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Quantum transfer energy in the framework of time-dependent dipole-dipole interaction

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ABSTRACT

In this work, we examine the process of the quantum transfer of energy considering time-dependent dipole-dipole interaction in a dimer system characterized by two-level atom systems. By taking into account the effect of the acceleration and speed of the atoms in the dimer coupling, we demonstrate that the improvement of the probability for a single-excitation transfer energy extremely benefits from the incorporation of atomic motion effectiveness and the energy detuning. We explore the relevance between the population and entanglement during the time-evolution and show that this kind of nonlocal correlation may be generated during the process of the transfer of energy. Our work may provide optimal conditions to implement realistic experimental scenario in the transfer of the quantum energy.

Introduction

The absorption of light energy by an atom is typically followed by its electronic transition from the ground state to the excited state. This electronic energy relocated to another nearby atom by a process known as resonance energy transfer. The most favoring spectral features for better capture of solar light and efficient resonance energy transfer occur when the spectral and spatial cross section in a photosynthetic light-harvesting system is high [1–7]. The quantum transfer of energy between a donor atom (the one that gets excited) to an acceptor atom is usually described by an incoherent process. In this context, the energy transfer with the impact of inter-atomic interaction in the framework of dipole-dipole coupling is described using electronic coupling elements. Coherent energy transfer, however, is considered as an interesting period of photosynthesis, by which excitation energy get transferred efficiently from the photosensitizers (pigments) to the reaction center as recently reported [8–14]. In general, the transfer of energy via a network of pigments is a very complicated process. To have an idea about the mechanism of light harvesting complex, a simple model representing the light harvesting complex based on a dimer system consists of a donor (the one excited) and an acceptor (the one photosensitized) is proposed. A number of both theoretical and experimental studies have been recently investigated using the coherence in the transport of the quantum energy [15,16]. Studies in multichromophoric quantum systems indicated that exciton delocalization together with pure dephasing has been considered as effective parameters in improving the efficiency of quantum transfer [17,18]. On the other hand, the correlations introduced by a bath in different site energies are shown to affect the dephasing noise.

Recently, some experiments have been revealed the existence of quantum processes that enjoy the coherence alive for a long time in space ranges [19]. Especially, within the photosynthetic processes in light-harvesting complex processes, a typical oscillatory dynamics can include the quantum coherence. The result obtained clarified that in the quantum systems of photosynthetic

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antenna the correlation may be eliminated in the dynamic processes. The longest living of the quantum coherence alone, however, will not be suitable to get a high efficiency of quantum energy transfer. Furthermore, the quantum coherence provides an essential role in controlling the dynamical properties of a system dynamics, considering dissipative and phase damping, and its populations of excitation in a given quantum state.

As known that the entanglement is one of the most promising phenomena in quantum technology, which proposed the nonlocal correlations between different physical systems [20–28]. In this way the investigation of entanglement as the main type of quantum correlation and its outcomes of quantum measurements led to understand and solve different physical problems [29,30]. More recently, the development of quantum information processing (QIP) has been provided rise to a large knowledge and also augmented the literature of entanglement phenomenon, which has performed the optimal tasks of QIP and quantum metrology [31–37]. The significance of entanglement in different applications has led to analysis and investigation of high-dimensional quantum systems and bring the new role of this kind of correlation in many-particle quantum systems [38].

Understanding the very fundamental mechanism responsible for high-efficiency energy transfer in photosynthesis is expected to lead to both fundamental and practical implications. Our results reported recently on a single-excitation energy transfer have shown that the enhancement probability for this process benefits well from the photon-number transition, energy detuning, classicality of the field and time-dependent coupling effect for a dimer system displayed by two-level systems (TLSs) interacting with a cavity field [39]. In this paper, a model that almost describes a realistic experimental scenario based on an atom-atom interaction will be adapted to study the acceleration and speed effects in the interaction between the pigments. We consider the coupling term as a sinusoidal function of a second degree of the time. In a single excitation from a donor to an acceptor where each one is modeled by a TLS, the coupling effect, and energy frequencies, which might affect the efficiency of the coherent energy transfer will be explored in details. This form of the coupling term could include the acceleration and speed effects of the TLSs on the physical quantities during the process of the energy transfer. Additionally, the dynamical behavior of the entanglement of the pigment states through the energy transfer process will be investigated.

This paper is structured as follows. In Section 'Model of the physical system', we present the formalism that describes the model of the quantum transfer energy in the framework of time-dependent dipole-dipole interaction and showing the dependence of the physical parameters on the population dynamics for a single-excitation and entanglement in the dimer system. In Section 'Result and discussions', we present the numerical results and explain the physical phenomena that can be observed in the framework of the atomic motion. Finally, some conclusions are given in Section 'Conclusion'.

Model of the physical system

Thus, a dimer system with its dipole-dipole interaction and time-dependent coupling effect is the undertaken physical system.

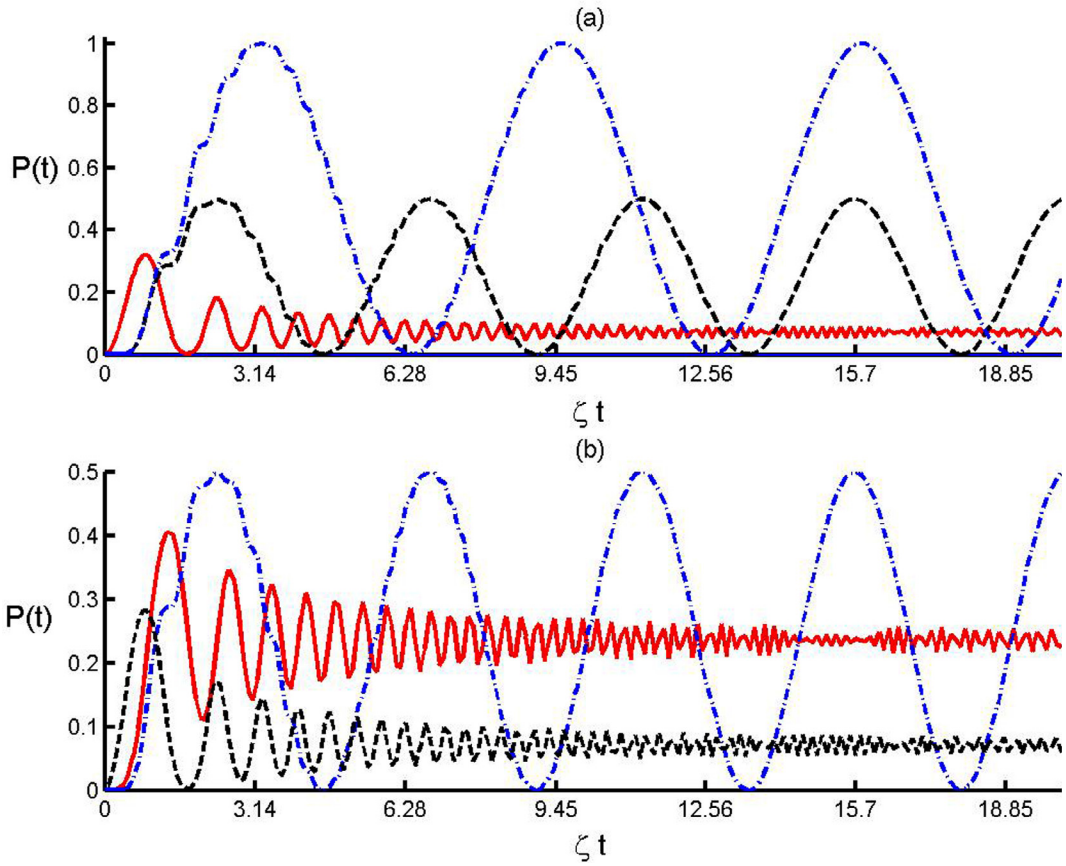

Fig. 1. The probability to get the acceptor in an excited state as a function of the scaled time ζt. Fig. 1(a) presents the case of resonance $\omega_d = 0$ and Fig. 1(b) is corresponds to the case of the energy detuning $\omega_d = 1$. The solid red line is for the time-dependent coupling $\lambda(t) = \xi \sin(t^2 + t)$, the dashed black line is for the time-dependent coupling $\lambda(t) = \xi \cos(t^2 + t)$, and the dashed-dotted blue is for the time-dependent coupling $\lambda(t) = \xi \sin^2(t^2 + t)$. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

The dimer is defined as a pair of TLSs, which composes of TLS1 and TLS2 as donor and acceptor systems with their energy separations ω_1 and ω_2, respectively. The Hamiltonian for the donor and acceptor systems can be written as

$$H_{\mathrm{TLSs}} = \frac{\omega_1}{2}\sigma_1^z + \frac{\omega_2}{2}\sigma_2^z + \lambda(t)\left(\sigma_1^+\sigma_2^- + \sigma_1^-\sigma_2^+\right), \quad \hbar = 1, \tag{1}$$

where $\lambda(t)$ presents the dipole–dipole interaction strength between TLS1 and TLS2 and $\sigma_j^+ = |e_j\rangle\langle g_j|$ (raising), $\sigma_j^- = |g_j\rangle\langle e_j|$ (lowering), and $\sigma_j^z = |e_j\rangle\langle e_j| - |g_j\rangle\langle g_j|$, where $|e_j\rangle$ (resp.$|g_j\rangle$) is the excited (resp. ground) states of the j$^{\mathrm{th}}$ ($j = 1, 2$) TLS. The physical process for excitation energy transfer and the nonlocal correlation between TLS1 and TLS2 is assured by the dipole–dipole interaction defined in time-dependent coupling. The generalization from the constant coupling ζ to arbitrary time dependent coupling $\lambda(t)$ provides us to explore new physical situations not discussed before. In this manuscript we consider that the coupling term is modelled by the following three cases: $\lambda(t) = \zeta\cos(t^2 + t), \lambda(t) = \zeta\sin(t^2 + t)$, and $\lambda(t) = \zeta\sin^2(t^2 + t)$.

In order to investigate the populations of the transfer of energy in single excitation from the donor to the acceptor, we consider that the donor is initially defined in excited state $|e_1\rangle$ and the acceptor is in a ground state $|g_2\rangle$

$$|\psi_{12}\rangle = |e_1 g_2\rangle, \tag{2}$$

and the probability to get the acceptor in an excited state (single excitation energy transfer) at time t will be

$$P(t) = \mathrm{Tr}\left(\rho_2\sigma_2^+\sigma_2^-\right). \tag{3}$$

In this paper, the entanglement of the formation is considered to measure the nonlocal correlation between the donor and acceptor. The entanglement of formation is widely explored to implement various tasks in the quantum information theory as quantum key distribution [40], the quantum teleportation [41], etc. For a bipartite quantum system, entanglement of formation is defined as a von Neumann entropy of the reduced density matrix

$$E = -\mathrm{Tr}(\rho_1\log_2\rho_1) = -\mathrm{Tr}(\rho_2\log_2\rho_2), \tag{4}$$

where ρ_1 (resp. ρ_1) is the reduced density matrix of TLS1 (resp. TLS2).

Result and discussions

The coherence property is of prime importance in the theory of quantum mechanics. In this regard, oscillation phenomena that widely found in a quantum system, are the result of coherent aspects. Tentatively, the light harvesting complex was demonstrated to show that the dynamics of electronic oscillation has inspired a great interest for understanding the nature of this process and whether it plays role in biological systems [42,43]. Previous studies reported that complete classical systems may also comprise oscillations [44]. Therefore, it is of prime importance to shed light on these oscillations by means of quantum mechanics, so as to disclose the fundamentals of light harvesting mechanism in nature, which may inspire scientists to harness the solar light for better clean energy for the future.

Using the coupling λ and the frequency ω_d as controllable parameters, we plot in Fig. 1 the dynamics of the population for

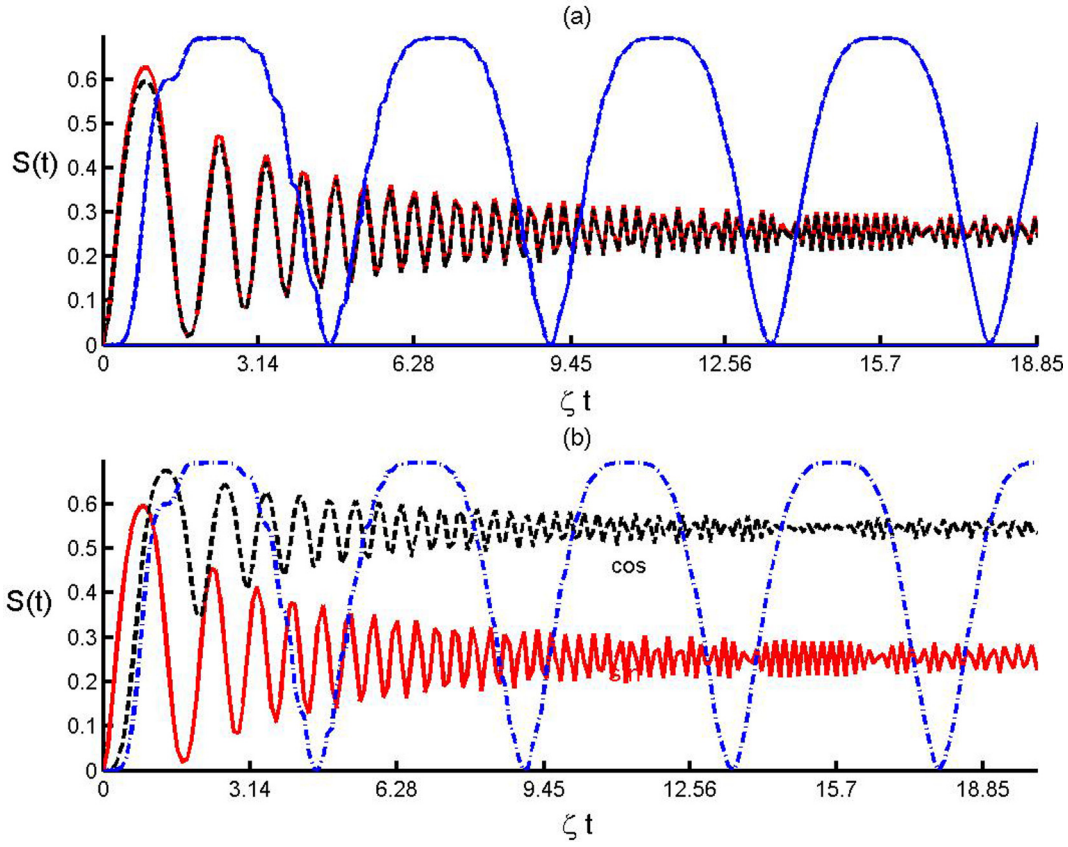

Fig. 2. The entanglement between the pigments as a function of the scaled time ζt. Fig. 1(a) presents the case of resonance $\omega_d = 0$ and Fig. 1(b) is corresponds to the case of the energy detuning $\omega_d = 1$. The solid red line is for the time-dependent coupling $\lambda(t) = \xi\sin(t^2 + t)$, the dashed black line is for the time-dependent coupling $\lambda(t) = \xi\cos(t^2 + t)$, and the dashed-dotted blue is for the time-dependent coupling $\lambda(t) = \xi\sin^2(t^2 + t)$. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

single-excitation energy transfer for the different kinds of the dipole–dipole interactions. Interestingly, we observe that the population exhibits oscillatory behavior during the time evolution and its amplitude and periodicity time are dependent on the form of the dipole–dipole interaction $\lambda(t)$ and value of the energy detuning $\omega_d = \omega_1 - \omega_2$. From Fig. 1(a) and 1(b), the dynamics of the population is profoundly impacted by the form of the function that describes the dipole–dipole interaction. Depending on the choice of the coupling term, the time-dependent effect reduces the oscillations and enhances the probability amplitude. It appears that there exists a period of time within which the probability reaches its maximum. This period of time is dependent on the coupling $\lambda(t)$ and becomes much larger when $\lambda(t) = \zeta \sin^2(t^2 + t)$. On the other hand, we find that the decrease of the detuning leads to increase the amplitude of the population and then the quantum transfer of energy in the dimer. The energy emitted by the donor may cause excitation for several acceptors, if the detuning energy parameter is large. In this case, the excitation of several acceptors would decrease the time of periodicity and thus enhance oscillations during the evolution time. Therefore, proper choice of detuning energy and the form of the coupling term describing the dipole-dipole interaction during the energy transfer process would greatly favor the optimal steady population value for a single excitation energy transfer.

Let us now analyze the behavior of entanglement for the dimer state as a function of the physical parameters for the three kinds of the dipole-dipole interaction. The quantum entanglement of the dimer system states (TLS1 and TLS2) with some interesting properties are shown in Figs. 2. It is observed that the entanglement of formation suffers periodic oscillations during the time-evolution, with the phenomena of sudden death and birth for the case of the coupling $\lambda(t) = \xi \sin^2(t^2 + t)$. On the other hand, the amount of entanglement exhibits damping oscillations and remains constant as the time becomes large for other forms of coupling terms. It may also be interesting to see that the parameter ω_d and its choice may greatly affects the entanglement variation during the evolution time. The degree of the entanglement of the dimer state TLS1 and TLS2 decreases and thus reduces and/or inhibit the quantum coherence effect in the dimer system as the detuning energy gets far from the resonant case. It may also be interesting to mention that the enhancement of entanglement amount for the pair system state TLS1 and TLS2 may be benefit by the choice of the time-dependent coupling and takes its maximal values for the case of $\lambda(t) = \xi \sin^2(t^2 + t)$. This result confirms that the appropriate choice of the physical parameters leads to the high generation of the quantum entanglement within the process of coherent energy transfer.

Conclusion

Photosynthesis, in which photosynthetic pigments possess the solar light as photosensitizers and convey the excitation energy to the reaction center is very much affected by coherent excitation energy transfer. The transmit of a single excitation from the photosensitizer to the center of reaction is a complicated physical process. Thus the mechanism of such process can be revealed by studying a dimer system of a donor–acceptor type and modeled by bipartite two-level systems. In summary, the coherent excitation energy transfer for the studied model in the presence of the acceleration and speed effects of the atoms in the dimer have been investigated. The necessary parameters that simulate the real experimental scenario for optimal generation of nonlocal quantum correlation and energy transfer have been analyzed and explored. The results indicated that the enhancement of the process benefits well from both detuning energy and time-dependent coupling effect. Furthermore, the degree of quantum entanglement in the dimer system which generated during the energy transfer process using the von Neumann entropy as a quantifier of entanglement was also investigated. Finally, the physical parameters that describe the relationship between the entanglement and the transfer probability during the evolution time is explored.

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