Thermal quantum discord of one-dimensional in three-qubit spin chain with nearest-neighbor and next-nearest neighbor and Dzyaloshinskii-Moriya interaction

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Abstract: We have studied thermal quantum discord in three-qubit Ising model with nearest-neighbor and next-nearest neighbor and Dzyaloshinskii-Moriya (DM) interaction. Lack of inversion symmetry in the presence of the DM interaction stimulated us to study quantum correlations of the three-qubit through symmetric (SY) and non-symmetric (NYS) ways for both ferromagnetic (FM) and antiferromagnetic (AF) Cases. We found that the discord with increasing the temperature $T$, at first the quantum correlations in the system increase, smoothly reach the maximum, and then turn again into zero.

Key words: Ising model, quantum discord, qubit, Dzyaloshinskii-Moriya interaction

Introduction

Quantum discord (QD) is a more general measure of quantum correlation than entanglement (Modi, Brodutch, Cable, Paterik, Vedral, 2012). The computation of discord is mostly confined to two-qubit systems for which an analytical formula (Ali, Rau, Alber, 2010) is available for the arbitrary X density matrices (Yu, Eberly, 2007. Rau, 2009.). The notion quantum discord has been introduced in the quantum information theory by Zurek (2000). Discord was regarded as “a measure of a violation of classicality of a joint state of two quantum subsystems” (Zurek, 2000). However later its initial definition undergone some changes. In 2001, Henderson and Vedral and then independent of them Ollivier and Zurek in their papers (Henderson, Vedral, 2001. Ollivier, Zurek, 2001. Vedral, 2003. Zurek, 2003.) performed analysis of every possible correlations $\mathcal{L}$ in a bipartite system and suggested the ways to extract from them, on the one hand, the purely classical parts $C$ and, on the other hand, only the quantum contribution $QD$. The quantum excess of correlations, $QD = \mathcal{L} - C$, has been called “discord” in the modern understanding of this term. The authors of above papers established also that the quantum correlation can be non zero even in separable (but mixed) states. In other words, quantum correlations are not exhausted by entanglement (E). Entanglement, which can relate the different parts of a system even when there are no interactions between the parts (the Einstein-Podolsky-Rosen effect), is only a special kind of quantum correlations. Since the 80–90s of past century the entanglement was considered as a fundamental resource for quantum information processing, teleportation, cryptography, metrology, and other tasks in quantum technology (Nielsen, Chung, 2000. Horodecki, Horodecki, Horodecki, Horodecki, 2009). It is remarkable that quantum discord can also lead to a speedup over classical computation and lead even without containing much entanglement (Datta, Shaji, Caves, 2008. Lanyon, Barbieri, Almeida, White, 2008. Dillenschneider, 2008. Sarandy, 2009. Verlang, Trippe, Ribeiro, Rigolin, 2010. Ferraro, Aolita, Cavalcanti, Cucchietti, Ac’ in, 2010.). This important property of discord evoked extremely great interest to the new kind of correlations. Achieved up to now results on the theory and applications of quantum discord are given in the recent reviews (Celeri, Maziero, Serra, 2011. Modi, Brodutch, Cable, Paterik, Vedral, 2012). Recently, C. Yi-Xin and et al (Yi-Xin, Zhi, 2010.) have studied thermal QD (TQD) of a two-qubit anisotropic XXZ model with DM interaction. They have reported an exotic opposite behavior of TQD versus entanglement for both Dzand Dx tunable parameters. In a very recent work, L.J. Tian (Tian, Yanand, Qin, 2011.) have studied the pair wise QD in a three-qubit XXZ model with
DM interaction. The Hamiltonian considered by them satisfies periodic boundary condition. The three-qubit system considered in this paper has the structure of an open chain and the quantum correlation features turn out to be different from the ring structure. In a multi-qubit system it is intriguing to define monogamy of entanglement. If two qubits are fully entangled then they cannot be correlated with other(Bennett, Divincenzo, Smolin, Wootters,1996.). For three-qubit system it can be possible to focus on two types of entanglement: pair wise, i.e. between two qubits and three-party entanglement involving all the three qubits. The goal of this paper is to study the behavior of thermal quantum discord in Ising model with added Dzyaloshinskii Morriya interaction and exchange coupling. A lack of inversion symmetry make ones, who works in the strongly correlated systems, to consider an extra exchange coupling between spins in the magnetic materials than the usual and well known isotropic exchange JSi.Sj . In this respect, Dzyaloshinskii has shown (Dzyaloshinsky, 1958.) that an antisymmetric exchange should be considered in these magnetic materials. Later, Moriya has shown(Moriya,1960.) that inclusion of spin orbit coupling on magnetic ions in 1st and 2nd order leads to antisymmetric and anisotropic exchange respectively. This interaction is, however, rather difficult to handle analytically, but it is one of the agents responsible for magnetic frustration. Generally the DM interaction for two spin can be written as \( \vec{D} \times \vec{S} \).

Since this interaction may induce spiral spin arrangements in the ground state (Sudan, Luscher, Lauchli,2009.), it is closely involved with ferroelectricity in multi ferroic spin chains1(Seki, Yamasaki, Soda, Matsuura, Hirotaand, Tokura,2008. Huvonen, Nagel, Room, Choi, Zhang, Park, Cheong 2009. Besides, the DM interaction plays an important role in explaining the electron spin resonance experiments in some one-dimensional antiferromagnets (Oshikawa, Affleck ,1999. Affleck, Oshikawa, 1999.). Moreover, the DM interaction modifies the dynamic properties(Derzhko, Verkholyak, Krokhmalskii, Buttner,2006.) and quantum entanglement(Kargarian, Jafari,. Langari,2009.) of spin chains(Garate, Affleck,2010.) . Behaviors of quantum and classical correlations in spin chain with DM interaction also was discussed(Liu, Shao, Li, Zou J, Wu, 2011.). In the present paper, we are interested to study the spin-1/2 Ising model with added DM interaction from quantum correlation point of view. The Hamiltonian is given by

\[
H = J_1 \sum_{j=1}^{N} S_j^z S_{j+1}^z + J_2 \sum_{j=1}^{N} S_j^z S_{j+2}^z + D \sum_{j=1}^{N} \vec{S}_j \times \vec{S}_{j+1} \tag{1}
\]

where \( \vec{S}_j \) is spin-1/2 operator on the j-th site, \( J_1, J_2 \) denote the coupling constant and \( \vec{D} \) denotes the DM interaction vector.

**Quantum Discord**

In order to quantify quantum discord, Ollivier and Zurek(Ollivier, Zurek,2001.) suggested the use of von Neumann type measurements which consist of one-dimensional projectors that sum to the identity operator. Let the projection operators \( \{B_k\} \) describe a von Neumann measurement for subsystem \( B \) only, then the conditional density operator \( \rho_k \) associated with the measurement result \( k \) is

\[
\rho_k = \frac{1}{p_k}(I \otimes B_k)\rho(I \otimes B_k), \tag{2}
\]

where the probability \( p_k \) equals \( \text{tr}((I \otimes B_k)\rho(I \otimes B_k)) \). The quantum conditional entropy with respect to this measurement is given by (Luo,2008.)

\[
S(\rho|\{B_k\}) := \sum_k p_k S(\rho_k) \tag{3}
\]

and the associated quantum mutual information of this measurement is defined as

\[
\mathcal{L}(\rho|\{B_k\}) := S(\rho A) - S(\rho|\{B_k\}) \tag{4}
\]

A measure of the resulting classical correlations is provided(Ollivier, Zurek,2001.Luo,2008. Li, Luo,2007.) by

\[
C(\rho) := \sup_{\{B_k\}} \mathcal{L}(\rho|\{B_k\}) \tag{5}
\]
The obstacle to computing quantum discord lies in this complicated maximization procedure for calculating the classical correlation because the maximization is to be done over all possible von Neumann measurements of $B$. Once $C$ is in hand, quantum discord is simply obtained by subtracting it from the quantum mutual information $Q(\rho) := \mathcal{L}(\rho) - C(\rho)$ (6)

In this section, we limit our discussion to initially prepared arbitrary two-qubit $X$ states. The density matrix of a two qubit $X$ state in the representation spanned by the two-qubit product states $\{|1\rangle = |0\rangle \otimes |0\rangle, |2\rangle = |0\rangle \otimes |1\rangle, |3\rangle = |1\rangle \otimes |0\rangle, |4\rangle = |1\rangle \otimes |1\rangle\}$ is of the general form

\[
\rho_{x} = \begin{pmatrix}
\rho_{11} & 0 & 0 & \rho_{14} \\
0 & \rho_{22} & \rho_{23} & 0 \\
0 & \rho_{32} & \rho_{33} & 0 \\
\rho_{41} & 0 & 0 & \rho_{44}
\end{pmatrix}
\]

that is, $\rho_{12} = \rho_{13} = \rho_{24} = \rho_{34} = 0$. The eigenvalues of the density matrix $\rho_X$ in Eq. (7) are given by

\[
\lambda_{1} = \frac{1}{2} \left[ (\rho_{11} + \rho_{44}) + \sqrt{(\rho_{11} - \rho_{44})^2 + 4|\rho_{14}|^2} \right],
\lambda_{2} = \frac{1}{2} \left[ (\rho_{11} + \rho_{44}) - \sqrt{(\rho_{11} - \rho_{44})^2 + 4|\rho_{14}|^2} \right],
\lambda_{3} = \frac{1}{2} \left[ (\rho_{22} + \rho_{33}) - \sqrt{(\rho_{22} - \rho_{33})^2 + 4|\rho_{23}|^2} \right],
\lambda_{4} = \frac{1}{2} \left[ (\rho_{22} + \rho_{33}) + \sqrt{(\rho_{22} - \rho_{33})^2 + 4|\rho_{23}|^2} \right].
\]

The quantum mutual information is given as

\[
\mathcal{L}(\rho_{x}) = S(\rho^{A}_{x}) + S(\rho^{B}_{x}) + \sum_{i=1}^{4} \lambda_{i} \log_{2} \lambda_{i}
\]

where $\rho^{A}_{x}$ and $\rho^{B}_{x}$ are the marginal states of $\rho_{x}$, an

\[
S(\rho^{A}_{x}) = -[(\rho_{11} + \rho_{22}) \log_{2}(\rho_{11} + \rho_{22}) + (\rho_{33} + \rho_{44}) \log_{2}(\rho_{33} + \rho_{44})]
\]

\[
S(\rho^{B}_{x}) = -[(\rho_{11} + \rho_{22}) \log_{2}(\rho_{11} + \rho_{22}) + (\rho_{33} + \rho_{44}) \log_{2}(\rho_{22} + \rho_{44})]
\]

After computing the quantum mutual information, we need next to compute the classical correlation $C(\rho X)$. We consider projective measurements for subsystem $B$ (the projective measurements for subsystem $A$ give the same results if we restrict to either $\rho_{11} = \rho_{44}$ or $\rho_{22} = \rho_{33}$). We follow the procedure of (Luo,2008.) except that we are considering a class of states that is more general than the three-parameter family of that study. It is known that any von Neumann measurement for subsystem $B$ can be written as Ref. (Luo,2008.)

\[
B = V \Pi_{i} V^{\dagger}, i = 0, 1, (11)
\]

where $\Pi_{i} = |i\rangle \langle i|$ is the projector for subsystem $B$ along the computational base $\{|i\rangle$ and $V = t I + i \vec{y} \cdot \vec{\sigma}$, $V \in SU(2)$, $t, y_{1}, y_{2}, y_{3} \in IR$ and $t^{2} + y_{1}^{2} + y_{2}^{2} + y_{3}^{2} = 1$. After the measurement, we have the ensemble $\{P_{i}, \rho_{i}\}$ the classical correlation is therefore given by

\[
C(\rho_{x}) = \sup_{B[i]}[\mathcal{L}(\rho_{x}[\{B_{i}\}])](12)
\]

\[
= S(\rho^{A}_{x}) - \min_{B[i]}[S(\rho_{x}[\{B_{i}\}])]
\]

Where $S(\rho_{x}[\{B_{i}\}])$ is the quantum conditional entropy

\[
S(\rho_{x}[\{B_{i}\}]) = R_{0} S(\rho_{0}) + R_{1} S(\rho_{1})(14)
\]

by the parameter transformation

\[
k = t^{2} + y_{3}^{2}, \quad l = y_{1}^{2} + y_{2}^{2} (15)
\]

\[
m = (ty_{1} + y_{2}y_{3})^{2}, \quad n = (ty_{2} - y_{1}y_{3})(ty_{1} + y_{2}y_{3})
\]

\[
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\]
With \( k + l = 1 \), \( k \in [0, 1] \), \( m \in \left[ -\frac{1}{b}, \frac{1}{b} \right] \). Then according to Ref. (Wootters, 1998), the minimum of Eq (19) lies at \( k = l = \frac{1}{2} \) or at the end points \( k = 0 \) or \( k = 1 \) and using theorem defined in Ref. (Vidal, Werner, 2002.), the classical correlation of \( \rho_x \) is given by

\[
C(\rho_x) = S(\rho_x^A) - \min\{S_1, S_2\}(16)
\]

where \( S_1, S_2, \) and \( S_2 \) are defined by Eq. (16), (17) and (18) in Ref. (Garate, Affleck, 2010. Ali, Rau, Alber, 2010.).

**Hamiltonian And Densitymatrix**

We consider the Hamiltonian (Eq.(1)) for three qubit then reduces to

\[
H = J_1(S_x^1S_x^2 + S_z^1S_z^2) + J_2(S_y^2S_z^2) + D(S_x^0S_y^0 - S_x^0S_z^0) + D(S_x^2S_y^2 - S_x^2S_z^2)(17)
\]

Where \( S_x^1, S_y^2 \) and \( S_z^2 \) have \( z \)-component of spin particles and we choose \( \hat{D} = D \hat{z} \). Hamiltonian matrix form for Eq.(17) as follows:

\[
H = \frac{1}{4}\begin{bmatrix}
2J_1 + J_2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -J_2 & 2iD & 0 & 0 & 0 & 0 & 0 \\
0 & -2iD & -J_2 + J_2 & 0 & 2iD & 0 & 0 & 0 \\
0 & 0 & 0 & -J_2 & 0 & 2iD & 0 & 0 \\
0 & 0 & 0 & -2iD & 0 & -J_2 & 0 & 0 \\
0 & 0 & 0 & 0 & -2iD & 0 & -J_2 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 2J_1 + J_2 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 2J_1 + J_2
\end{bmatrix}(18)
\]

In what follows, we focus on thermal entanglement behavior of three qubits in the SY and NSY ways. The thermal elements of the density matrix operator \( \rho(T) = \exp(-\beta H) \), where \( Z = \text{Tr}(\exp(-\beta H)) \) is the partition function and \( \beta = 1/kT \).

**Finite-Temperature Behavior**

In this section, we study quantum correlation of three qubit with open boundary condition in two in equivalent SY and NSY pair wise ways. Let’s labeling the three qubit as 1, 2, 3 sequentially. The SY reduced density matrix \( \rho_{\text{SY}} \) is defined as \( \rho_{\text{SY}} = \text{Tr}_2(\rho) \), where \( \rho \) is the density matrix of three-qubit and the NSY reduced matrix is \( \rho_{\text{NSY}} = \text{Tr}_3(\rho) \) for SY and NSY ways are presented in sequence. In the NSY case \( \rho_{\text{NSY}}(T) \) is given as

\[
\rho_{11} = \rho_{44} = \frac{1}{Z} \left[ \frac{1}{2} e^{-\beta E_1} + e^{-\beta E_2} + \frac{1}{b^2 + 2} e^{-\beta E_5} + \frac{1}{a^2 + 2} e^{-\beta E_7} \right]
\]

\[
\rho_{22} = \rho_{33} = \frac{1}{Z} \left[ \frac{1}{2} e^{-\beta E_1} + \frac{2b^2}{b^2 + 2} e^{-\beta E_5} + \frac{2a^2}{a^2 + 2} e^{-\beta E_7} \right]
\]

\[
\rho_{23} = (\rho_{32})^* = -\frac{2i}{Z} \left[ \frac{b}{b^2 + 2} e^{-\beta E_5} + \frac{a}{a^2 + 2} e^{-\beta E_7} \right](19)
\]

and in the SY case \( \rho_{\text{SY}}(T) \) is written as

\[
\rho_{11} = \rho_{44} = \frac{1}{Z} \left[ e^{-\beta E_1} + \frac{b^2}{b^2 + 2} e^{-\beta E_5} + \frac{a^2}{a^2 + 2} e^{-\beta E_7} \right]
\]

\[
\rho_{22} = \rho_{33} = \frac{1}{Z} \left[ e^{-\beta E_1} + \frac{2}{b^2 + 2} e^{-\beta E_5} + \frac{2}{a^2 + 2} e^{-\beta E_7} \right]
\]
\[ \rho_{z3} = \rho_{32} = \frac{1}{Z} \left[ e^{-\beta E_1} - \frac{2}{b^2 + 2} e^{-\beta E_5} - \frac{2}{a^2 + 2} e^{-\beta E_7} \right] (20) \]

where \( Z = 2 \exp \left( \frac{J_z}{4T} \right) + 4 \exp \left( \frac{J_1}{4T} \right) \cos \hbar \left( \sqrt{\left( \frac{J_z}{4} \right)^2 + 8D^2} / 4T \right) + 2 \exp \left( - \frac{J_1}{2T} \right) \exp \left( - \frac{J_z}{2T} \right) \exp \left( \frac{\left( J_1 - J_z \right)^2}{2D} \right) \),

\[ b = \frac{\left( J_1 - J_z \right)^2}{2D}, \quad q = \sqrt{\left( J_1 - J_z \right)^2 + 8D^2}. \]

The eigenvalues of Eq(1) are given as

\[ E_1 = E_2 = - \frac{J_z}{4}, \quad E_3 = E_4 = \frac{J_1}{2} + \frac{J_z}{4}, \]

\[ E_5 = E_6 = - \frac{1}{4} (J_1 + q), \quad E_7 = E_8 = - \frac{1}{4} (J_1 - q) (21) \]

In what follows, we focus on thermal quantum correlation behavior of three qubit in the SY and NSY ways. In the low temperatures, spins live in states which have both quantum correlations and thermal fluctuations. When the temperature grows, the role of thermal fluctuations exceeds quantum ones.

Figure 1. The thermal quantum discord thought symmetric way case for \( J_z = 2 J_1 \) and different DM as function of temperature

Figure 2. The thermal quantum discord thought non-symmetric way case for \( J_z = 2 J_1 \) and different DM as function of temperature
In the AF and FM case in Fig(1,2) with \( \frac{J_2}{J_1} = 2 \) TQD at zero temperature is not zero for all values of DM interaction. When temperature increases from zero, TQD remains constant and resists against the thermal fluctuations up to a critical temperature \( T \). It is clear that the \( T \) depends on the strength of DM interaction and in principle increases by increasing \( D \). in Fig(3,4) with \( \frac{J_2}{J_1} = 1 \) we have plotted TQD through SY and NSY ways for Ferro-Anti(magnetic) cases as function of temperature for four different values of DM interaction. As soon as the DM interaction turn on, a significant quantum correlations creates in the NSY way. By increasing the DM interaction QD in the SY way decreases which is in sharp contrast to the SY way. In addition, the QD in the NSY way is stronger than the SY way in all values of the DM interaction.

**CONCLUSION**

To summarize, we have investigated the effect of a Dzyaloshinsky-Moriya (DM) and nearest neighbor and next nearest neighbor interaction on the thermal state QD of Ising spin-1/2 model through the SY and the NSY ways. We have calculated ground state QD through the SY and the NSY ways for FM and AF cases. Our calculations show that in both FM and AF cases through the SY and NSY ways, TQD shows the same qualitative behavior. The amount of TQD through the SY way is almost equal in both FM and AF cases and the same story also exists in the NSY way. However, the amount of TQD is different through the SY and the NSY ways, in which for low temperature the TQD_{NSY} is almost two times bigger than TQD_{SY}. This effect is because of the influence of coupling constant \( J \) and DM interaction which makes quantumness considerable. Finally, in all the considered cases, both SY and NSY show the same qualitative behavior and the higher DM interaction is the larger TQD.
ACKNOWLEDGMENT

N.Nikdel and M.R.Soltani thank to Dr.S.Mahdavifar for very helpful discussions.

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