Quantum correlations in two-level atomic system over Herring-Flicker coupling

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In this article we study the thermal quantum correlations in tripartite atomic system under the existence of Herring-Flicker coupling among the atoms. Topologically different arrangements of three atom system is considered differing in their coupling pattern. These configurations are well known in classical networking theory. Quantum analogue of these configurations are found to play an important role in the design of quantum data buses that can transfer the quantum states to establish quantum communication. We specifically study the thermal pairwise quantum correlations in these topologies with Herring-Flicker coupling and found that atoms can be maximally entangled or quantum mechanically correlated in a controlled manner depending on arrangement of atoms. It is observed that asymmetrically arranged atomic systems are more strongly entangled as compared to the symmetrically arranged one, with the quantum correlations being unity for particular set of parameters. Thus, these systems will be propitious for various quantum protocols such as secure communication, quantum cryptography, quantum key distribution etc.

Keywords: Two-level atoms, Quantum discord, Entanglement, Herring-Flicker coupling

I. INTRODUCTION

Entanglement [1] and quantum discord [2, 3] are fascinating quantum correlations (QCs), which are crucial to quantum information processing. Varieties of algorithms have been developed based on these correlations for prime factorization [4], database search [5], phase estimation, and linear equation solving, to name a few. The development of quantum algorithms [6] is an active area of research, presently being extended to domains like machine learning [7], quantum cryptography [8], quantum key distribution [9], image processing, communication, game theory and many others [10]. Execution of various applications in a quantum computer requires an optimal architecture for the quantum computer. To fulfill this requirement the scientific community has been taking recourse to photonic systems, NMR, Bose Einstein condensate, superconducting qubits, ion trap, ultra cold atoms, quantum dots, nitrogen defects in diamond etc., based quantum computing experimental techniques [11].

There are efforts to design the important parts of the quantum computer, such as arithmetic logic unit, quantum memory and data buses [12, 13]. Quantum data bus is a very important ingredient of quantum computer, used to transport the data and supply it to various constituent units. One of the successful models of quantum data buses are spin chains [14, 15]. Experimentalists have successfully demonstrated quantum teleportation, quantum state transfer over the quantum data buses, wherein QCs play an important role. In the spin chains entanglement manifest in various physical quantities, such as temperature, susceptibility, heat capacity, and pressure are a measurable manner [16–18]. The first analysis of thermal entanglement has been provided by Nielsen 1998 [10] using the two-qubit Gibbs quantum state. Multiparticle thermal entanglement has been exploited by Brukner and Vedral in 2004 [19] and by Toth in 2005 [20] independently. Experimentally thermal entanglement has been identified even at 100 Kelvin in high temperature superconductors. In parallel, it is also important to investigate thermal behavior of quantum discord along with entanglement in spin chains as discord can be useful in certain quantum tasks. There are extensive studies on thermal QCs in spin chains equipped with varieties of configurations modeled with Heisenberg and Ising type interactions primarily. There are few investigations which include the coupling strength, Ωij, as function of position in diverse configurations of spin chains. Because of the quantum fluctuations and noises the coupling strength in quantum systems can vary with respect to the distance among quantum particles in realistic situations. Scaling and controlling of QCs, energy of the systems and phase transition can be tuned by varying the distance and hence the coupling strength. This approach can be used to perform better quantum applications. Investigating the phenomenon of entanglement sudden death [21–26] over the varying coupling distance is also an interesting area. The first attempt for the study of entanglement in the spin chain with long-range interactions has been done in 1988 by Haldane and Shastry [27, 28], in which the coupling strength follow the inverse square law. In the same direction, in XXZ Heisenberg spin chain with long-range interactions has been studied by B. Lin [29], XX Heisenberg spin chain with Calogero Moser type interaction has been studied by MA XiaoSan [30]. Further, in 2005, Huang and Kais [31] have shown the dependency of entanglement on Herring-Flicker (HF) coupling distance.
of a XY spin chain. The HF coupling has been experimentally implemented in designing the silicon based nuclear spin quantum computer [32, 33]. Recently, Sharma [34] has shown the dependency of thermal quantum discord and entanglement in XXX Heisenberg spin chain and has found the robust behaviour of quantum discord over the HF coupling distance. HF coupling arises from the differences of triplet and singlet configurations [35]:

$$\Omega(R) = E_{\text{triplet}} - E_{\text{singlet}} = 0.821 e^{-2R} R^{5/2} + O(R^2 e^{2R}).$$

Here $R$ is the distance between spins or atoms. It plays an important role in determining the energy difference between triplet and singlet state of the Hydrogen molecule. Here, we investigate the impact of HF coupling on QCs in a tripartite system equipped with three two-level atoms arranged in two topologically different configurations, such as line and loop configuration. It is important to mention that these topologies play an important role in designing data buses, spin star networks and studying the behavior of thermal pairwise QCs, it gives crucial insight regarding the quantum discord and entanglement with symmetric and asymmetric arrangement of atoms.

The paper is organized as follows: in Sec. II, we describe the Hamiltonian of two-level atomic system coupled via Herring-Flicker coupling. Sec. III is devoted to the study of QCs in symmetric arrangement of atoms followed by Sec. IV which deals with the study of QCs in asymmetric arrangement of atoms. Finally, we conclude with a summary of results and direction for future research.

II. THEORY AND MODEL

We consider a tripartite system equipped with three identical atoms coupled via HF coupling. We divide the study in two phases, first we consider the symmetric arrangement of atoms and asymmetric arrangement of atoms. Further, each arrangement is divided into two inequivalent topologies, line topology and the ring topology. The Hamiltonian for the system of two-level atoms is given by

$$H = \sum_{i=1}^{3} \omega_i S_i^z + \sum_{i\neq j=1}^{3} \Omega_{ij} S_i^+ S_j^-.$$  (1)

The first term describes the energy of isolated atom (in excited state) and the second term represents the dipole-dipole interaction between the ground state of one atom and the excited state of another atom, with $\Omega_{ij}$ is the dipole-dipole interaction strength (HF coupling), which is a function of the inter-atomic separation $'R'$. The nature of dipole-dipole interaction prohibits interaction between two atoms which are both in excited / ground state. In the above, $S_i^+ = (|1\rangle\langle0|)$, and $S_i^- = (|0\rangle\langle1|)$, are the raising and lowering operators of the $i^{th}$ atom in the spin representation. For simplicity, we consider the transition frequencies of all the three atoms to be the same, i.e., $\omega_A = \omega_B = \omega_C = \omega$. The presence of the coupling, $\Omega_{ij}$, between the atoms causes mixing of the energy levels leading to the creation of states with different correlations.

We now take into account the thermal effects, where, at finite temperature, the thermal density operator given by

$$\hat{\rho} = \frac{1}{\text{Tr}} \left( \sum_{i=1}^{8} |\psi_i\rangle \langle\psi_i| e^{-\beta\epsilon_i} \right).$$  (2)

Here $|\psi_i\rangle$ is an eigenstate with $\epsilon_i$ its eigenvalue. For pairwise thermal entanglement, one can obtain the reduced density matrices $\rho_{ijk}$ by taking partial trace of $\rho = \rho_{ijk}$ with respect to $k$, given by

$$\rho_{ij} = Tr_k(\rho_{ijk}).$$  (3)

In the next few subsections, we define the different measures of QCs.

A. Concurrence

Concurrence is a measure of entanglement [36] defined as,

$$C = \max\{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\}$$  (4)

where $\lambda_i$’s are the square root of the eigenvalues of the non-Hermitian matrix $R = \rho \hat{\rho}$ (or eigenvalues of Hermitian matrix $R \equiv \sqrt{\rho \rho^*}$) in decreasing order with $\hat{\rho}$

$$\rho = \sigma_y \otimes \sigma_y \rho^* \sigma_y \otimes \sigma_y.$$  (5)

Here asterisk denotes the complex conjugate and $\sigma_y$ is the Pauli matrix. The matrix $\hat{\rho}$ is known as spin flip matrix.

B. Quantum Discord

Quantum discord is non-classical correlation apart from entanglement which can even exist for separable states [2, 3]. Quantum discord is defined as the difference between mutual information and classical correlation. The difference arises because of the role played by measurement on the system. Quantum discord is physically described as a measure of the quantumness of correlations. It can easily be computed for specific reduced density matrices of the form X-type [37]. In the following
sections, we explore the behavior of QCs present in the symmetric and asymmetric arrangements of atoms, with each arrangement separated into line and loop configurations.

III. PAIRWISE CORRELATIONS: ASYMMETRIC ARRANGEMENT OF ATOMS

In this section, we introduce the schematic of arrangements of atom placed symmetrically along a line and on the vertices of an equilateral triangle, as depicted in Fig. 1. In the subsequent subsections, we investigate QCs present in the following configurations. The HF coupling between two atoms along with their inter-atomic distances is presented in respective subsections.

![Schematic diagram of the atomic system](image)

**FIG. 1.** (Color online) Schematic diagram of the atomic system in the line and loop configurations, with the identical two-level atoms localized at positions (a) A to C and (b) at the vertices of an equilateral triangle.

A. Line configuration

In this configuration, a system of three identical dipole-coupled two-level atoms are placed symmetrically along a line. The dipole-dipole interactions $\Omega_{AB} = \Omega_{BC} = 0.821 e^{-2R\sqrt{5}/2}$ and $\Omega_{AC} = 0.821 e^{-4R(2R)^{3/2}}$, since $AB = BC = R$ and $AC = 2R$. As depicted in Fig. 1(a), atoms are localized at positions A, B, and C, with equal spacing $R$ between adjacent atoms.

![Concurrence of bipartite system AB and AC](image)

**FIG. 2.** (Color online) Concurrence of bipartite system AB and AC as a function of transition frequency and inter-atomic spacing for two different temperatures. Here atoms are placed symmetrical along a line.

![Quantum discord of bipartite system AB and AC](image)

**FIG. 3.** (Color online) Quantum discord of bipartite system AB and AC as a function of transition frequency and inter-atomic spacing for two different temperatures. Here atoms are placed symmetrical along a line.
Fig. 2 and 3 show three dimensional plot of concurrence and quantum discord, respectively, as a function of transition frequency and inter-atomic distance for atoms arranged in line configuration symmetrically, for two temperatures $T = 0.005$ and $T = 0.1$. The maximum value of entanglement and discord for subsystem $AB$ is less than that of subsystem $AC$. At $T = 0.005$, from $R = 0$ to $R = 0.88$, QCs are zero for subsystem $AB$ while for subsystem $AC$ QCs attain their maximum value. The amount of QCs reduces as transition frequency and temperature increase. Fig. 4 shows the comparison between entanglement and discord as a function of inter-atomic distance for distinct values of temperature and transition frequency. The decrease in QCs is less when transition frequency increases while increase in temperature causes rapid decrease of amplitude of QCs. The increase in $\omega$ reduces the width of plot along axis $R$. The sharp fall in entanglement, at high temperature, is due to transition of eigenstates from pure to mixed and finally to separable states. Also, at lower temperatures entanglement dominates discord while at high temperature behavior reverses. At high temperature, discord remain non-zero even if entanglement vanishes and sustains over long range of $R$.

### B. Loop configuration

In this configuration, a system of three identical dipole-coupled two-level atoms are placed on vertices of an equilateral triangle. The dipole-dipole interactions $\Omega_{AB} = \Omega_{BC} = \Omega_{AC} = 0.821 e^{-2R R^2/2}$. Here, the distance between adjacent atoms is $R$. As illustrated in Fig. 1(b), atoms are localized at positions $A$, $B$, and $C$ on the vertices of an equilateral triangle.

Fig. 5 shows the variation of QCs for bipartite subsystem $AB$ as a function of transition frequency and inter-atomic spacing for two temperatures $T = 0.005$ and $T = 0.10$ while Fig. 6 shows the two dimensional plot of concurrence and discord as a function of inter-atomic space for different transition frequencies and temperatures. From both the figures it is evident that increasing the temperature and transition frequency decreases the amplitude of QCs. The decrease in amplitude of QCs is steeper with increase in temperature than transition frequency. The plot of QCs become narrower along $R$ with increasing the transition frequency. At high temperature, discord persists even if entanglement vanishes. The amount of QCs diminishes due to transition of eigenstates from pure to mixed and finally to separable states. Actually, thermal fluctuation dominates over quantum fluctuation.
FIG. 6. (Color online) QCs (concurrency blue and QD red) for subsystem $AB$ of loop configuration as a function of interatomic distance for different temperatures and transition frequencies. Here atoms are placed on vertices of an equilateral triangle.

FIG. 7. (Color online) Schematic diagram of the system in the line and loop configurations with identical two-level atoms localized at positions (a) $A$ to $C$, (b) atoms at the vertices of an isosceles, and (c) atoms at the vertices of a scalene.

IV. PAIRWISE CORRELATIONS: ASYMMETRIC ARRANGEMENT OF ATOMS

In this section, we present the schematic of asymmetric arrangements of atoms placed asymmetrically along a line and vertices of triangles, as depicted in Fig. 7. Here we consider Isosceles and Scalene as loop configurations. The plots of underlying QCs of following configurations is shown in next subsections. The HF couplings between two atoms along with inter-atomic distances between them are provided in subsequent subsections. The results with discussion are also present there.

A. Line configuration

In this configuration, a system of three identical dipole-coupled two-level atoms are placed asymmetrically along a line. The dipole-dipole interactions $\Omega_{AB} = 0.821 e^{-2R_{5/2}}$, $\Omega_{BC} = 0.821 e^{-2gR(gR)^{5/2}}$, and $\Omega_{AC} = 0.821 e^{-2R_{5/2}}$, considering $AB = R$, $BC = gR$, and $AC = (1 + g)R$. As depicted in Fig. 7(a), atoms have occupied positions $A$, $B$, and $C$. We have used $g = 1.5$.

Figs. 8 and 9 show concurrence and discord, respectively, for bipartite subsystems $AB$, $BC$, and $AC$ as a function of transition frequency and inter-atomic distance with $A$, $B$, and $C$ located asymmetrically along a line. The maximum value of entanglement and discord is close proximity to one for $T = 0.005$. Also, at $T = 0.005$, the extent of QCs for subsystem $AB$ is less than subsystem $AC$ for $R$ ranging from 0 to 0.80 but behavior reverses after $R = 0.80$ till QCs vanish clearly. The amplitude of QCs decrease with increasing transition frequency and temperature. Fig. 10 shows the comparison between entanglement and discord as a function of inter-atomic distance for different temperatures and transition frequencies. This displays that entanglement prevails discord at low temperature while discords exceeds entanglement at high temperature.
B. Loop configuration

In this configuration, a system of three identical dipole coupled two-level atoms are placed on vertices of Isosceles and Scalene. As shown in Figs. 7(b) and 7(c), atoms are localized at positions A, B, and C.

1. Atoms are placed on vertices of an Isosceles

The dipole-dipole interactions $\Omega_{AB} = 0.821 e^{-2R} R^{5/2}$ and $\Omega_{BC} = \Omega_{AC} = 0.821 e^{-gR}(gR)^{5/2}$ with $AB = R$ and $AC = BC = gR$. Atoms are positioned at A, B, and C as can be seen in Fig. 7(b). The value of $g$ use is 1.5.
FIG. 13. (Color online) QCs (concurrency blue and QD red) as a function of inter-atomic spacing for subsystems (a) $AB$ and (b) $AC$ for different transition frequencies and temperatures. Here atoms are placed on vertices of Isoceles.

FIG. 14. (Color online) Concurrence for bipartite systems $AB$, $BC$, and $AC$ as a function of transition frequency and inter-atomic distance for two different temperatures. Here atoms are placed on vertices of Scalene.

FIG. 15. (Color online) Quantum discord for bipartite systems $AB$, $BC$, and $AC$ as a function of transition frequency and inter-atomic distance for two different temperatures. Here atoms are placed on vertices of Scalene.

Figs. 11 and 12 show the variation of concurrence and discord, respectively, for bipartite subsystem $AB$ and $AC$ as a function of transition frequency and inter-atomic spacing. The maximum value of QCs is one for subsystem $AB$ while it is less than one for subsystem $AC$. The amount of QCs reduces at higher temperatures. This reduction is due to dominance of thermal fluctuations over quantum one. The amplitude of QCs for subsystem $AB$ is less than that of subsystem $AC$ for $R < 1$ and greater for $R > 1$ at $T = 0.005$. Also, Entanglement and discord eclipse each other for $\omega = 0.05$ and $T = 0.005$. The increase in transition frequency compresses the curve along $R$. Fig. 13 shows relative analysis of QCs as function of $R$ for several values of transition frequency and temperature. Entanglement dominates discord at low temperatures while discord surpasses entanglement at high temperatures. Further, discord remain non-zero even in the absence of entanglement.

2. Atoms are placed on vertices of a Scalene

The dipole-dipole interactions $\Omega_{AB} = 0.821 e^{-2R R^{5/2}}$, $\Omega_{AC} = 0.821 e^{-g_1 R (g_2 R)^{5/2}}$ and $\Omega_{BC} = 0.821 e^{-g_2 R (g_2 R)^{5/2}}$, as $AB = R$, $AC = g_1 R$, and $BC = g_2 R$. On e can see in Fig. 7(c) that atoms fill the positions $A$, $B$, and $C$ of vertices of Scalene. We have used $g_1 = 1.5$ and $g_2 = 2.0$. 

FIG. 16. (Color online) QCs (concurrency blue and QD red) as a function of inter-atomic spacing for subsystems (a) \( AB \) and (b) \( AC \) for different transition frequencies and temperature. Here atoms are placed on vertices of Scalene.

Figs. 14 and 15 display the change in amplitude of concurrence and discord, respectively, for bipartite subsystems \( AB \), \( BC \), and \( AC \) as a function of transition frequency and inter-atomic spacing. The maximum value of QCs is in neighbourhood of one. The amount of QCs reduces at higher temperatures and transition frequencies. However, loss is more with respect to temperature than transition frequency. Also, increase in \( \omega \) compresses the plot along \( R \) as can be seen in Fig. 16. The amount of QCs is more for bipartite subsystem \( AC \) than \( AB \) for \( R < 0.85 \) and less for \( R > 0.85 \) until QCs die out. The variation of QCs with inter-atomic distance for distinct values of temperature and transition frequency is displayed in Fig. 16. One can see that the nature of entanglement and discord look alike for all parameters. It is observed that discord persists significantly up to high temperature and over long range of \( R \).

V. CONCLUSION

In conclusion, we have systematically investigated the thermal behavior of QCs for three particle atomic system over HF coupling. We have plotted entanglement and discord as a function of system parameters (\( \omega \) and \( R \)) for two different temperatures. Three dimensional plots are presented in order to realize the nature of amplitude of QCs for different values of transition frequency (\( \omega \)) and inter-atomic distance (\( R \)) at fixed temperature. It is observed that arrangements of atoms play a significant role for the construction of maximally entangled systems. The systems having asymmetric arrangement of atoms are quantum mechanically correlated more strongly than systems having symmetric arrangement of atoms. Therefore, asymmetric arrangements of atoms must be favoured more over symmetric arrangements for various quantum protocols, such as secure communication, quantum internet, quantum cryptography, quantum key distributions etc. It is admitted that shareability of QCs vanishes for maximally entangled sources, as maximally entangled sources cannot share entanglement with third party \( C \). Further, at lower temperatures, entanglement eclipses discord while at higher temperatures discord surpasses over entanglement. The nature of entanglement and discord are almost same for all system parameters differing only in numerical value. Further, at high temperature, entanglement vanishes while discord persist in the system displaying the robustness of discord. Discord sustains over the large range of inter-atomic distance. These systems can be used as a source for emitting highly focused or superradiant light [38, 39]. Highly focused nature of light is effective for lithography.

VI. ACKNOWLEDGEMENTS

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