Non-classical correlations in a Heisenberg spin model with Heitler–London approach

Youssef Khedif[1] · **Saeed Haddadi[2,3]** · **Mohammed Daoud[4,5]** ·
Hazhir Dolatkhah[6] · **Mohammad Reza Pourkarimi[7]**

Abstract

The isotropic Heisenberg two-spin-1/2 model in the XXX configuration under an external transverse nonuniform magnetic field is considered at thermal equilibrium. In the context of the Heitler–London approach, the variation of the spin–spin exchange coupling strength in terms of the position is adopted. The effects of the inter-spin relative coupling distance r and nonuniform magnetic field on the thermal evolution of quantum correlations are studied in detail. By tuning the coupling distance r, temperature T and nonuniform magnetic field B, quantum correlations can be scaled in the bipartite system. Astonishingly, we find the long sustainable behavior of geometric quantum discord in comparison with entanglement over the coupling distance r. Moreover, we show the existence of separable quantum states with nonzero quantum correlations in terms of trace discord. Besides, the quantum correlations shared between the considered bipartite system parts are only the entanglement type for a fixed temperature and suitable strong nonuniform magnetic field values. An entangled-unentangled phase transition at $T = 0.1$ with threshold relative distance r_f can be detected by the entanglement behavior in terms of B and r. A kind of correspondence between thermal entanglement and thermal non-classical correlations for a strong value of B can be

✉ Youssef Khedif
    youssef.khedif@gmail.com

[1] Laboratory of High Energy and Condensed Matter Physics, Department of Physics, Faculty of Sciences Aïn Chock, University Hassan II, P.O. Box 5366, 20100 Maarif, Casablanca, Morocco

[2] Faculty of Physics, Semnan University, P.O. Box 35195-363, Semnan, Iran

[3] Saeed's Quantum Information Group, P.O. Box 19395-0560, Tehran, Iran

[4] Department of Physics, Faculty of Sciences, University Ibn Tofail, Kenitra, Morocco

[5] Abdus Salam International Centre for Theoretical Physics, Strada Costiera 11, 34151 Trieste, Italy

[6] RCQI, Institute of Physics, Slovak Academy of Sciences, Dúbravská Cesta 9, 84511 Bratislava, Slovakia

[7] Department of Physics, Salman Farsi University of Kazerun, Kazerun, Iran

observed. It is our hope that this research may open a new path to consider the role of Heitler–London approach in non-classical correlations preservation.

Keywords   Thermal quantum correlations · Trace distance discord · Heitler–London approach

1 Introduction

Quantum correlations have been intensively studied in recent decades as a fundamental resource in quantum information theory such as quantum teleportation [1], quantum computation [2], quantum communication [3], and so forth [4, 5]. Quantum correlations reveal non-classical aspects of quantum mechanics, which has no classical counterpart. One kind of well-known quantum correlations is quantum entanglement. Until a few years ago, it was believed that quantum entanglement alone can explain all quantum correlations in a typical system. In this direction, many proper quantifiers, namely concurrence [6, 7], negativity [8, 9], global entanglement [10], Scott measure [11, 12] and many others [13–18], have been introduced to characterize the entanglement concept in the bipartite as well as multipartite quantum systems. However, some studies have shown that entanglement cannot grasp all quantum correlations of a system well [19, 20]. Indeed, Ollivier and Zurek showed that the quantum discord (QD) is another promising quantifier which goes beyond entanglement [19]. Strictly speaking, QD reveals the quantumness of correlations even in the separable mixed states [19, 20]. But despite this advantage, an analytical evaluation of this information-theoretic measure remains, generally, very difficult. Alternatively, various metrics based correlations measures such as geometric QD [21], global geometric QD [22], super QD [23], trace distance discord (TDD) [24, 25], and quantum consonance (QC) [26, 27] were proposed.

In recent years, the solid-state systems formed a milestone for several studies in realm of the quantum information theory [28–34]. In the perspective of the Heisenberg model [35], the dynamics of quantum correlations in a three-qubit with phase decoherence was studied [36]. Moreover, the dynamics of nonlocal correlations in an anisotropic two-qubit Heisenberg XYZ model under the effect of the phase damping was examined [37]. In the intrinsic decoherence framework, the temporal evolution of quantum correlations in a two-qubit Heisenberg spin chain model with the interaction of anti-symmetric and symmetric contributions of spin–orbit coupling [30, 31] has been also recently studied [38]. Meanwhile, the Heisenberg spin models have been used to characterize the thermal features of the bipartite entropic uncertainty [31, 39]. But excepting some few studies [40, 41], a varieties of Heisenberg spin chains, in various configurations like XXX, XXZ, and XYZ, have been studied without assuming the coupling strength as a function of position. However, in view to expand the effect of coupling distance on quantum correlations, we present in the current paper a study of pairwise Heisenberg quantum correlations in the context of the Heitler–London (HL) approach.

Historically, the first quantum-mechanical description of the chemical bonding is generally credited to W. Heitler and F. London [42], who proposed it just a year
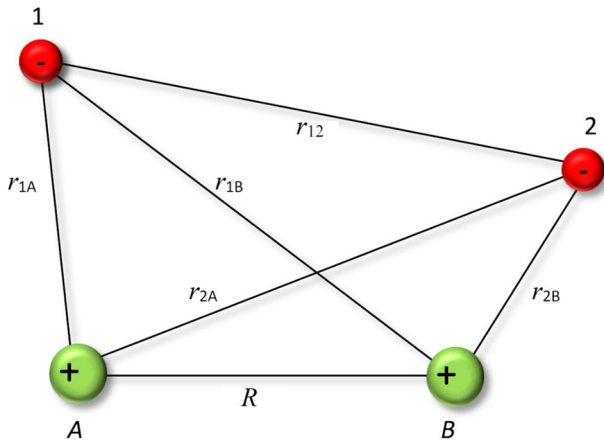
Fig. 1 Valence bond treatment of H_2 molecule. In the scheme, $r_{1A(B)}$ and $r_{2A(B)}$ denote the distance from the first (second) electron labeled as 1(2) to the nuclei labeled as $A(B)$, while r_{12} is the distance between the electrons 1 and 2. Also, R is the distance between the nuclei A and B

after the presentation of Schrödinger equation [43, 44]. The HL approximation [42] is typically conceived to explain the interaction between a pair of spins, resulting from Coulomb forces between two electrons of the two adjoining atoms [45]. It is an example of the valence bond (VB) method [46], which was introduced to describe the bonding of a hydrogen molecule H_2. It is worth mentioning that the VB method views molecules as composed of atomic cores (nuclei plus inner shell electrons) and bonding valence electrons (Fig. 1 scheme is devoted to the procedure of H_2 molecule). Heitler and London began with the atomic orbitals toward setting up an approximate solution. They found that the suitable linear combinations of the hydrogen $1s$ wave functions centered at two atoms **A** and **B** are given by the symmetric $A_1 B_2 + B_1 A_2$ and anti-symmetric $A_1 B_2 - B_1 A_2$ wave functions (Fig. 1). It is assumed that the atomic orbitals A and B are suitably normalized, and therefore, the normalized functions are obtained as $\psi_{\pm} = (A_1 B_2 \pm B_1 A_2)/\sqrt{2\left(1 \pm S^2\right)}$ where the amount $S = \int A_1 B_1 dv_1$ is the overlap integral [47].

The concept of exchange coupling of the cluster spins of nonsinglet atoms was proposed in the molecular binding theory of HL and the Heisenberg theory of ferromagnetic [42, 48]. In literature, some few works have been done on HL approach with exchange coupling [45–51]. On the other hand, so far no work has been published on quantum information that uses HL exchange coupling. So given the obvious importance of this issue, we consider a two-qubit Heisenberg XXX model with HL exchange coupling approach subjected to an external transverse nonuniform magnetic field. The purpose of the present work is to probe the behavior of quantum correlations captured by concurrence, TDD, and QC for our realistic Hamiltonian model at thermal equilibrium. Hence, the layout of the work is structured as follows. In Sect. 2, we briefly present the two-qubit Heisenberg XXX spin system with HL exchange coupling for the quantum system. In Sect. 3, the thermal evolution of mentioned quantifiers in the background of our model has been examined in detail, under the influence of the tem-
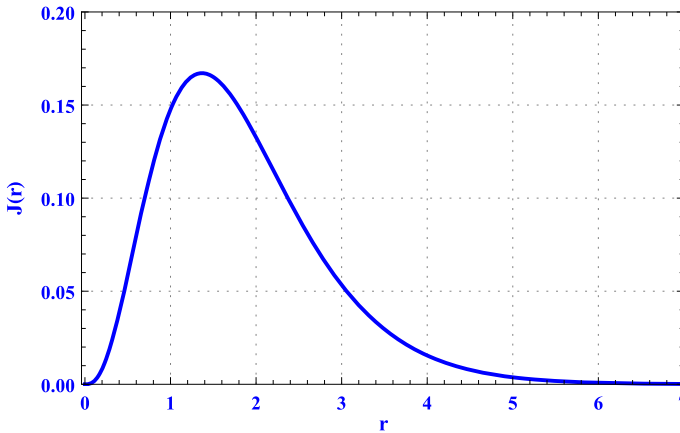
Fig. 2 HL coupling strength $J(r)$ with respect to inter-spins relative distance r

perature, the external magnetic field, and the exchange coupling. In Sect. 4, we give the main results with detailed analysis. Finally, some concluding remarks are given in Sect. 5.

2 Hamiltonian model

This section is devoted to describe a system of two nearest neighboring Heisenberg spin model subjected to an external transverse magnetic field. The model of Hamiltonian is given by [52]

$$H = \frac{1}{2}\left[\left(J_x \sigma_1^x \sigma_2^x + J_y \sigma_1^y \sigma_2^y + J_z \sigma_1^z \sigma_2^z \right) + B \left(\sigma_1^z - \sigma_2^z \right) \right], \tag{1}$$

where $\sigma_{i=1,2}^{j}$ with $j \in \{x, y, z\}$ are the 2D-Pauli spin matrices, while B is the nonuniform magnetic field directed along the z-axis. To proceed further, we concentrate in our study on the case of the isotropic XXX configuration of Heisenberg antiferromagnetic spin chain characterized by $J_x = J_y = J_z = J > 0$. Besides, we assume that the exchange spin constant J is identical to HL coupling, namely $J(r)$, given as [47]

$$J \equiv J(r) = \left(\frac{56}{45} - \frac{4\gamma}{15} - \frac{4}{15} \ln r \right) r^3 e^{-2r} + O\left(r^2 e^{-2r} \right), \tag{2}$$

where $\gamma = 0.5772$ is Euler's constant and r refers to the inter-spins relative distance defined as the ratio of the distance between spins R and Bohr radius $a_0 = \hbar^2/m_{\oplus}e^2$ ($r = R/a_0$). Figure 2 displays the plot of the function $J(r)$ in terms of the inter-spins relative distance r.

So, the modified Hamiltonian for XXX configuration with HL coupling in the two-qubit standard computational basis $\mathcal{B} \equiv \{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$ can be written under the following matrix form

$$H = \begin{pmatrix} \frac{J(r)}{2} & 0 & 0 & 0 \\ 0 & -\frac{J(r)}{2} + B & J(r) & 0 \\ 0 & J(r) & -\frac{J(r)}{2} - B & 0 \\ 0 & 0 & 0 & \frac{J(r)}{2} \end{pmatrix}. \tag{3}$$

The diagonalization of H leads to the following eigenspectrum and the associated eigenvectors

$$E_{1,4} = \frac{J(r)}{2}, \qquad\qquad |\psi_1\rangle = |00\rangle, \ |\psi_4\rangle = |11\rangle, \tag{4a}$$

$$E_2 = -\frac{J(r)}{2} + \eta, \qquad\qquad |\psi_2\rangle = \frac{1}{\sqrt{1+\xi^2}} \left(|10\rangle + \xi |01\rangle \right), \tag{4b}$$

$$E_3 = -\frac{J(r)}{2} - \eta, \qquad\qquad |\psi_3\rangle = \frac{1}{\sqrt{1+\xi^2}} \left(|01\rangle - \xi |10\rangle \right), \tag{4c}$$

where $\eta := \sqrt{J^2(r) + B^2}$ and $\xi := (B + \eta)/J(r)$. The kets $|0\rangle$ and $|1\rangle$ are taken here, respectively, as the spin-up and spin-down states and $\{|0\rangle, |1\rangle\}$ form a computational basis of a qubit.

3 Thermal quantum correlations over HL approximation

To quantify the amount of quantum correlations in a bipartite quantum system, various indicators are suggested in the literature [6–19]. In our study, we employ three main figures of merit, namely concurrence, TDD, and QC. To describe the behavior of the quantum correlations, we calculate firstly the thermal state of our mentioned Hamiltonian which describes a system state in equilibrium at temperature T.

3.1 Thermal state

In order to study the thermal behavior of quantum correlations in a two coupled spin-1/2 Heisenberg model, we will be focused on systems that are in a state of thermal equilibrium. Such state called thermal state and described by the Gibbs density matrix

$$\varrho(T) = \frac{1}{\mathcal{Z}} \exp(-\beta H), \tag{5}$$

with $\mathcal{Z} = \mathrm{Tr}\left[\exp(-\beta H)\right]$ being the partition function and the inverse temperature $\beta = 1/(k_B T)$ wherein k_B is the Boltzmann's constant. Throughout this paper, we use $k_B = 1$ for convenience.

The matrix form of $\varrho(T)$ can be obtained through the spectral decomposition of the Hamiltonian (3). Accordingly, for the considered two-qubit system, Eq. (5) can be rewritten as

$$\varrho(T) = \frac{1}{\mathcal{Z}} \sum_{m=1}^{4} e^{-\beta E_m} |\psi_m\rangle\langle\psi_m|. \tag{6}$$

Reporting Eqs. (4a-4c) in Eq. (6), the density matrix describing the suggested system in thermal equilibrium can be written in the standard computational basis $\mathcal{B}$ as

$$\varrho_T = \frac{1}{\mathcal{Z}} \begin{pmatrix} a & 0 & 0 & 0 \\ 0 & b^+ & c & 0 \\ 0 & c & b^- & 0 \\ 0 & 0 & 0 & a \end{pmatrix}, \tag{7}$$

where

$$a = e^{\frac{-\beta J(r)}{2}},$$
$$b^\pm = e^{\frac{\beta J(r)}{2}} \left(e^{\pm\beta\eta} + \xi^2 e^{\mp\beta\eta} \right) / (1 + \xi^2),$$
$$c = -2\xi e^{\frac{\beta J(r)}{2}} \sinh\left(\beta\eta\right) / (1 + \xi^2),$$
$$\mathcal{Z} = 2a + b^+ + b^-.$$

3.2 Trace distance discord

The concept of quantum correlations beyond entanglement can be quantified by quantum discord [19]. It measures all non-classical correlations in a quantum bipartite system. Let ρ^{ab} be a state describing any bipartite system ab in a composite Hilbert space $H = H^a \otimes H^b$, where H^a and H^b are the Hilbert spaces corresponding to the subsystems a and b of ab, respectively. The total correlation shared between a and b can be quantified by the quantum mutual information defined as [53],

$$I\left(\rho^{ab}\right) := S\left(\rho^a\right) + S\left(\rho^b\right) - S\left(\rho^{ab}\right), \tag{8}$$

where the quantity $S(\rho) = -\text{Tr}\left[\rho \log_2 \rho\right]$ stands for the von Neumann entropy and $\rho^{a(b)} = \text{Tr}_{b(a)}[\rho^{ab}]$ denotes the marginal state describing the subsystem $a(b)$, which is determined by tracing out the subsystem $b(a)$. Given that a local measurement was performed on the party b, the quantum discord is given by the quantity [19, 20]

$$D\left(\rho^{ab}\right) := I\left(\rho^{ab}\right) - CC\left(\rho^{ab}\right), \tag{9}$$

which is expressed as the difference between the mutual information $I\left(\rho^{ab}\right)$ and classical correlation $CC\left(\rho^{ab}\right)$ of the bipartite state ρ^{ab}, with

$$CC\left(\rho^{ab}\right) = S\left(\rho^a\right) - \min_{\left\{\Pi_{(j)}^b\right\}} \sum_j p_j S\left(\rho^{a|j}\right). \tag{10}$$

We look that the optimization in Eq. (10) is performed over the set $\left\{ \Pi_{(j)}^b \right\}$ comprising all one-dimensional orthogonal projectors. The density matrix $\rho^{a|j} = p_j^{-1} \mathrm{Tr}_b \left[\left(\mathbb{1}^a \otimes \Pi_{(j)}^b \right) \rho^{ab} \left(\mathbb{1}^a \otimes \Pi_{(j)}^b \right) \right]$ refers to the post-measurement state of a after obtaining outcome j on subsystem b with probability $p_j = \mathrm{Tr} \left\{ \left(\mathbb{1}^a \otimes \Pi_{(j)}^b \right) \rho^{ab} \left(\mathbb{1}^a \otimes \Pi_{(j)}^b \right) \right\}$, and $\mathbb{1}^a$ is the 2×2 identity operator on the subsystem a. In order to obtain a simple and reliable analytical result of the quantum discord, the best way is to treat this quantifier from a geometric perspective. One of the reliable geometric measures of quantum discord is that based on TDD concept which has been proposed recently [21, 24]. It quantifies the quantum correlation through the nearest Schatten 1-norm distance between the state under study and the quantum-classical state $\rho^{qc} = \sum_{k=1}^{2} p_k \rho_k^a \otimes |k\rangle^b \langle k|$ with zero discord [54, 55]. For a bipartite state ρ^{ab}, TDD is defined by [21, 24].

$$D_{\mathrm{T}}(\rho^{ab}) = \min_{\rho^{qc} \in \Omega_0} \| \rho^{ab} - \rho^{qc} \|_1, \tag{11}$$

where Ω_0 denotes the set of all zero discord states and $\|.\|_1$ is the usual trace norm. An explicit formula of TDD was derived when the shape of considering two-qubit state ρ^{ab} is X-structured [25]. It is given by

$$D_{\mathrm{T}}(\rho^{ab}) = \sqrt{\frac{\max\{R_{33}^2, R_{22}^2 + R_{30}^2\} \cdot R_{11}^2 - \min\{R_{11}^2, R_{33}^2\} \cdot R_{22}^2}{\max\{R_{33}^2, R_{22}^2 + R_{30}^2\} - \min\{R_{11}^2, R_{33}^2\} + R_{11}^2 - R_{22}^2}}, \tag{12}$$

where $R_{\mu\nu} = \langle \sigma_\mu^a \otimes \sigma_\nu^b \rangle$ in Eq. (12) being the components of the correlation matrix occurring after decomposing the state ρ^{ab} in the Fano–Bloch representation as [56]

$$\rho^{ab} = \frac{1}{4} \sum_{\mu,\nu=0}^{3} R_{\mu\nu} \sigma_\mu^a \otimes \sigma_\nu^b. \tag{13}$$

In the case of the thermal state ϱ_T, which belongs to X-states family, its corresponding TDD can be easily computed. Indeed, by making use of Eqs. (7), (12), and (13), one straightforwardly finds that

$$D_T(\varrho_T) = \frac{4e^{\frac{\beta J(r)}{2}}}{\mathcal{Z}} \frac{|\xi|}{(1 + \xi^2)} \sinh(\beta\eta). \tag{14}$$

3.3 Concurrence

To quantify the quantum entanglement contained in an arbitrary two-qubit mixed state ρ^{ab}, shared between two subsystem a and b, we present here the concurrence [6, 7]. It can be evaluated by using the formula

$$\mathcal{C}(\rho^{ab}) = \max\left\{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\right\}, \tag{15}$$

where λ_i represents the square roots of the eigenvalues of the operator $\rho^{ab}\left(\sigma_y^a \otimes \sigma_y^b\right)$ $(\varrho^{ab})^*\left(\sigma_y^a \otimes \sigma_y^b\right)$ in descending order. Here $(\rho^{ab})^*$ denotes the complex conjugate of the density matrix ρ^{ab} in the standard two-qubit computational basis $\mathcal{B}$, while $\sigma_y^{i=a,b}$ being the well known 2D-Pauli spin matrix for the two level systems. For the two-qubit X-shaped thermal density operator (7), the amount of the thermal entanglement can be straightforwardly evaluated. By using Eqs. (7) and (15), one finds

$$\mathcal{C}(\varrho_T) = \frac{2e^{\frac{\beta J(r)}{2}}}{\mathcal{Z}} \max\left\{0, \frac{2|\xi|}{1+\xi^2}\sinh(\beta\eta) - e^{-\beta J(r)}\right\}. \tag{16}$$

3.4 Quantum consonance

In the following, we deal with the QC [26] as quantum correlations quantifier. This measure is defined as a sum of the entanglement and some other quantum correlations after omitting, by means of a local unitary operations, the local coherence from the total one [27]. By considering a bipartite quantum state ρ^{ab}, the QC is defined mathematically according to the following expression

$$\mathcal{Q}_C(\rho^{ab}) = \sum_{ijmn}\left|\rho_{ijmn}^c\,(1-\delta_{im})\left(1-\delta_{jn}\right)\right|, \tag{17}$$

where $\rho^c = (U_1 \otimes U_2)\,\rho^{ab}\,(U_1 \otimes U_2)^\dagger$ stands for the transformed state achieved by making specific local unitary operations U_1 and U_2 on the original state ρ^{ab}. Interestingly, QC is simplified for a two-qubit X-state as the sum of off-diagonal terms of the density matrix [31].

The QC for thermal state ϱ_T can be easily computed because it belongs to X-states. By using (7), we indeed find that

$$\mathcal{Q}_C(\varrho_T) = \frac{4e^{\frac{\beta J(r)}{2}}}{\mathcal{Z}} \frac{|\xi|}{\left(1+\xi^2\right)}\sinh(\beta\eta), \tag{18}$$

which is identical to the analytical expression of TDD (14). Hence, we restrict in our analysis to compare only the thermal TDD behavior with the thermal entanglement.

4 Results and discussions

In the present section, we examine the behavior of thermal quantum correlations in the isotropic two-qubit XXX Heisenberg model in the HL approach described by the thermal state (7). More precisely, we are concerned in our analysis by studying the
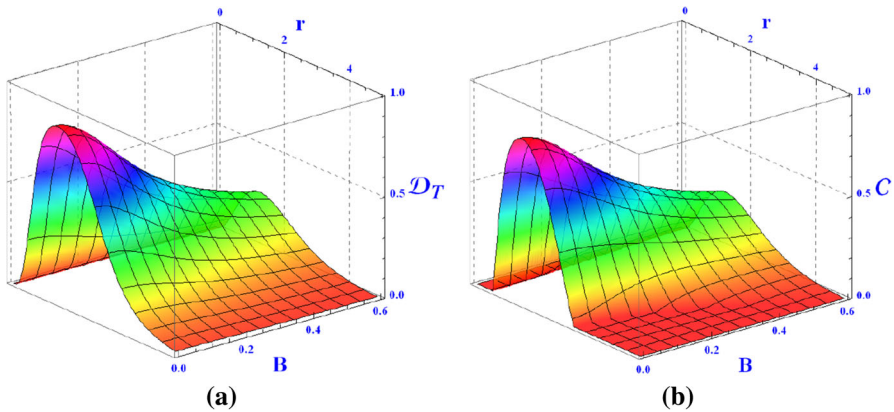
Fig. 3 (Color online) XXX model for fixed temperature $T = 0.1$. TDD (**a**) and concurrence (**b**) versus the HL coupling relative distance r and nonuniform magnetic field B

quantum correlations quantified by the geometric trace discord and quantum entanglement over the HL coupling relative distance r with the varying parameters; absolute temperature T and nonuniform magnetic field B.

In Fig. 3, we have plotted the TDD (14) and the concurrence (16) as functions of the nonuniform magnetic field B and the inter-spins relative distance r for fixed value of the absolute temperature $T = 0.1$. The results show that the thermal quantum correlations amounts are always zero for $r \to 0$ whatever the B values. That is to say that there are no pairwise thermal quantum correlations when the two spins are uncoupled $J(r) \to 0$. This happens due to the fact that for $r \to 0$, the two-spin system is uncoupled. We notice also that for a fixed value of B, the amounts of quantum correlations become more significant for $r = 1.357$ wherein the exchange coupling constant $J(r)$ is maximal (see Fig. 2). Figure 3 depicts that the quantumness of correlations undergoes an amplitude decreasing with B advancing. Furthermore, it turns out that as HL coupling relative distance increases, both entanglement and geometric quantum discord slowly vanish after a certain range of r. It is interesting to notice that for $T = 0.1$, the entanglement dies at $r_0 \approx 3$ for $B = 0$ while the TDD sustains over the larger ranges of HL coupling relative distance r and weak values of B. The entanglement vanishing moves away from r_0 when the intensity of B increases. This can be perceived by the fact that, for $\beta = 10$, that is $T = 0.1$, and fixed values of B, an entangled-unentangled phase transition takes place for a threshold value r_f of HL relative distance r.

According to Eq. (16), this threshold value r_f can be achieved by resolving the following nonlinear equation

$$e^{10J(r_f)} \sinh\left(10\eta_f\right) = \frac{1 + \xi_f^2}{2|\xi_f|}, \tag{19}$$
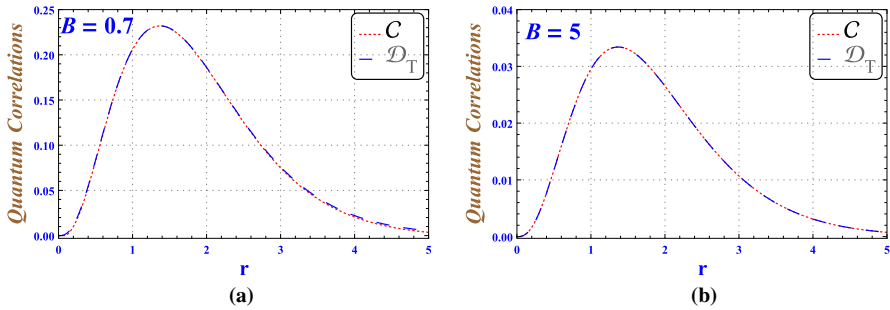
Fig. 4 (Color online) Thermal quantum correlations over the HL coupling relative distance r with fixed $T = 0.1$ and $B = 0.7$ (**a**) and $B = 5$ (**b**). Here, dotted red line represents the entanglement and dashed blue line represents the TDD

where $\eta_f = \sqrt{J^2(r_f) + B^2}$ and $\xi_f = (B + \eta_f)/J(r_f)$. It is worth of mentioning that TDD (QC) reveals the non-classical correlations even in the absence of the entanglement. This implies that the TDD can capture the quantum correlations even in the separable mixed states.

Figure 4 shows that for $T = 0.1$ and $B = 0.7$ (Fig. 4a) and $B = 5$ (Fig. 4b), the TDD and concurrence are considerably matched. This typical behavior emerges due to the link between the quantum entanglement and the quantum coherence concept, quantified here by QC, which is a fundamental manifestation of the quantum superposition principle on which based the quantum entanglement [57].

The thermal behaviors of TDD (QC) and concurrence as functions of the HL coupling distance r and nonuniform magnetic field B are plotted in Figs. 5 and 6, where the temperature is chosen to be $T = 0.3$ and $T = 0.6$, respectively. As can be seen in Fig. 5, the TDD behavior is similar to the previous case (Fig. 3), which means TDD decreases gradually with increasing B; however, the only difference is that its maximum value is less than the previous case. The entanglement behavior here is different from TDD. The amount of the magnetic field in which entanglement reaches its maximum value is larger than the previous case. It is interesting to note that, as the temperature increases, this difference becomes more apparent (see Fig. 6). As seen from Fig. 6, when $B < 2$, the entanglement is zero while TDD reaches its maximum value in this interval. In other words, although the quantum correlation captured by TDD achieves its maximum in this range, the entanglement does not have any role in this correlation. Moreover, it is observed that the non-classical correlation quantified by TDD decreases whereas entanglement increases to reaches its maximum value to coincide, therefore, with TDD for strong magnetic field values. This indicates that increasing the nonuniform magnetic field plays a positive role in the production of the entanglement in high temperatures.

Furthermore, by comparing Figs. 3, 4, 5 and 6, it can be found that the behavior of both quantum correlations is the same with varying the HL coupling distance r. One can note that when the HL coupling distance r increases, the quantum correlations after reaching their maximum value then monotonically decrease down to zero. The physical reason for this observation may be rooted in the behavior of HL coupling
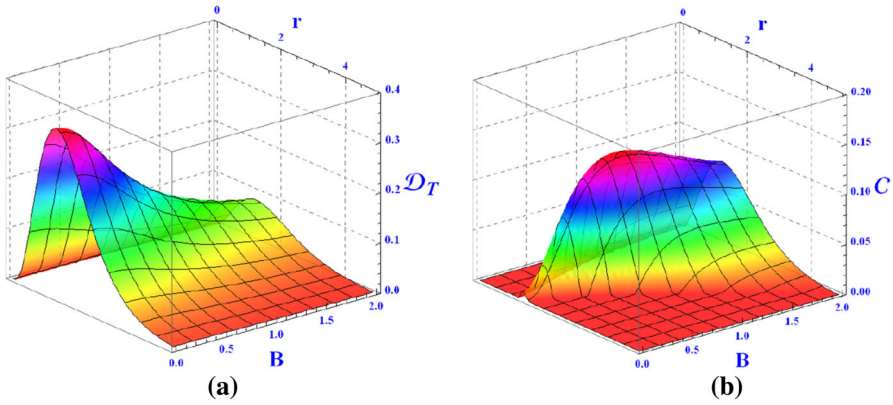
Fig. 5 XXX model for fixed temperature $T = 0.3$. TDD (**a**) and concurrence (**b**) versus r and B
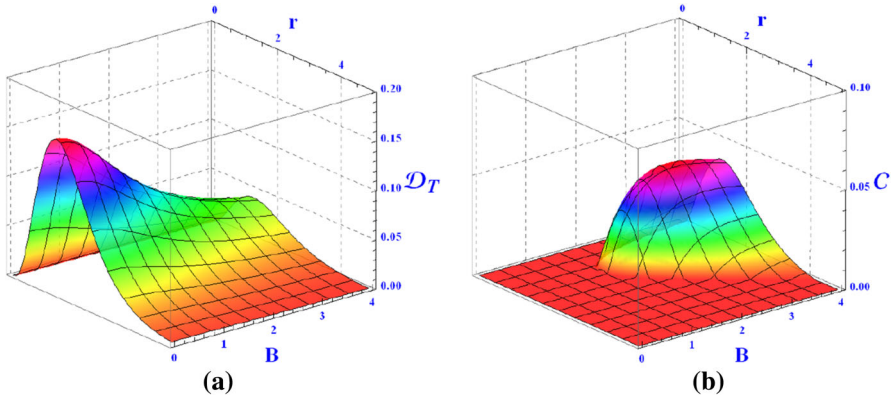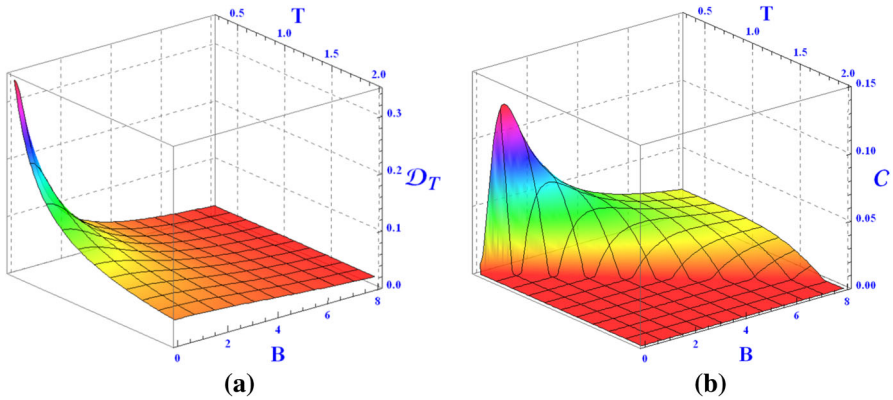

Fig. 6 XXX model for fixed temperature $T = 0.6$. TDD (**a**) and concurrence (**b**) versus r and B

strength $J(r)$ in terms of the inter-spins relative distance r (see Fig. 2). On the other hand, the correspondence of TDD and thermal entanglement for sufficient magnetic field values may be understood by the fact that the strong nonuniform magnetic field induces entangled phase in the two-qubit (antiferromagnetic XXX model) thermal state.

Finally, Fig. 7 shows the thermal evolution of TDD and concurrence over the nonuniform magnetic field B and temperature with fixed HL coupling relative distance r. As can be seen, the behaviors of TDD and entanglement are almost the same although the rate of changes in entanglement is slower than that of TDD. Also, one can observe that for any given magnetic field, the entanglement is equal to zero for temperatures greater than a certain threshold temperature. It is intriguing to note that by increasing B, the critical temperature above that entanglement disappears increases. That is to say, the high value of nonuniform magnetic field plays a crucial role in sustaining entanglement at high temperatures; however, the role of the magnetic field is destructive at low temperatures (see Fig. 3). It seems that the possibility of maintaining entanglement in such a quantum system at high temperatures requires stronger magnetic fields.

Fig. 7 XXX model for fixed HL relative distance $r = 1.357$. TDD (**a**) and concurrence (**b**) versus B and absolute temperature T

5 Concluding remarks

In summary, we have investigated the thermal quantum correlations shared between the bipartite system parts in the ambit of the Heitler–London scheme. We dealt with a system composed of two XXX Heisenberg spins subjected to a transverse external nonuniform magnetic field. For $T = 0.1$, we have found that the amplitude of quantum correlations decrease with nonuniform magnetic field increasing. Furthermore, it is observed that the TDD surpasses the entanglement for small values of B and therefore persists over the large range of HL coupling relative distance r in comparison with entanglement. Besides, the entanglement behavior in terms of B and r detects an entangled-unentangled phase transition. When the temperature increases, TDD retains the same appearance but with a reduced amount. Correspondingly, the thermal entanglement exhibits a completely different behavior to the one of $T = 0.1$, especially for a small range of B. However, there is a kind of correspondence between thermal entanglement and thermal non-classical correlations for a strong value of B. TDD can detect the quantum correlations even in the absence of the entanglement, which is generally an expected behavior of quantum discord. The obtained results confirmed that the suitable strong value of the nonuniform magnetic field helps to sustain entanglement even for higher absolute temperatures. However, the magnetic field has a destructive effect on the entanglement at low temperatures. We mention that the adopted model may be useful for designing quantum wires, data bus, solid-state gates, and quantum processors [41]. Therefore, we think that our observations may provide a new insight into the dynamics of non-classical correlations in Heisenberg spin chains and shed light on the maintenance of quantum correlations within the framework of real quantum systems, especially solid-state ones.

As a prolongation, the present study can be extended to another spin chain configurations such as XXZ and XYZ in the presence of the Dzyaloshinskii–Moriya and Kaplan–Shekhtman–Entin–Wohlman–Aharony interactions [30, 32, 38] to know the

behavior of quantum discord and entanglement in the Heitler–London approach. We think this can be useful for quantum information processing.

Author Contributions YK and MD have proposed the main idea and performed the calculations. YK, SH, HD, and MRP all contributed to the development of the idea, writing and discussions of the manuscript, and analyzing the results. Thorough checking of the paper was done by YK and SH.

Data Availability All data generated or analyzed during this study are included in this paper.

Declarations

Disclosures The authors declare that they have no known competing financial interests.

References

1. Bennett, C.H., Brassard, G., Crepeau, C., Jozsa, R., Peres, A., Wooters, W.K.: Teleporting an unknown quantum state via dual classical and Einstein–Podolsky–Rosen channels. Phys. Rev. Lett. **70**, 1895 (1993)
2. Sheng, Y.B., Pan, J., Guo, R., Zhou, L., Wang, L.: Efficient N-particle W state concentration with different parity check gates. Sci. China Phys. Mech. Astron. **58**, 060301 (2015)
3. Sheng, Y.B., Deng, F.G., Long, G.L.: Complete hyperentangled-Bell-state analysis for quantum communication. Phys. Rev. A **82**, 032318 (2010)
4. Ekert, A.K.: Quantum cryptography based on Bell's theorem. Phys. Rev. Lett. **67**, 661 (1991)
5. Bennett, C.H., Wiesner, S.J.: Communication via one- and two-particle operators on Einstein–Podolsky–Rosen states. Phys. Rev. Lett. **69**, 2881 (1992)
6. Hill, S., Wootters, W.K.: Entanglement of a pair of quantum bits. Phys. Rev. Lett. **78**, 5022 (1997)
7. Wootters, W.K.: Entanglement of formation of an arbitrary state of two qubits. Phys. Rev. Lett. **80**, 2245 (1998)
8. Vidal, G., Werner, R.F.: Computable measure of entanglement. Phys. Rev. A **65**, 032314 (2002)
9. Plenio, M.B.: Logarithmic negativity: a full entanglement monotone that is not convex. Phys. Rev. Lett. **95**, 090503 (2005)
10. Love, P.J., Van den Brink, A.M., Smirnov, A.Y., Amin, M.H.S., Grajcar, M., Ilichev, E., Izmalkov, A., Zagoskin, A.M.: A characterization of global entanglement. Quant. Inf. Process. **6**, 187 (2007)
11. Scott, A.J.: Multipartite entanglement, quantum-error-correcting codes, and entangling power of quantum evolutions. Phys. Rev. A **69**, 052330 (2004)
12. Haddadi, S.: A brief note on the Scott measure as a multipartite entanglement criterion. Laser Phys. Lett. **17**, 075201 (2020)
13. Vedral, V., Plenio, M.B., Rippin, M.A., Knight, P.L.: Quantifying entanglement. Phys. Rev. Lett. **78**, 2275 (1997)
14. Carvalho, A.R.R., Mintert, F., Buchleitner, A.: Decoherence and multipartite entanglement. Phys. Rev. Lett. **93**, 230501 (2004)
15. Hu, M.L., Hu, X., Wang, J., Peng, Y., Zhang, Y.R., Fan, H.: Quantum coherence and geometric quantum discord. Phys. Rep. **762–764**, 1 (2018)
16. Akhound, A., Haddadi, S., Chaman Motlagh, M.A.: Analyzing the entanglement properties of graph states with generalized concurrence. Mod. Phys. Lett. B **33**, 1950118 (2019)
17. Haddadi, S., Akhound, A., Chaman Motlagh, M.A.: Efficient entanglement measure for graph states. Int. J. Theor. Phys. **58**, 3406 (2019)
18. Haddadi, S., Bohloul, M.: A brief overview of bipartite and multipartite entanglement measures. Int. J. Theor. Phys. **57**, 3912 (2018)

19. Ollivier, H., Zurek, W.H.: Quantum discord: A measure of the quantumness of correlations. Phys. Rev. Lett. **88**, 017901 (2001)

20. Henderson, L., Vedral, V.: Classical, quantum and total correlations. J. Phys. A: Math. Gen. **34**, 6899 (2001)

21. Dakić, B., Vedral, V., Brukner, C.: Necessary and sufficient condition for nonzero quantum discord. Phys. Rev. Lett. **105**, 190502 (2010)

22. Qiang, W.C., Zhang, H.P., Zhang, L.: Geometric global quantum discord of two-qubit X states. Int. J. Theor. Phys. **55**, 1833 (2016)

23. Singh, U., Pati, A.K.: Quantum discord with weak measurements. Ann. Phys. **343**, 141 (2014)

24. Paula, F.M., de Oliveira, T.R., Sarandy, M.S.: Geometric quantum discord through the Schatten 1-norm. Phys. Rev. A **87**, 064101 (2013)

25. Ciccarello, F., Tufarelli, T., Giovannetti, V.: Toward computability of trace distance discord. New J. Phys. **16**, 013038 (2014)

26. Pei, P., Wang, W., Li, C., Song, H.S.: Using nonlocal coherence to quantify quantum correlation. Int. J. Theor. Phys. **51**, 3350 (2012)

27. Gebremariam, T., Li, W., Li, C.: Dynamics of quantum correlation of four qubits system. Phys. A **457**, 437 (2016)

28. Khedif, Y., Errehymy, A., Daoud, M.: On the thermal nonclassical correlations in a two-spin XYZ Heisenberg model with Dzyaloshinskii–Moriya interaction. Eur. Phys. J. Plus **136**, 336 (2021)

29. Haseli, S., Haddadi, S., Pourkarimi, M.R.: Probing the entropic uncertainty bound and quantum correlations in a quantum dot system. Laser Phys. **31**, 055203 (2021)

30. Yurischev, M.A.: On the quantum correlations in two-qubit XYZ spin chains with Dzyaloshinsky–Moriya and Kaplan–Shekhtman–Entin–Wohlman–Aharony interactions. Quant. Inf. Process. **19**, 336 (2020)

31. Khedif, Y., Haddadi, S., Pourkarimi, M.R., Daoud, M.: Thermal correlations and entropic uncertainty in a two-spin system under DM and KSEA interactions. Mod. Phys. Lett. A **36**, 2150209 (2021)

32. Fedorova, A.V., Yurischev, M.A.: Behavior of quantum discord, local quantum uncertainty, and local quantum Fisher information in two-spin-1/2 Heisenberg chain with DM and KSEA interactions. Quant. Inf. Process. **21**, 92 (2022)

33. Mohamed, A.B.A., Abdel-Aty, A.H., Qasymeh, M., Eleuch, H.: Non-local correlation dynamics in two-dimensional graphene. Sci. Rep. **12**, 3581 (2022)

34. Haddadi, S., Pourkarimi, M.R., Khedif, Y., Daoud, M.: Tripartite measurement uncertainty in a Heisenberg XXZ model. Eur. Phys. J. Plus **137**, 66 (2022)

35. Heisenberg, W.: Zur Theorie des Ferromagnetismus (On the theory of ferromagnetism). Z. Phys. **49**, 619 (1928)

36. Mohamed, A.B.A.: Pairwise quantum correlations of a three-qubit XY chain with phase decoherence. Quant. Inf. Process. **12**, 1141 (2013)

37. Mohamed, A.B.A., Farouk, A., Yassen, M.F., Eleuch, H.: Quantum correlation via skew information and Bell function beyond entanglement in a two-Qubit Heisenberg XYZ model: Effect of the phase damping. Appl. Sci. **10**, 3782 (2020)

38. Hashem, M., Mohamed, A.B.A., Haddadi, S., Khedif, Y., Pourkarimi, M.R., Daoud, M.: Bell nonlocality, entanglement, and entropic uncertainty in a Heisenberg model under intrinsic decoherence: DM and KSEA interplay effects. Appl. Phys. B **128**, 87 (2022)

39. Abdelghany, R.A., Mohamed, A.B.A., Tammam, M., Obada, A.S.F.: Dynamical characteristic of entropic uncertainty relation in the long-range Ising model with an arbitrary magnetic field. Quant. Inf. Process. **19**, 392 (2020)

40. Ma, X., Qiao, Y., Zhao, G., Wang, A.: Quantum discord of thermal states of a spin chain with Calogero-Moser type interaction. Sci. China Phys. Mech. Astron. **56**, 600 (2013)

41. Sharma, K.K.: Herring-Flicker coupling and thermal quantum correlations in bipartite system. Quant. Inf. Process. **17**, 321 (2018)

42. Heitler, W., London, F.: Wechselwirkung neutraler Atome und homöopolare Bindung nach der Quantenmechanik. Z. Physik **44**, 455 (1927)

43. Schrödinger, E.: An undulatory theory of the mechanics of atoms and molecules. Phys. Rev. **28**, 1049 (1926)

44. Griffiths, D., Schroeter, D.: Introduction to Quantum Mechanics. Cambridge University Press (2018)

45. Misra, P. K.: *Physics of condensed matter, chapter 13: magnetic ordering* (Academic Press, 409, 2012)

46. Cooper, D. L.: *Valence Bond Theory* (Ed. Elsevier, 2002)

47. Wu, W.: *Exchange Calculations Between Donors in Silicon and Metal-Phthalocyanine Dimer* (Doctoral thesis, University of London, 2007)
48. Heisenberg, W.: Zur theorie des ferromagnetismus. Z. Physik **49**, 619 (1928)
49. Gorkov, L. P., and Pitaevsky, L. P.: *The Energy Splitting of Terms of the Hydrogen Molecule* (DokladyAkademiiNauk. USSR. 151, 1963)
50. Herring, C., Flicker, M.: Asymptotic exchange coupling of two hydrogen atoms. Phys. Rev. **134**, A362 (1964)
51. Smirnov, B.M.: *Asimptotic Methods in Theory of Collisions of Atoms*. (Atomizdat, 1973)
52. Zhang, G.F., Li, S.S.: Thermal entanglement in a two-qubit Heisenberg XXZ spin chain under an inhomogeneous magnetic field. Phys. Rev. A **72**, 034302 (2005)
53. Groisman, B., Popescu, S., Winter, A.: Quantum, classical, and total amount of correlations in a quantum state. Phys. Rev. A **72**, 032317 (2005)
54. Luo, S.: Using measurement-induced disturbance to characterize correlations as classical or quantum. Phys. Rev. A **77**, 022301 (2008)
55. Khedif, Y., Daoud, M.: Pairwise nonclassical correlations for superposition of Dicke states via local quantum uncertainty and trace distance discord. Quant. Inf. Process. **18**, 45 (2019)
56. Bloch, F.: Nuclear induction. Phys. Rev. **70**, 460 (1946)
57. Qi, X., Gao, T., Yan, F.: Measuring coherence with entanglement concurrence. J. Phys. A: Math. Theor. **50**, 285301 (2017)