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Quantum Discord and Entanglement of Hydrogen Molecule under Thermal Fluctuation and Noise

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Abstract: This article is devoted to analyze the measures of electron–electron correlation for hydrogen molecule in ground and thermal states in presence of applied magnetic field. It is found that quantum discord is more robust then the entanglement in the sense that quantum discord have significant correlation as compared to the entanglement. It is further discovered that the quantum discord and entanglement can be controlled by thermal and magnetic effects. In addition it is investigated that the decoherence degrades both the entanglement and quantum discord. However, phase damping channels degrades more heavily compared to the amplitude damping. Finally, both the entanglement and quantum discord vanish asymptotically under decoherence, with no ESD is seen.

Keywords: Quantum correlations; Hydrogen molecule; Decoherence

1 Introduction

Quantum entanglement is a major resource for a diversity of quantum information processing tasks, such as quantum cryptography, quantum error correction and superdense coding [1,2,3,4]. Although entanglement is a valuable resource in quantum information processing and being used for a long time to study the quantum correlations [5] but it does not describe all the aspects of the quantum correlations, also resides only in non-separable states. There are some other kinds of quantum correlations besides entanglement that are also responsible for the quantum advantages over their classical counterparts [6,7]. Olivier and Zurek [8] suggest a more fundamental degree of quantum correlation than entanglement called quantum discord (QD). Quantum discord can also exist in separable states and is defined as a measure of nonclassical correlations between the two subsystems of a quantum system. Investigation of quantum discord is currently a very active area and has been studied intensely due to its potential applications in quantum communications and information processing[9, 10,11,12,13,14,15,16].

Recovering the electrons correlations for large systems remains one of the most challenging problems in quantum physics, and has a strong influence on many atomic, molecular [17], and solid properties [18]. Recently a lot of attention has been paid to the quantum correlations in the spin system, such as the Ising model [19] and all kinds of Heisenberg XX, XY, XXZ, XYZ models [20,21,22,23]. There exist many measuring kits for electrons correlation strength in the literature such as the statistical correlation coefficients [24], the Shannon entropy, entanglement, and the quantum discord [25,26]. Beyond the theoretical spin model in solid state physics, more realistic physical systems have been considered. For example, a detailed investigation on spin-3/2 electron and nuclear spin states [27] and the thermal quantum discord in hydrogen atom and Li atom has been presented [28, 29]. Huang and Kais [30] measure the electron–electron correlation for hydrogen molecule by using Ising model. They presented the entanglement as an alternative measure of the electron-electron correlation in quantum calculations for atoms and molecules.

The behavior of correlations under the action of decoherence is another important problem. Implementation of decoherence on dynamics of the quantum correlation for a certain class of states in a two-qubit, qubit-qutrit and qutrit-qutrit system shows that the entanglement may exhibit a sudden death (ESD), while quantum discord vanish asymptotically [31,32,33, 34].

In this work we measures the electron–electron correlation for hydrogen molecule in ground and thermal

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states using entanglement and quantum discord. In addition we also investigate the effects of decoherence on the properties of entanglement and quantum discord. Our finding shows that the thermal and decoherence effects degrades both the entanglement and quantum discord. Further more, the entanglement and quantum discord both vanish asymptotically under decoherence, with no ESD is seen.

2 Formalism

In this section, we introduce the measures of quantum discord used in our work. The quantum discord that measures the amount of non-classical correlations, is defined as the difference between total and classical correlations.

$$D(\rho^{12}) = I(\rho^{12}) - C(\rho^{12}), \tag{1}$$

The total mutual correlations in defined as

$$I(\rho^{12}) = S(\rho^{1}) + S(\rho^{2}) - S(\rho^{12}), \tag{2}$$

where $S(\rho) = -Tr(\rho\log_2\rho)$ is the von-Neumann entropy with ρ^{12} and ρ^{1}, ρ^{2} being the density matrix of the total system and reduced density matrices of subsystems, respectively. The amount of classical correlations present in a quantum state is measured by [8,35]

$$C(\rho^{12}) = S(\rho^{2}) - \min_{[\mho_k^1]} \sum_k p_k S(\rho_k^2), \tag{3}$$

where $[\mho_k^1]$ defines a set of orthonormal projection operators, acting on the subsystem 1 and $\rho_k^2 = Tr_1((\mho_k^1 \otimes I)\rho^{12})/p_k$ is the remaining state of the subsystem 2 after obtaining the outcome k with the probability $p_k = Tr((\mho_k^1 \otimes I^2)\rho^{12})$. The two projection operators for a qubit system can be expressed as [36]

$$\mho_A^1 = \frac{1}{2}(I + \sum_{j=1}^{3} n_j\sigma_j), \tag{4}$$

$$\mho_B^1 = \frac{1}{2}(I - \sum_{j=1}^{3} n_j\sigma_j), \tag{5}$$

where I stands for identity matrix, σ_j are the three Pauli spin matrices and $n = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)^T$ is a unit vector on Bloch sphere with $\theta \in [0,\pi]$ and $\phi \in [0,2\pi]$.

Vidal and Werner [37] gives negativity as a quantitative way for judging whether the state is entangled or not, it is defined as,

$$N(\rho) = \sum_i |\mu_i|\,,$$

where μ_i is the negative eigenvalue of ρ^{T_1}, and T_1 denotes the partial transpose with respect to the first system. The negativity can also defined as,

$$N(\rho) = \frac{\left\|\rho^{T_1}\right\|_1 - 1}{2},$$

where the trace norm of ρ^{T_1} is equal to the sum of the absolute values of the eigenvalues of ρ^{T_1}.

3 The Model

We use the same model as described in reference [30], This is a model of two spin-$1/2$ electrons with an exchange coupling constant J in an effective transverse magnetic field of strength B. The Hamiltonian for such a system is given by

$$H = -J/2(1+\gamma)\sigma_1^x \otimes \sigma_2^x - J/2(1-\gamma)\sigma_1^y \otimes \sigma_2^y - B\sigma_1^z \otimes I - BI \otimes \sigma_2^z, \tag{6}$$

where σ^a are the Pauli matrices($a = x,y,z$) and γ is the degree of anisotropy. For $\gamma = 1$ Eq.(6) reduces to the Ising model, where as for $\gamma = 0$ it is the XY model. The exchange coupling constant (J), between the spins of the two electrons, can be calculated as half the energy difference between the lowest singlet and triplet states of the hydrogen molecule. Herring and Flicker [38] have shown that J for H_2 molecule can be estimated as a function of the interatomic distance R. In atomic units, the expression for large R is given by

$$J(R) = -0.821R^{5/2}e^{-2R} + O(R^2e^{-2R}),$$

this model admits an exact solution, with the following four eigenvalues

$$\lambda_1 = -J,\ \lambda_2 = J,\ \lambda_3 = -\sqrt{4B^2 + J^2\gamma^2},\ \lambda_4 = \sqrt{4B^2 + J^2\gamma^2},$$

and the corresponding eigenvectors

$$|\Phi_1\rangle = \begin{pmatrix} 0 \\ 1/\sqrt{2} \\ 1/\sqrt{2} \\ 0 \end{pmatrix}, |\Phi_2\rangle = \begin{pmatrix} 0 \\ -1/\sqrt{2} \\ 1/\sqrt{2} \\ 0 \end{pmatrix}, |\Phi_3\rangle = \begin{pmatrix} \sqrt{\frac{\alpha+2B}{2\alpha}} \\ 0 \\ 0 \\ \sqrt{\frac{\alpha-2B}{2\alpha}} \end{pmatrix}, |\Phi_4\rangle = \begin{pmatrix} -\sqrt{\frac{\alpha-2B}{2\alpha}} \\ 0 \\ 0 \\ \sqrt{\frac{\alpha+2B}{2\alpha}} \end{pmatrix},$$

where $\alpha = \sqrt{4B^2 + J^2\gamma^2}$.

For simplicity we take $\gamma = 1$, Eq. (6) reduces to the Ising model with the ground state energy λ_3 and the corresponding eigenvector $|\Phi_3\rangle$. Excited state of typical system at thermal equilibrium is given by

$$\rho(T) = \frac{e^{-\beta H}}{Z},$$

where H is the Hamiltonian, $\beta = \frac{1}{k_BT}$ and $Z = Tr(e^{-\beta H})$ is the partition function. From this point onward we choose the Boltzmann constant $k_B = 1$. The density operator for the above system in thermal equilibrium can be written as

$$\rho(T) = \frac{1}{Z}(e^{\beta J}|\Phi_1\rangle\langle\Phi_1| + e^{-\beta J}|\Phi_2\rangle\langle\Phi_2| + e^{\beta\alpha}|\Phi_3\rangle\langle\Phi_3| + e^{-\beta\alpha}|\Phi_4\rangle\langle\Phi_4|, \quad (7)$$

The interaction between a system and its environment is studied in terms of various quantum channels such as phase damping channels and amplitude damping channels. The dynamics of a system in the presence of quantum channels are best described using the Kraus operators formalism. The Kraus operators for phase damping channels are

$$E_1 = \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{1-p} \end{pmatrix}, \; E_2 = \begin{pmatrix} 0 & 0 \\ 0 & \sqrt{p} \end{pmatrix},$$

and for amplitude damping channels are

$$E_1 = \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{1-p} \end{pmatrix}, \; E_2 = \begin{pmatrix} 0 & \sqrt{p} \\ 0 & 0 \end{pmatrix},$$

where p represents the quantum noise parameter.

The evolved states of the initial density matrix of such a system when it is influenced by environments can be given compactly by

$$\rho(t) = \sum_{i,j=1}^{2} F_j E_i \rho(0) F_j^{\dagger} E_i^{\dagger} \qquad (8)$$

here, the operators E_i and F_j are the Kraus operators which are used to describe the noise channels acting on the qubit A and B, respectively. They satisfy the completeness $\sum_i^2 E_i^{\dagger} E_i = I$ and $\sum_i^2 F_i^{\dagger} F_i = I$ relations for all t.

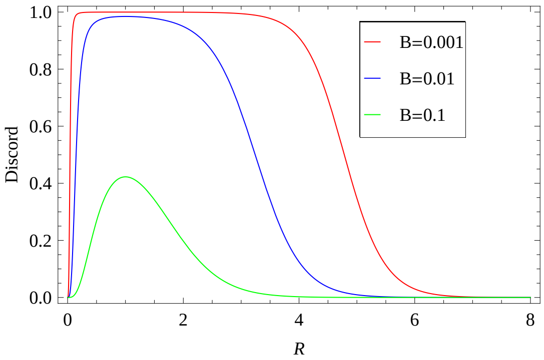

Fig. 1: Quantum discord is plotted against the inter atomic distance R for three different values of magnetic field

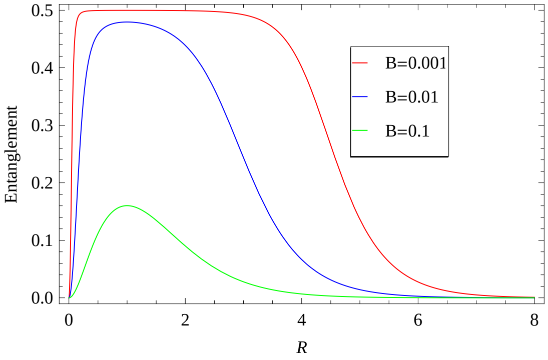

Fig. 2: Entanglement is plotted against the inter atomic distance R for three different values of magnetic field B.

4 Results and Discussions

Quantum discord and entanglement as a function of interatomic distance R, for different values of the magnetic field strength B is plotted in Figure 1 and Figure 2. One can see that at the united atom limit, $R = 0$, both quantum discord and entanglement are zero because exchange coupling constant $J = 0$. As R increases, the exchange interaction increases leading to increasing quantum discord and entanglement. However this increase reaches a maximum limit and then finally decreases exponentially with R.

Overall behaviors of quantum discord and entanglement are similar where as one can observed that the value of correlation for quantum discord is almost two times greater then that of entanglement for each values of magnetic field B, hence quantum discord have significant correlation as compared to entanglement. Figure 1 and Figure 2 also shows that the quantum discord and entanglement decreases with increasing the magnetic field strength B.

Figure 3 reveals the thermal effect on quantum discord of hydrogen molecule in an external tunable magnetic field. In the case of $B = 0.001$ the quantum discord for ground state is non zero for $R \leq 7A^{\circ}$ but when thermal effects are applied the quantum discord is almost reaches to zero for $R \leq 5A^{\circ}$. Similarly the maximum values of correlation for ground state is 1 but when thermal effects are applied the correlation decreases to 0.2.

hence when thermal effects are applied not only the value of quantum discord decreases but also dies earlier with R.

We analyze the influence of temperature on quantum discord with the inclusion of magnetic field. Figure 4 depicts that for quantum discord, there exist two completely different regions of the magnetic field, namely $0 \leq B \leq 1/2$ and $B > 1/2$. In the case of $0 \leq B \leq 1/2$, the quantum discord will start from a finite value at zero temperature and in the case of $B > 1/2$ it decreases with the increasing temperature.

The higher temperature can make quantum discord weaker, but quantum discord is always non-vanishing even at higher temperatures. It can be seen that by decreasing the thermal and magnetic effect an increases in quantum discord has been observed. So the quantum

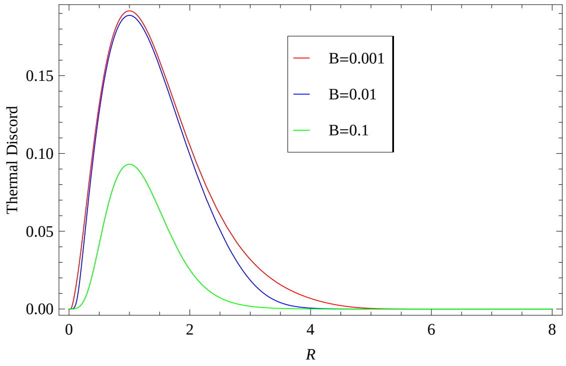

Fig. 3: Quantum discord is plotted against the inter atomic distance R for three different values of magnetic field B

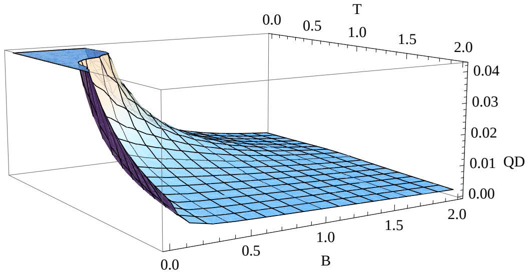

Fig. 4: The quantum discord is plotted as a function of temperature T and the external magnetic field B for $R = 1$.

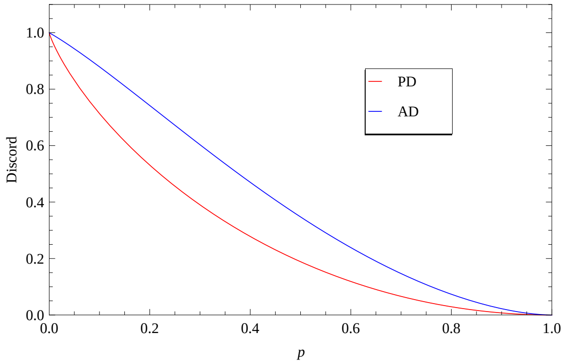

Fig. 5: The quantum discord is plotted as a function of quantum noise parameter p for phase damping channels and amplitude damping channels with the external magnetic field $B = 0.001$ for $R = 1$.

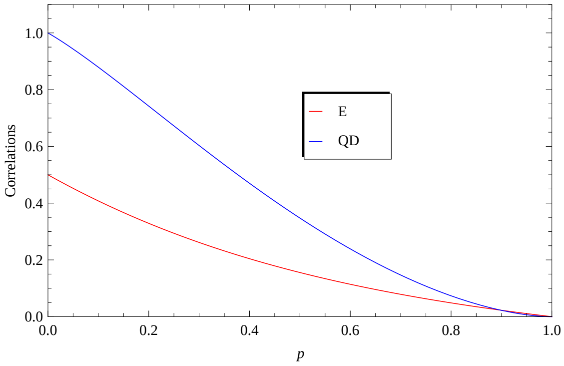

Fig. 6: Correlation is plotted as a function of quantum noise parameter p for entanglement and quantum discord with the external magnetic field $B = 0.001$ for $R = 1$.

discord and entanglement can be controlled by thermal and magnetic effects.

In Figure 5 we investigated the effects of phase damping and amplitude damping on the properties of quantum discord for ground state at inter atomic distance $R = 1$ against quantum noise parameter. We observed that the effect of these decoherences are to degrades the quantum discord, however, phase damping channels degrades more heavily as compared to the amplitude damping, same results are true for entanglement.

Finally the results of quantum discord and entanglement of amplitude damping channels as a function of quantum noise parameter are compared in Figure 6. It is found that both the quantum discord and entanglement vanishes only in the asymptotic limit, with no entanglement sudden death (ESD) is seen.

5 Conclusion

In conclusion, we have calculated the measures the electron–electron correlation for hydrogen molecule in ground and thermal states in presence of the applied magnetic field. It is shown that by decreasing the thermal and magnetic effect an increases in quantum discord and entanglement has been observed, so the quantum discord and entanglement can be controlled by thermal and magnetic effects. We also depicted that quantum discord is more robust then the entanglement in the sense that quantum discord have significant correlation as compared to entanglement. Moreover The effect of decoherence is observed to, degrades the entanglement and quantum discord. However, phase damping channels degrades more heavily as compared to the amplitude damping. Finally both the entanglement and quantum discord vanish asymptotically under decoherence, with no ESD is seen. Therefore, we expect that these features of quantum discord revealed in the hydrogen molecule may have some significant applications in quantum communications and information processing.

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