Thermal and Magnetic Quantum Discord in Heisenberg models

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We investigate how quantum correlations (quantum discord (QD)) of a two-qubit one dimensional XYZ Heisenberg chain in thermal equilibrium depend on the temperature $T$ of the bath and also on an external magnetic field $B$. We show that the behavior of thermal QD differs in many unexpected ways from thermal entanglement. For example, we show situations where QD increases with $T$ when entanglement decreases, cases where QD increases with $T$ even in regions with zero entanglement, and that QD signals a quantum phase transition even at finite $T$. We also show that by properly tuning $B$ or the interaction between the qubits we get non-zero QD for any $T$ and we present a new effect not seen for entanglement, the “regrowth” of thermal QD.

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Introduction. Since the seminal work of John S. Bell [1], who brought to the realm of experimental Physics the ideas of Einstein, Podolsky, and Rosen [2] concerning the non-local aspects of Quantum Mechanics, it became clear that the constituents of some quantum composite systems possessed correlations among themselves unachievable in the classical world. Those states belong to the class of entangled states although not all entangled states possess stronger-than-classical correlations in the sense of violating Bell inequalities [3]. However, given a composite quantum state whose constituents are correlated, how can one tell the origin of the correlations? In other words, how can one divide the total correlation into a classical and a purely quantum one? This is particularly important for mixed states since their quantum correlations are many times hidden by their classical correlations. An answer to these questions is given by the quantum discord (QD), a measure of the quantumness of correlations introduced in Ref. [4]. QD is built on the fact that two classical equivalent ways of defining the mutual information turn out to be inequivalent in the quantum domain. In addition to its conceptual role, some recent results [5] suggest that QD and not entanglement may be responsible for the efficiency of a mixed state based quantum computer.

Due to its fundamental and practical significance we wish to investigate the amount of QD in a concrete system such as a pair of qubits (spin-1/2) within a solid at finite temperature, whose interaction is given by the Heisenberg model (XYZ model in general). Such Heisenberg models can describe fairly well the magnetic properties of real solids [6] and is well adapted to the study of the interplay of disorder and entanglement as well as of entanglement and quantum phase transitions [7]. We characterize the dependence of QD on the temperature and also on external magnetic fields applied to the qubits. We also compare the behavior of QD against the entanglement of formation (EoF) between the two qubits [8][10]. We obtain several interesting and novel results for the behavior of QD at non-zero $T$, many of them in contrast to the behavior of EoF. First, we show that QD can increase with temperature in the absence of external fields applied to the qubits. This is in sharp contrast to the behavior of EoF since one can show [10] that this effect never occurs without the presence of an external magnetic field. We also show that there exist regions where QD is different from zero while EoF is always zero, confirming a generic feature of QD [11]. In particular, we show that for the isotropic XXX model, both the ferromagnetic and anti-ferromagnetic Hamiltonians possess relatively high values of QD while EoF is absent for the ferromagnetic model [8]. These properties of QD have important practical consequences for the realization of a quantum computer at finite temperatures. Indeed, once it is established that what is at stake for the correct functioning of a quantum computer is the existence of a certain level of QD (just having non-null QD might not be enough since almost all states have QD [11]), we have shown that Heisenberg solids are better than previously thought as good candidates for the construction of a quantum computer at $T > 0$: for some parameter sets they have high values of QD while having no EoF at all. We also show that by properly adjusting the coupling constants [9] one can achieve any desired level of QD for any $T$. Finally, we show that for finite $T$ we observe the sudden-change of QD [12] as we change the coupling constant of the Hamiltonian and we show a new effect, namely the “regrowth” of the thermal QD with increasing $T$.

The thermalized Heisenberg system. The Hamiltonian of the XYZ model with an external magnetic field acting on both qubits is

$$ H = B(S_x^1 + S_x^2) + J_x S_x^1 S_x^2 + J_y S_y^1 S_y^2 + J_z S_z^1 S_z^2, \quad (1) $$

with $J_x$, $J_y$, and $J_z$ the coupling constants, $S_{x,y,z}^j = \sigma_{x,y,z}^j/2$, $\sigma_{x,y,z}^j$ the usual Pauli matrices acting on qubit $j$, and $B$ the external magnetic field. We have assumed $\hbar = 1$. The density matrix describing a system in equilibrium with a thermal reservoir at temperature $T$ (canonical ensemble) is $\rho = \exp(-H/kT)/Z$, where $Z$ is the partition function.

$$ Z = \text{Tr} \exp(-H/kT). $$

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where $f = I$ is Boltzmann’s constant. Therefore, Eq. $[1]$ leads to the following thermal state in the standard basis

$$\rho = \frac{1}{Z} \begin{pmatrix} A_{11} & 0 & 0 & A_{12} \\ 0 & B_{11} & B_{12} & 0 \\ 0 & B_{12} & B_{11} & 0 \\ A_{12} & 0 & 0 & A_{22} \end{pmatrix}. \quad (2)$$

Here $A_{11} = e^{-\alpha} \left( \cosh(\beta) - 4B \sinh(\beta)/\eta \right)$, $A_{12} = -\Delta e^{-\alpha} \sinh(\beta)/\eta$, $A_{22} = e^{-\alpha} \left( \cosh(\beta) + 4B \sinh(\beta)/\eta \right)$, $B_{11} = e^{\alpha} \cosh(\gamma)$, $B_{12} = -e^{\alpha} \sinh(\gamma)$, and $Z = 2 \left( \exp(-\alpha) \cosh(\beta) + \exp(\alpha) \cosh(\gamma) \right)$, where $\Delta = J_x - J_y$, $\Sigma = J_x + J_y$, $\eta = \sqrt{\Delta^2 + 16B^2}$, $\alpha = J_z/(4kT)$, $\beta = \eta/(4kT)$, and $\gamma = \Sigma/(4kT)$.

**Entanglement.** For a pair of qubits there exists an analytical expression to quantify its amount of entanglement called Entanglement of Formation (EoF) [13]. Given the density matrix $\rho$ describing thermalized two qubits, EoF is the average entanglement of the pure state decomposition of $\rho$, minimized over all possible decompositions, $EoF(\rho) = \min \sum_j p_j H(\phi_j)$, where $\sum_j p_j = 1$, $0 < p_j \leq 1$, and $\rho = \sum_j p_j \ketbra{\phi_j}{\phi_j}$. $H(\phi)$ is the entanglement of the pure state $\ket{\phi_j}$ [14]. For a pair of qubits Wootters [13] has shown that EoF is a monotonic increasing function of the concurrence $C$ (an entanglement monotone), $EoF = -f(C) \log_2 f(C) - (1-f(C)) \log_2 (1-f(C))$, where $f(C) = (1+\sqrt{1-C^2})/2$. The concurrence is simply [15] $C = \max \{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4 \}$, where $\lambda_1, \lambda_2, \lambda_3,$ and $\lambda_4$ are the square roots of the eigenvalues, in decreasing order, of the matrix $\rho = \rho^*$. Here $\rho^*$ is the time reversed matrix $\rho^* = (\sigma_y^x \otimes \sigma_y^y) \rho^* (\sigma_y^x \otimes \sigma_y^y)$. The symbol $\rho^*$ means complex conjugation of the matrix $\rho$ in the standard basis $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$. For a density matrix in the X-form above $C = 2\max \{0, \lambda_1, \lambda_2 \}/Z$, with $\lambda_1 = |B_{12}| - \sqrt{A_{11}A_{22}}$ and $\lambda_2 = |A_{12}| - B_{11}$.

**Quantum Discord.** In classical information theory (CIT) the total correlation between two systems (two sets of random variables) $A$ and $B$ described by a joint distribution probability $p(A,B)$ is given by the mutual information (MI),

$$I(A,B) = H(A) + H(B) - H(A|B), \quad (3)$$

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 to systems $A, B$, or to the joint system $AB$. Using Bayes’s rule we may write MI as

$$I(A,B) = H(A) - H(A|B), \quad (4)$$

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 [3]. The first quantum extension of MI, denoted by $I(\rho)$, is obtained directly replacing the Shannon entropy in $I(A,B)$ 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 $I(A,B)$ 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 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 $S(\rho \mid \{\Pi_j\}) = \sum_j p_j S(\rho_j)$ and, consequently, the second quantum extension of the classical MI as $\mathcal{I}(\rho \mid \{\Pi_j\}) = \sum \mathcal{J}(\rho \mid \{\Pi_j\})$, where $\mathcal{J}(\rho \mid \{\Pi_j\})$ depends on the choice of $\{\Pi_j\}$. Henderson and Vedral [16] have shown that the maximum of $\mathcal{J}(\rho \mid \{\Pi_j\})$ with respect to $\{\Pi_j\}$ can be interpreted as a measure of classical correlations. Therefore, the difference between the total correlations $I(\rho)$ and the classical correlations $\mathcal{Q}(\rho) = \sup_{\{\Pi_j\}} \mathcal{J}(\rho \mid \{\Pi_j\})$ is defined as

$$D(\rho) = I(\rho) - \mathcal{Q}(\rho), \quad (5)$$

giving, finally, a measure of quantum correlations [4] called quantum discord (QD). For pure states QD reduces to entropy of entanglement [14], highlighting that in this case all correlations come from entanglement. However, it is possible to find separable (not-entangled) mixed states with nonzero QD [4], 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 only locally [17]. For more insights into QD the reader is referred to [18]. In this work, when $B = 0$ the density operator $\rho$ is such that QD is given by an analytical expression obtained in [19]. When $B \neq 0$ we computed QD numerically [20].

**Results.** Let us start presenting the important result that QD increases with temperature without an external field acting on the qubits $(B = 0)$. This effect can be clearly seen when we deal with the XXZ model ($J_x = J_y = J$ and $J_z \neq 0$). Looking at Fig. 1, panels $a$ and $b$, we see that this effect happens for several configurations of coupling constants being, thus, dense around this region. We should note that such behavior can be found for other models than the XXZ as well. As we mentioned before, in the absence of external fields [10] such increase with T only occurs for QD and not for EoF. Note also that QD starts at zero and then increases with T. In particular, for the set of coupling constants shown in Fig. 1, the EoF is always zero [10]. Furthermore, one can show that the classical correlation decreases when QD increases (See Fig. 1c). We have, therefore, a genuine
a mixed state density operator in the limit $J = 0$. (a) Here $kT \to 0$ while $J < 0$, achieving the value zero at $\Delta = 7$, and various values of $kT$. For the dotted/black line $kT = 0.01$, dashed/red line $kT = 0.1$, dash-dotted/blue line $kT = 0.6$, and solid/orange line $kT = 1$.

When the magnetic field $B$ is not zero we first analyze what happens to the Ising model ($J_x = J$ and $J_y = J_z = 0$). Looking at Fig. 4 we see that for the regions where EoF is zero QD is negligible. However, as well as with EoF, QD initially increases as we increase the value of $B$, going to zero with increasing field. This is
true since the density operator is separable state when . On the other hand, as we will shortly see, this is not a general result. The behavior of QD and EoF can be quite different from each other if we work with another model.

For the XY model ( and ) with a transverse magnetic field ( ), for example, QD behaves in quite different (and interesting) ways from what we have seen for the Ising model. Also, for the XY model we see a new effect, the regrowth of QD. Contrary to the behavior of EoF, where we see its sudden death and then a revival, for QD there is no sudden death. See Fig. for QD decreases with , retaining appreciable values and then after a critical temperature , it starts increasing again. This is what we call regrowth. Note that in the behavior of EoF we never see a regrowth. Indeed, EoF decreases after decreasing with only after reaching the value zero (sudden death).

Moreover, looking at (a) and (c) of Fig. we see that QD becomes non-null before the appearance of EoF. Also, QD continues to be non-null after EoF disappears. If we now analyze (b) and (d) of Fig. we notice that we have for all three curves regimes in which QD increases while EoF decreases. This is a quite remarkable behavior since the decrease of a certain quantum aspect (entanglement) is simultaneous to the increase of another quantum aspect (quantum correlations), illustrating clearly the distinctive aspects of these two concepts.

**Conclusions.** We examined the behavior of the quantum discord (QD) for a pair of qubits described by the Heisenberg model in thermal equilibrium with a reservoir at temperature . By changing the temperature and also by applying an external magnetic field we observed several remarkable effects for QD, many of them in sharp contrast to the behavior observed for the entanglement of formation (EoF) between the two qubits. We found that for the XXX model QD signals a quantum phase transition for finite while EoF does not. Also, we observed regimes where QD increases while EoF decreases with . Moreover, and surprisingly, we showed that for the XXZ model there exist regions in the parameter space in which EoF is zero while the classical correlation decreases and only QD increases with . Finally, we also observed a new effect for QD which we called regrowth: QD decreases with and starts increasing again after reaching a minimum different from zero.

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