described as follows.

Consider a two-qubit state ρ^{AB} expressed in its Bloch representation as

$$
\rho^{AB} = \frac{1}{4} \left[I^A \otimes I^B + \sum_{i=1} (x_i \sigma_i \otimes I^B + I^A \otimes y_i \sigma_i) + \sum_{ij=1} R_{ij} \sigma_i \otimes \sigma_j \right],
$$
\n(5)

where $\{\sigma_i\}$ are the usual Pauli spin matrices. $x_i =$ $Tr(\rho^{AB}(\sigma_i \otimes I))$ and $y_i = Tr(\rho^{AB}(I \otimes \sigma_i))$ are the components of the local Bloch vector. $R_{ij} = Tr(\rho^{AB}(\sigma_i \otimes \sigma_j))$ are the components of the correlation matrix [\[21\]](#page-6-0). Then its geometric measure of quantum discord is given by

$$
D_A^g = \frac{1}{4} (||\vec{x}||^2 + ||R||^2 - k_{max}),
$$
\n(6)

 $\vec{x} = (x_1, x_2, x_3)^T$ and k_{max} is the largest eigenvalue of the matrix $K = \vec{x}\vec{x}^T + RR^T$, where R is the matrix with elements R_{ij} . To measure the quantum entanglement (QE) one uses the

negativity [\[41\],](#page-6-0) in which, the negative eigenvalues of the partial transposition of ρ^{AB} are used to measure QE of the qubits system. Therefore, the negativity of a state ρ^{AB} is defined as

$$
N(\rho) = \max\left(0, -2\sum_{j} \mu_j\right),\tag{7}
$$

where μ_i is the negative eigenvalue of $(\rho^{AB}(t))^{T_B}$, and T_B denotes the partial transpose with respect to the system B.

3. The model and quantum correlations

One considers a one-dimensional spin-chain interaction, the Hamiltonian H for the four-qubit Heisenberg XX spin chain with uniform magnetic field can be described by

$$
H = J \sum_{j=1}^{4} \frac{1}{2} \left(\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y + B \sigma_j^z \right), \tag{8}
$$

where J is the coupling constant for the spin interaction, and σ_j^i , $i = x, y, z$ are the Pauli matrices of the *j*th qubit. The eigenvalues and eigenstates of the Hamiltonian in Eq. (8) are calculated analytically in Ref. [\[36\]](#page-6-0). The time evolution of the system is given by

$$
\rho(t) = e^{-iHt}\rho(0)e^{iHt},\qquad(9)
$$

this density matrix is used to study the dynamical character of the quantum correlations, including entanglement and discord with its geometric measure, of two qubits $(A, B, C \text{ and } D)$ for several different initial states, where the coupling system is initially in pure state $\rho(0) = |\psi(0)\rangle \langle \psi(0)|$. To study the pairwise correlations via quantum discord and its geometric measure in a four-qubit spin chain, one compares pairwise correlations between the nearest and alternate spin pairs. Where the quantum correlations of the nearest neighbor qubits A and B are calculated by tracing out the qubits C and D . But the correlations of the alternate qubits A and C are calculated by tracing out the qubits B and D . Therefore, the states of the resulted two-qubit systems are mixed states and their correlations differ. In the following one offers QE, QD and GMQD of these two-qubit systems AB and AC.

Case1: Therefore, one considers the initial state $|\psi(0)\rangle$ = - $\cos\theta$ 0000) + sin θ 1100). In this state, the nearest neighbor qubits A and B are initially prepared in the Bell-like state $|\psi_{AB}(0)\rangle = \cos\theta|00\rangle + \sin\theta|11\rangle$, and qubit C and D are initially in $|00\rangle_{CD}$. The time evolution of $\rho(t)$ can be obtained by this initial state $\rho(0)$ and Eq. (9). To calculate the quantum correlations between nearest neighbor qubits A and B , one traces out the qubits C and D . Therefore, the reduced density matrix $\rho^{AB}(t)$ is given by

$$
\rho^{AB}(t) = x|00\rangle\langle00| + w|00\rangle\langle11| + w^*|11\rangle\langle00| + y(|01\rangle)
$$

$$
\times \langle01| + |10\rangle\langle10|) + d(|01\rangle\langle10| + |10\rangle\langle01|)
$$

$$
+ z|11\rangle\langle11|,
$$
 (10)

with the abbreviation

$$
x = \sin^2 \theta + \frac{1}{32} \cos^2 \theta \left(3 - 4 \cos 2\sqrt{2} Jt + \cos 4\sqrt{2} Jt \right),
$$

\n
$$
y = \frac{1}{32} \cos^2 \theta \left(5 - 4 \cos 2\sqrt{2} Jt - \cos 4\sqrt{2} Jt \right),
$$

\n
$$
w = \frac{1}{8} \left(\cos 2\sqrt{2} Jt + 3 \right) \sin 2\theta e^{4itB},
$$

\n
$$
z = \frac{1}{32} \cos^2 \theta \left(19 + 12 \cos 2\sqrt{2} Jt + \cos 4\sqrt{2} Jt \right), \quad d = 0.
$$
 (11)

Case2: When the initial state $|\psi(0)\rangle = \cos\theta|0000\rangle + \sin\theta$ θ 1010) is considered, the alternate qubits A and C are initially prepared in the Bell-like state $|\psi_4|$ $C(0)$ = cos θ 00) + sin θ 11), and qubits B and D are initially in $|00\rangle_{BD}$. Substituting $\rho(0)$ into Eq. (9), one can obtain the time evolution of $\rho(t)$ in this case. To study the pairwise correlations of the alternate qubits, including entanglement and discord with its geometric, in the qubits A and C , one traces out the qubits B and D , and then the reduced density matrix $\rho^{AC}(t)$ is given by

$$
\rho^{AC}(t) = x|00\rangle\langle00| + w|00\rangle\langle11| + w^*|11\rangle\langle00| + y(|01\rangle)
$$

$$
\times \langle01| + |10\rangle\langle10|) + d(|01\rangle\langle10| + |10\rangle\langle01|)
$$

$$
+ z|11\rangle\langle11|,
$$
 (12)

with the abbreviation

$$
x = \sin^2 \theta + \frac{1}{8} \cos^2 \theta \left(3 + \cos 4\sqrt{2}Jt - 4\cos 2\sqrt{2}Jt \right),
$$

\n
$$
y = d = \frac{1}{8} \cos^2 \theta \left(1 - \cos 4\sqrt{2}Jt \right),
$$

\n
$$
w = \frac{1}{4} \left(\cos 2\sqrt{2}Jt + 1 \right) \sin 2\theta e^{4itB},
$$

\n
$$
z = \frac{1}{8} \cos^2 \theta \left(3 + \cos 4\sqrt{2}Jt + 4\cos 2\sqrt{2}Jt \right).
$$

From Eqs. (10) and (12), one finds that the reduced density matrices $\rho^{AB}(t)$ and $\rho^{AC}(t)$ have X-form. Such X-states occur in many contexts and include pure Bell states as well as Werner mixed states. It is straightforward to calculate the analytic expression of GMQD for the density matrix (10) or (12):

$$
D_A^g(\rho^{AB}) = \frac{1}{4} [8(|w|^2 + |d|^2) + k_3 - \max\{k_1, k_2, k_3\}],
$$
 (13)

where $k_1 = 2(|d_1 - |w_1|^2, \quad k_2 = 2(|d_1 + |w_1|)$ and $k_3 = 2(x - y)^2 + 2(y - z)^2$ are the eigenvalues of the matrix K. The analytic form of the QD for the density matrix Eq. (10), was recently calculated in Ref. [\[20\]](#page-6-0). Where, this solution provides us a simple analytic expression of quantum discord for a subclass of the X-structured density matrix. Therefore, the analytic expression for the quantum discord can be calculated as [\[19\]](#page-6-0):

$$
D(\rho^{AB}) = S(\rho^A) + S(\rho^{AB})
$$

-
$$
-\max\left[x\log_2\left(\frac{x}{x+y}\right) + y\log_2\left(\frac{y}{y+x}\right) + z\log_2\left(\frac{z}{z+y}\right)\right)
$$

+
$$
y\log_2\left(\frac{y}{y+z}\right), \sum_{i=+,-} v_i\log_2 v_i\right],
$$
(14)

where $v_{\pm} = \frac{1}{2} (1 +$ fifififififififififififififififi $\frac{1}{\sqrt{2}}$ $(x-z)^2+4(|w|+|d|)^2$ $\sqrt{2}$. It is easy to see that for this special case, the condition $S(\rho^A) = S(\rho^B)$ is satisfied and therefore the measurement performed on the subsytem A or B is irrespective [\[20\]](#page-6-0). It is easy to examine that the time evolution of quantum correlations are independent of the uniform magnetic field B.

Figs. 1–3, display the dynamics of GMQD, QD and QE as a function of scaled time $\tau = Jt$ for $\rho^{AB}(t)$ and $\rho^{AC}(t)$. When the initial states of the nearest neighbor qubits are maximally entangled state, $\theta = \frac{\pi}{4}$, the results are given in Fig. 1a and b for the two cases. As seen from Fig. 1a, GMQD, QD and QE of $\rho^{AB}(t)$ oscillate with scaled time τ and have the same behavior. But the values of QD are always greater than those of GMQD and QE, which approximately have the same values. Therefore, QD, GMQD and QE for the nearest neighbor qubits give almost the same information. But, for the alternate qubits (see Fig. 1b), QD and QE approximately have the same behavior and vanish at some time intervals. But, GMQD shows local maxima at the same time intervals. From Fig. 1a and b, one can easily find that the gradual vanishing of both QD and QE is exhibited for the alternate qubits AC , but it is not present for the nearest neighbor qubits AB , though the initial state of qubits AB in case(1) takes the same form as that of qubits AC in case(2).

If the degree of entanglement of the initial states of the qubits is weakened by putting $\theta = \frac{\pi}{6}$, the results are given in Fig. 2a and b for the two cases. From these figures, one finds that the correlations of the nearest neighbor qubits AB , which is resulted from GMQD, QD and QE, approximately are the same, but however with decreased values than the previous case. But the behavior of these correlations is different for the alternate qubits AC . Where QE can fall abruptly to zero and will remain to be zero for a period of time, which is called entanglement sudden death [\[13\]](#page-5-0) and several investigations have focused on this subject [\[14\]](#page-5-0). But QD decays continuously with respect to time even it tend to zero and then gradually evolves to its maximum values. This means that QD does not shows a phenomenon of sudden death. Under this condition, GMQD appears at the same death intervals of QD and QE and reaches a maximum values when the QD and QE vanish. Therefore, quantum correlations differ when the qubits state is initially in weak entangled state.

Figure 1 Time evolutions of the quantum discord (dash plots), geometric measure of QD (dash-dot plots) and negativity (sold plots) for $\rho^{AB}(t)$ in (a) and $\rho^{AC}(t)$ in (b).

Figure 2 The same as in Fig. 1 but $\theta = \frac{\pi}{6}$.

Figure 3 The same as in [Fig. 1](#page-3-0) but $\theta = \frac{\pi}{12}$.

Figure 4 Quantum discord for $\rho^{AB}(t)$ in (a) and $\rho^{AC}(t)$ in (b).

If the degree of entanglement of the initial states of the qubits is very weak by putting $\theta = \frac{\pi}{12}$, the results are given in Fig. 3a and b for $\rho^{AB}(t)$ and $\rho^{AC}(t)$. For $\theta = \frac{\pi}{12}$, one finds that phenomenon of sudden death appearers clearly for $\rho^{AB}(t)$, but GMOD, OD decreases as the angle θ decreases Therefore, appearance of sudden death of entanglement and decreasing of both GMQD and QD depend on the degree of entanglement of the initial state, the smaller the degree of the entanglement in the initial state, the longer the state will stay in the disentangled state. From Fig. 3a and b, one has found that for the initial state case(1), the appearance for sudden death entanglement is only for the smaller θ for which QE is weaker when $\tau = 0$. However, the sudden death always happens no matter how strong the entanglement of the initial state of case(2) is, which can be seen from Fig. 3b. By comparing Fig. 3a with Fig. 3b, one can observe that the state case(2) has longer period of time for the disentanglement than that of state case(1). Also GMQD and QD of nearest qubits approximately have the same behavior, but for alternate qubits AC they are different. Where QD decays continuously with respective to time until it tends to zero and will remain zero for a period of time. At same time of quantum discord death, GMQD grows with time and even reaches its local maximum value (see Fig. 3b). Therefore, the pairwise correlations in alternate qubits affect the degree of entanglement of the initial

state stronger than that for strongly interacting nearest qubits. Thus, it seems that GMQD is more robust than QD and QE to describe pairwise quantum correlations with nonzero values which offers a valuable resource for quantum computation.

To evidently see the effect of the degree of entanglement of the initial state on resulted pairwise correlations from GMQD and QD, the dynamics of GMQD and QD as a function of θ and QD, the dynamics of SINQD and QD as a rancelor of θ are introduced with $\theta \in [0, \frac{\pi}{2}]$ in Fig. 4a and b and [Fig. 5](#page-5-0)a and b. At $\theta = 0$ (disentangled initial states), for nearest qubits, one notes that the dynamics of quantum discord is constant and equal to zero, but the geometric measure of quantum discord oscillates with time. This is noted for alternate qubits AC , but the period of GMQD is smaller than that for nearest qubits. But, at $\theta = \frac{\pi}{2}$ there is a preservation for a long time in both quantum discord(at zero value) and geometric measure of quantum discord (at constant value). Therefore, in the interval of $\theta \in [0, \frac{\pi}{2}]$, one notes that the dynamics of geometric measure of quantum discord and quantum discord differ and they are sensitive for any change in θ .

4. Conclusions

The dynamic evolution of pairwise quantum correlations, including GMQD, QD and QE, is shown in the four-qubit Heisenberg XX spin chain. For some initial states, the phe-

Figure 5 Geometric measure of quantum discord for $\rho^{AB}(t)$ in (a) and $\rho^{AC}(t)$ in (b).

nomenon of entanglement sudden death occurs in the time evolution of entanglement. The pairwise correlations in alternate qubits affect the degree of entanglement of the initial state stronger than that for strongly interacting nearest qubits. It is found that GMQD is more robust than QD and QE to describe pairwise quantum correlations with nonzero values which offers a valuable resource for quantum computation. A comparison of the dynamics of geometric measure of quantum discord with quantum discord for $\theta \in [0, \frac{\pi}{2}]$ is made. It is found that the dynamics of GMQD and QD differ and they are sensitive to any change in the degree of entanglement of the initial state.

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