Abstract

In this paper, we study thermal quantum correlations as quantum discord and entanglement in bipartite system imposed by external magnetic field with Herring–Flicker coupling, i.e., \( J(R) = 1.642 e^{-2R} R^{5/2} + O(R^2 e^{-2R}) \). The Herring–Flicker coupling strength is the function of \( R \), which is the distance between spins and systems carry XXX Heisenberg interaction. By tuning the coupling distance \( R \), temperature and magnetic field quantum correlations can be scaled in the bipartite system. We find the long sustainable behavior of quantum discord in comparison with entanglement over the coupling distance \( R \). We also investigate the situations, where entanglement totally dies but quantum discord exists in the system.

Keywords  Herring–Flicker coupling · Quantum discord · Thermal entanglement · Bipartite spin system

1 Introduction

Entanglement [1] is the back bone for quantum information processing tasks, such as teleportation, quantum cryptography, quantum games and many others [2]. Fundamental role of entanglement in developing quantum computer has a significant importance. As far as the quantum computer architecture is concerned, the quantum bus [3] has an important role which is used to connect the quantum devices over the bus and routing the information. Although there is no perfect model for quantum computer architecture as yet, quantum bus based on spin chains [4,5] plays the role to transport the data over the bus among quantum registers and the flow of data can be controlled by tuning the relative coupling among spins. So, in this direction, it becomes very important to study the quantum correlations and their variations through coupling dis-
tance in spin chains. Varieties of spin chains have been studied by various authors in various configurations like XXX, XYZ, XXZ, which miss the coupling strength as function of position. Very few studies have been done for the effect of coupling distance on quantum correlations. In 1988, Haldane and Shastry have studied the spin chains for long-range interactions [6,7], in which the coupling strength follow the inverse square law. Relatively in the same direction, XXZ Heisenberg spin chain with long-range interactions has been studied by BO. Li [8], XX Heisenberg spin chain with Calogero–Moser-type interaction has been studied by MA XiaoSan [9]. Very recent studies for the same has been found in the literature [10–13]. In 2005, Zhen Huang and Sabre Kais have shown the dependency of entanglement on Herring–Flicker (HF) coupling distance [14] of XY spin chain governed by Ising modal [15]. The authors have found that the increasing amount of magnetic field decreases the entanglement over the HF coupling distance. HF coupling has its importance in determining the energy difference between triplet and singlet state of the Hydrogen molecule [14], which is given by $J(R) = E_{\text{triplet}} - E_{\text{singlet}} = 1.642 e^{-2R} R^{5/2} + O(R^2 e^{-2R})$. So by tuning the coupling distance $R$, the energy difference can be scaled. The HF coupling has been experimentally implemented in designing the silicon-based nuclear spin quantum computer [16,17]. By taking the motivations from the above studies in continuation of Zhen Huang and Sabre Kais study [15], we study the effect of HF coupling distance on thermal quantum correlations in XXX configuration of Hisenberg bipartite system and investigated that thermal quantum discord [18–20] sustain over the larger range of $R$ in comparison with thermal entanglement [21–23]. Further, we find the parameter values of temperature and magnetic field over which entanglement vanish in the system but thermal quantum discord exists over $R$. Here, we mention that quantum information processing community is always interested to search such systems which can persist long quantum correlations and avoid the phenomenon of entanglement sudden death [24–31] for practical applicability of the system. In the present study, we study only thermal entanglement and quantum discord, but on the other hand, quantum correlations based on nonlocal inequalities such as measurement-induced nonlocality [32], quantum steering [33,34] are also subject of investigation. In the present article, finding the properties of thermal quantum correlations through HF coupling distance can be useful to construct the quantum buses, solid-state quantum gates and quantum processors. To the best of our knowledge, this study presents the first outcome of the comparison of thermal quantum discord and entanglement dynamics over the HF coupling distance.

The plan of the paper is as follows in Sect. 2. We discuss the Hamiltonian, thermal density matrix and concurrence. In Sect. 3, we study the dynamics of thermal quantum discord and entanglement with the varying values of parameters temperature and magnetic field over the coupling distance $R$. In the last with Sect. 4, we present the conclusion of the paper.

2 Hamiltonian, thermal density matrix, concurrence and discord

In this section, we give the Hamiltonian of the bipartite spin system, thermal density matrix, concurrence and quantum discord. The Hamiltonian of bipartite system is given as below:
In this letter, we consider the anti-ferromagnetic case with 
\( J_x = J_y = J_z = J > 0 \)
for XXX configuration of Heisenberg spin chain. Further, we assume the coupling \( J \) is HF coupling, i.e., \( J(R) \), given as:
\[
J(R) = 1.642e^{-2R} R^{5/2} + O(R^2 e^{-2R}).
\]
So the modified Hamiltonian for XXX configuration with HF coupling can be obtained as follows:
\[
H = J(R)[\sigma_1^x \sigma_2^x + \sigma_1^y \sigma_2^y + \sigma_1^z \sigma_2^z + B(\sigma_1^z + \sigma_2^z)].
\]

The plot of the function \( J(R) \) is shown in Fig. 1. In order to study the thermal behavior \cite{35} of entanglement, we need to calculate the thermal density matrix of the system, which can be obtained as:
\[
\rho_T = \frac{e^{-H/ KT}}{Tr(e^{-H/ KT})}.
\]

The matrix form of \( \rho_T \) can be obtained by calculating the eigenspectrum of the Hamiltonian given in Eq. 3, this matrix is obtained as follows:
\[
\rho_T = [c_1, c_2, c_3, c_4].
\]

with
\[
c_1 = [a_{11}, 0, 0, 0]^T, \quad c_2 = [0, a_{22}, a_{32}, 0]^T \\
c_3 = [0, a_{23}, a_{33}, 0]^T, \quad c_4 = [0, 0, 0, a_{44}]^T
\]
Further, the format of thermal density matrix gives the clue to obtain the concurrence [36] in a $4 \times 4$ dimensional matrix. Here we mention that concurrence is a good measure of entanglement for bipartite system. The concurrence is a $4 \times 4$ dimensional matrix is given by

$$C(\rho) = \max \{0, p - q - r - s\}$$

where $(p > q > r > s)$ with $(p = \sqrt{\lambda_1}, q = \sqrt{\lambda_2}, r = \sqrt{\lambda_3}, s = \sqrt{\lambda_4})$. Here $(\lambda_1, \lambda_2, \lambda_3, \lambda_4)$ are the eigenvalues of the matrix $\rho \rho^f$. Where $\rho^f$ is the spin flip matrix given as,

$$\rho^f = (\sigma_y \otimes \sigma_y) \rho^*(\sigma_y \otimes \sigma_y)$$

Here, $\rho^*$ is the complex conjugate of the density matrix. Here, we calculate the concurrence in the thermal density matrix given in Eq. 5. In this case, the concurrence is the function of three parameters $(KT, B, R)$. Here, we mention another quantum correlation called quantum discord, which is a measurement-based quantum correlation. To give the deep insights into quantum discord, we proceed with the derivation of its mathematical expression. Let assume two random variables $X$ and $Y$, then their classical mutual information is given by:

$$I(X : Y) = H(X) + H(Y) - H(X, Y)$$

$$I(X : Y) = H(X) - H(X|Y)$$

where $H(X) = - \sum p_i \log p_i$ and $H(Y) = - \sum q_i \log q_i$ are Shannon entropies. $H(X, Y)$ is the joint entropy, and $H(X|Y)$ is the conditional entropy of $X$ and $Y$. Both Eqs. 16 and 17 are same in classical sense. One can write the quantum mechanical equivalent versions of both the equations in nonfactual sense by replacing the random variables $X$ and $Y$ by density matrices $\rho^A$ and $\rho^B$, which are given below:
\[ I(\rho^{AB}) = S(\rho^A) + S(\rho^B) - S(\rho^{AB}) \]  
(18)

\[ I(\rho^{AB}) = S(\rho^A) - S(\rho^A | \rho^B) \]  
(19)

where \( S(\rho^A) = -Tr(\rho^A \log_2 \rho^A) \) and \( S(\rho^B) = -Tr(\rho^B \log_2 \rho^B) \) are Von-Neumann entropies of subsystems \( \rho^A \) and \( \rho^B \), respectively. The term \( S(\rho^{AB}) = Tr(\rho^{AB} \log_2 \rho^{AB}) \) is the joint Von-Neumann entropy. It is important to mention that factually both Eqs. 18 and 19 are not same, because the factor \( S(\rho^A | \rho^B) \) depends on quantum measurements performed on either party \( A \) or \( B \) of the composite system \( AB \). Mathematical \( S(\rho^A | \rho^B) \) can be written as:

\[ S(\rho^A | \rho^B) = S(\rho^{AB} | O_P) \]  
(20)

with \( P \in \{A, B\} \). The \( O_K \) is the set of projective measurement operators given as,

\[ O_K = U M_K U^+ \]  
(21)

With

\[ M_K = |K\rangle\langle K|, K = \{0, 1\} \]  
(22)

\[ U = tI + y.\sigma \]  
(23)

with the trace condition,

\[ t^2 + y_1^2 + y_2^2 + y_3^2 = 1. \]  
(24)

where \( t \in R, y \in (y_1, y_2, y_3) \in R^3, \sigma \) is the Pauli vector, and \( I \) is the identity matrix. From Eq. 20, we conclude that the quantity \( S(\rho^A | \rho^B) \) depends on the set of subsystems, i.e., \( P \). This quantity is not symmetric, and hence, the quantum discord is also not symmetric in general. The amount of quantum discord is sensitive to the subsystem chosen for quantum measurement. Here, in the present work, we choose the subsystem \( A \) for the measurement \( O_K \). After the quantum measurement, the state of subsystem as well as of the whole system collapse and the ensemble is projected to \( (\rho^B, n_K) \). Hence, the whole state \( \rho^{AB} \) after the measurement can be written as:

\[ \rho^{AB}_K \rightarrow \frac{(O_K^A \otimes I_B)\rho^{AB}(O_K^{A\dagger} \otimes I_B)}{n_K} \]  
(25)

with, \( n_K = Tr[(O_K^A \otimes I_B)\rho^{AB}(O_K^{A\dagger} \otimes I_B)] \). Now rewriting the Eq. 19 in concise form after the measurement,

\[ I(\rho^{AB} | O_K^A) := S(\rho^B) - S(\rho^{AB} | O_K^A) \]  
(26)

with \( S(\rho^{AB} | O_K^A) = \sum_K n_K S(\rho^{AB}_K) \). We can extract the classical correlations by getting the supremum of the quantity \( I(\rho^{AB} | O_K^A) \) over all the projective measurements. Hence, the classical correlations are defined as:
\[ C(\rho^{AB}) := \sup_{\{O_k^A\}} I(\rho^{AB}|O_k^A) \]  

(27)

by simplification we get,

\[ C(\rho^{AB}) := S(\rho^R) - \min_{\{O_k\}} S(\rho^{AB}|O_k^A) \]  

(28)

Now we have two equations as Eqs. 18 and 28, then the quantum discord is defined as the difference of both of these equations, which is computed as:

\[ Q(\rho^{AB}) = S(\rho^A) + S(\rho^B) - S(\rho^{AB}) - S(\rho^B) + \min_{\{O_k\}} S(\rho^{AB}|O_k^A) \]  

(29)

\[ Q(\rho^{AB}) = S(\rho^A) - S(\rho^{AB}) + \min_{\{O_k\}} S(\rho^{AB}|O_k^A) \]  

(30)

Equation 30 gives the mathematical expression of quantum discord. The major problem to calculate the quantum discord arises because of the term \( S(\rho^B|O_k^A) \), which is to be minimized. It is easy to calculate Quantum discord with X-structured density matrices but become tedious for non-X-structured density matrices. Here, in the present work, the shape of the density matrix is X-structured and we use the method to calculate the quantum discord given in Ref. [37].

3 Thermal quantum correlations over HF coupling

In this section, we present the dynamics of thermal quantum correlations (quantum discord, entanglement), over the HF coupling distance \( R \) with the varying parameters of temperature and magnetic field. It is important to mention that thermal entanglement can survive in anti-ferromagnetic case. The results with two- and three-dimensional plots have shown in Figs. 2 and 3, respectively. Giving the glance to the results presented in the first row of Fig. 2. We observe the behavior of quantum correlations for a fixed value of the parameter \( KT = 0.2 \) and increasing amount of magnetic field \( B \in [0.2, 0.8] \). It is found that the amplitude of entanglement and quantum discord decreases with the advancement of the magnetic field \( B \) and both quantum correlations slowly vanish after a certain range of HF coupling distance \( R \). It is interesting to observe that quantum discord sustains over the large range of HF coupling distance \( R \), while entanglement dies at \( R = 3.2 \). To pint out the reason behind this phenomenon, we here mention that the thermal state given in Eq. 5 is a mixed state as it satisfies the condition \( Tr[\rho^2] < 1 \) with \( \forall KT, B \). Beyond the value of HF coupling, i.e., \( (R = 3.2) \), the state of the system converts into separable state and hence entanglement vanishes in the system. With a deep note, giving the look into the mathematical expression of concurrence which demand to calculate the eigenvalues of the matrix \( \rho \rho^T \), the expression capture the correlations from the composite state of the system \( (\rho^{AB}) \) and do not involve the entropic uncertainty features of subsystems \( (A, B) \). While on the
other hand, giving the insight into the mathematical expression of quantum discord in Eq. 30, we find, the factor $[S(\rho^A) + \min_{O_k^A} S(\rho^{AB}|O_k^A)]$ must be greater than $S(\rho^{AB})$, as quantum discord is always satisfy the condition, i.e., $Q(\rho^{AB}) \geq 0$. In other words, the sum of the Von-Neumann entropies of the subsystems $(A, B)$ may exceed the Von-Neumann entropy of the composite system $S(\rho^{AB})$. This situation may happen because of the classical correlations involved in the system or may be produced by measurement apparatus by any means. Quantum discord captures the entropic uncertainties involved by subsystems as well as classical correlations and gives the better insights for the quantum correlations in comparison with concurrence. It is known that, for a pure separable state of a bipartite system, the sum of the Von-
Neumann entropies of the subsystems is equal to the Von-Neumann entropy of the composite system, i.e., \[ S(\rho^A) + S(\rho^{AB})] = S(\rho^{AB}), \] but for mixed states, this case is not true. In fact, quantum discord, classical correlations and entanglement coincide for pure entangled states. But as our state in Eq. 5 is mixed, hence in results, the behavior of quantum discord and entanglement is different. With this explanation, we return to the behavior of quantum discord with \((KT = 0.2, R > 3.2)\) presented in Fig. 2; there is an increment in the entropies of the subsystems and hence the value of the factor \[ S(\rho^A) + \min_{\{O_k\}} S(\rho^{AB}\mid O_k^A) \] increases, which contribute to raising the sustainability of quantum discord over the entanglement. As the value of HF coupling distance \(R\) advances with \((R > 3.2)\), the factor \[ S(\rho^A) + \min_{\{O_k\}} S(\rho^{AB}\mid O_k^A) \] approaches the value equal to the factor \(S(\rho^{AB})\), which means the sum of entropies of the subsystems \((A, B)\) become equal to the total Von-Neumann entropy of the composite system, i.e., \(S(\rho^{AB})\), and system converts into separable state. With these explanations in terms of the interplay between subsystems entropies and composite system entropy, we investigate further results with higher values of the parameter \(KT\). As the value of \(KT\) increases with \((KT = 0.4)\), the amplitude of both quantum correlations decreases and sustainable range of entanglement also decreases; however, quantum discord still sustains over the large range of \(R\) and slowly surpasses over the entanglement. Further with \(KT = 0.6\), we again find the amplitude of quantum correlations decrease, and sustainable range of entanglement also decrease than previous cases. With the same value \(KT = 0.6\), quantum discord completely cover the entanglement and even present in the absence of entanglement in the system. Here, we mention that quantum discord is strong quantum correlation and has the long-range sustainability over HF coupling \(R\) in comparison with entanglement. Next we find that, with the parameter value \((KT \geq 0.7, \forall B)\) in Fig. 4, the entanglement totally vanished in the system, but quantum discord still survives, it is because of the beautiful property of quantum discord such that it can exist in mixed states even in the absence of entanglement. If there is no entanglement present in the systems, then quantum discord may be utilized for practical quantum applications. The three-dimensional plots of Fig. 4 are shown in Fig. 5 for better clarifications. The value \((KT \geq 0.7)\) is the threshold value at which the drastic change takes place in the system.
4 Conclusion

In this present article, we have studied thermal quantum correlations in the bipartite system with the existence of Herring–Flicker coupling. The system carries XXX Heisenberg interaction and imposed by external magnetic field. We have found that for the fixed value of temperatures with increasing amount of magnetic field, the amplitude of quantum correlations decreases. Further, it is observed that quantum discord sustains over the large range of HF coupling distance $R$ in comparison with entanglement. The increasing values of the temperature decrease the amplitude of quantum correlations and increasing values of magnetic field effect the sustainable range of entanglement. While the sustainable range of quantum discord has less influenced by increasing magnetic field. At the parameter value of temperature $(KT = 0.6)$, quantum discord became dominant over the entanglement and totally surpassed it. We also have found that increasing values of the parameters with $(KT \geq 0.7, \forall B)$ kill the entanglement, while quantum discord still exists in the system. So quantum discord is the more robust quantum correlation in comparison with entanglement, which is generally predicted the behavior of quantum discord. We have found long-range sustainability of the quantum discord over the entanglement as the coupling distance increases with increasing amount of magnetic field. The present study can be improved in another spin chain configurations like XXZ, XYZ, XXZ etc., for the investigation of the behavior of quantum discord and entanglement with Herring-Coupling and can be useful quantum information processing.

Acknowledgements The authors acknowledge support from the Ministry of Electronics & Information Technology, Government of India, through the Centre of Excellence in Nano-Electronics, IIT Bombay.

References

1. Einstein, A., Podolsky, B., Rosen, N.: Can quantum-mechanical description of physical reality be considered complete? Phys. Rev. 47, 777 (1935)
2. Nielsen, M.A., Chuang, I.L.: Quantum Computation and Quantum Information. Cambridge University Press, Cambridge (2000)
3. Bose, S., Bayat, A., Sodano, P., Banchi, L., Verrucchi, P.: Spin Chains as Data Buses, Logic Buses and Entanglers, Chapter: Quantum State Transfer and Network Engineering, pp. 1–37 (2013)
4. D’Amico, I.: Quantum dot-based quantum buses for quantum computer hardware architecture. Microelectron. J. 37, 1440 (2006)
5. Schirmer, S.G., Pemberton-Ross, P.J.: Fast high fidelity information transmission through spin chain quantum wires. Phys. Rev. A 80, 030301 (2009)
6. Haldane, F.D.M.: Exact Jastrow–Gutzwiller resonating-valence-bond ground state of the spin 1/2 antiferromagnetic Heisenberg chain with $\frac{1}{4}$ exchange. Phys. Rev. Lett. 60, 635 (1988)
7. Shastry, B.S.: Exact solution of an $S=\frac{1}{2}$ Heisenberg antiferromagnetic chain with long-ranged interactions. Phys. Rev. Lett. 60, 639 (1988)
8. Lin, B., Wang, Y.S.: Quantum correlations in a long range interaction spin chain. Phys. B 407, 77 (2012)
9. XiaoSan, M., Ying, Q., GuangXing, Z., AnMin, W.: Quantum discord of thermal states of a spin chain with Calogero–Moser type interaction. Sci. China 56, 600 (2013)
10. Bravo, B., Cabra, D.C., Gmez Albarracn, F.A., Rossini, G.L.: Long-range interactions in antiferromagnetic quantum spin chains. Phys. Rev. B 96, 054441 (2017)
11. Homrighausen, I., Abeling, N.O., Zauner-Stauber, V., Halimeh, J.C.: Anomalous dynamical phase in quantum spin chains with long-range interactions. Phys. Rev. B 96, 104436 (2017)
12. Neyenhuis, B., Zhang, J., Hess, P.W., Smith, J., Lee, A.C., Richerme, P., Gong, Z.X., Gorshkov, A.: Observation of prethermalization in long-range interacting spin chains. Sci. Adv. 3(8), e1700672 (2017)
13. Hunga, C.L., Gonzalez-Tudella, A., Ignacio, C.J., Kimble, H.J.: Quantum spin dynamics with pairwise-tunable long-range interactions. PNAS 113, 34 (2016)
14. Herrig, C., Flicker, M.: Asymptotic exchange coupling of two hydrogen atoms. Phys. Rev. 134, A362 (1964)
15. Huang, Z., Kais, S.: Entanglement as measure of electron–electron correlation in quantum chemistry calculations. Chem. Phys. Lett. 413, 1 (2005)
16. Kane, B.E.: A silicon-based nuclear spin quantum computer. Nature 393, 133 (1998)
17. Kamenev, D.I., Berman, G.P., Tsifrinovich, V.I.: Influence of qubit displacements on quantum logic operations in a silicon-based quantum computer with constant interaction. Phys. Rev. A 74, 042337 (2006)
18. Zurek, W.H.: Einselection and decoherence from an information theory perspective. Annalen der Physik 9, 855 (2000)
19. Ollivier, H., Zurek, W.H.: Quantum discord: a measure of the quantumness of correlations. Phys. Rev. Lett. 88, 017901 (2001)
20. Bera, A., Das, T., Sadhukhan, D., Singha Roy, S., Sen, De A., Sen, U.: Quantum Discord and Its Allies: A Review. arXiv:1703.10542v1
21. Nielsen, M.A.: Quantum information theory. Ph.D. thesis, University of Mexico, arXiv:quant-ph/0011036 (1998)
22. Arnesen, M.C., Bose, S., Vedral, V.: Natural thermal and magnetic entanglement in the 1D Heisenberg model. arXiv:quant-ph/0009060 (2000)
23. Maziero, J., Guzman, H.C., Cleri, L.C., Sarandy, M.S., Serra, R.M.: Quantum and classical thermal correlations in the XY spin-$\frac{1}{2}$ chain. Phys. Rev. A 82, 012106 (2010)
24. Yu, T., Eberly, J.H.: Finite-time disentanglement via spontaneous emission. Phys. Rev. Lett. 93, 140404 (2004)
25. Yu, T., Eberly, J.H.: Sudden death of entanglement. Science 30, 598 (2009)
26. Sharma, K.K., Awasthi, S.K., Pandey, S.N.: Entanglement sudden death and birth in qubit–qutrit systems under Dzyaloshinskii–Moriya interaction. Quantum Inf. Process. 12, 3437 (2013)
27. Sharma, K.K., Pandey, S.N.: Entanglement dynamics in two parameter qubit–qutrit states under Dzyaloshinskii–Moriya interaction. Quantum Inf. Process. 13, 2017 (2014)
28. Sharma, K.K., Pandey, S.N.: Influence of Dzyaloshinskii–Moriya interaction on quantum correlations in two qubit Werner states and MEMS. Quantum Inf. Process. 14, 1361 (2015)
29. Sharma, K.K., Pandey, S.N.: Dzyaloshinskii–Moriya interaction as an agent to free the bound entangled states. Quantum Inf. Process. 15, 1539 (2016)
30. Sharma, K.K., Pandey, S.N.: Dynamics of entanglement in two parameter qubit–qutrit states with x-component of DM interaction. Commun. Theor. Phys. 65, 278 (2016)
31. Sharma, K.K., Pandey, S.N.: Robustness of W and Greenberger Horne Zeilinger states against Dzyaloshinskii–Moriya interaction Quant. Inf. Proc. 15, 4995 (2016)
32. Luo, S., Fu, S.: Measurement-induced nonlocality. Phys. Rev. Lett. 106, 120401 (2011)
33. Cavalcanti, D., Skrzypczyk, P.: Quantum steering: a review with focus on semidefinite programming. Rep. Prog. Phys. 80, 024001 (2017)
34. Sainz, A.B., Aolita, L., Piani, M., Hoban, M.J., Skrzypczyk, P.: A formalism for steering with local quantum measurements, arXiv:1708.00756 (2017)
35. Arnesen, M.C., Bose, S., Vedral, V.: Natural thermal and magnetic entanglement in 1D Heisenberg model. Phys. Rev. Lett. 87, 017901 (2001)
36. Plenio, M.B., Virmani, S.: An introduction to entanglement measures. Quant. Inf. Comp. 7, 1 (2007)
37. Wang, C.Z., Li, C.X., Nie, L.Y., Li, J.F.: Classical correlation and quantum discord mediated by cavity in two coupled qubits. J. Phys. B At. Mol. Opt. 44, 015503 (2011)