Energy transfer and correlation dynamics in a three-quasi-spin-pigment system*

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(Received 28 November 2012; revised manuscript received 5 January 2013)

In this paper, the effects of quantum and classical correlations on the excitation energy transfer in a three-quasi-spin-pigment system are investigated. We first study the dependence of the energy transfer efficiency on various initial correlations of the donor pigments, and find that the initial concurrence is crucial to the efficiency no matter whether the initial states are pure or mixed. We then demonstrate the dynamics of correlations of the system and observe the appearance of sudden death of quantum correlations in the donor pigments. The relation between the energy transfer efficiency and the dynamics of correlations in the donor pigments is also discussed.

Keywords: energy transfer, correlation, quasi-spin-pigment system

PACS: 71.35.–y, 03.67.Mn, 03.65.Ud **DOI:** 10.1088/1674-1056/22/5/057104

1. Introduction

Young's double-slit interfering experiment, where the spatial coherence of light was proposed, not only plays a major role in the general acceptance of the wave theory of light,[1] but also opens the windows to the applications of wave optical techniques. In quantum aspects, the coherence has two types, classical and quantum. The quantum coherence, which corresponds to the quantum correlation among different sites, can be used to induce many nonclassical phenomena. Recent research shows that long-lived quantum coherence can be found in bio-systems, such as the light harvesting complex,[2–6] the compass system of robins,[7–9] and other biological systems.[10,11] Moreover, experiments performed on bacteriochlorophyll antenna complexes at 77 K[12] and even at room temperature[13,14] show that long-lasting quantum coherence exists in photosynthetic processes under normal conditions, and it influences the efficiency of excitation transfer. In the process of photosynthesis, the charge separation of multi-pigments is first stimulated by photons from solar light, and then the excitation energy is transferred through other pigments until it is accepted by a reaction center.[2] The wave packet of input photons with the classical or quantum coherence can induce the classical or quantum coherent charge excitation because the wave packet has a similar scale to the pigments of antenna proteins.[15,16] The initial excited coherence of the antenna pigments, just like the wave coherence in Young's experiments, makes the excitation transfer to the acceptor pigments in suitable sites have highly enhanced efficiency. The initial coherence is quantum if the initial excited states of the antenna pigments are pure, and the efficiency of the excitation transfer depending on the initial quantum coherence linearly in this case has already been investigated analytically and numerically.[17] However, the initial states of the antenna pigments are generally mixed before being transferred because of noise pollution or being excited by incoherent solar photons. In this case, we need to distinguish the effects coming from the classical and the quantum coherences of the initial states to the efficiency of the excitation transfer in detail. Moreover, it is necessary to investigate the dynamics of correlation and the entanglement distribution among pigments in the biological conditions because bio-systems are the natural potential materials for quantum information and quantum computing.[18,19] Usually, the transfer of excitation from antenna proteins to the reaction center is a very complicated physical process, since the practical transfer process takes place on a complicated network of pigments. However, the basic physical mechanism can be revealed by studying a trimer core unit in photosynthetic bacteria, which consists of two donors and one acceptor.

Based on the above consideration, in this article, we study the quantum dynamics of an ideal model including three quasi spins, where each spin has its ground and excited levels to model the charge separation of a protein pigment. We suppose that the donor system has two spins being excited initially, and the excitation energy transfers from the two donor spins to the remaining acceptor spin. We will also calculate the dynamics of quantum concurrence, quantum discord, and classical correlation of the trimer. We will give our numerical results by choosing all parameters for biological conditions.[20–25]

The paper is organized as follows. In Section 2, the theoretical model of a three-quasi-spin-pigment system is pro-

*Project supported by the National Natural Science Foundation of China (Grant No. 11174233) and the National Basic Research Program of China (Grant No. 2011CB311807).

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posed, and the necessary calculus is presented. In Section 3, we review the measures of classical correlation and quantum correlation. The main results and discussion are presented in Section 4. Conclusions are given in Section 5.

2. Theoretical model

The physical system under consideration is a three-quasi-spin-pigment system, which consists of two donor pigments and one acceptor pigment. Each pigment has a ground level $|g\rangle$ and an excited level $|e\rangle$, and the evolution of the quantum states will be restricted to the zero- and one-excitation subspaces.[3–6] We have four complete bases, where $|0\rangle = |g,g;g\rangle$ denotes that all three pigments are in the ground states, $|1\rangle = |e,g;g\rangle$ as well as $|2\rangle = |g,e;g\rangle$ denotes that one of the donor pigments is in the excited state, and $|3\rangle = |g,g;e\rangle$ denotes that the acceptor pigment is in the excited state. The Hamiltonian of the system is composed of two parts, $H = H_0 + H_{\rm I}$. Here H_0 represents the free energy of each pigment

$$H_0 = \sum_{\alpha=1}^{3} \varepsilon_\alpha \sigma_\alpha^+ \sigma_\alpha^-, \tag{1}$$

where $\sigma_\alpha^+ = |e_\alpha\rangle\langle g_\alpha|$ and $\sigma_\alpha^- = |g_\alpha\rangle\langle e_\alpha|$ are the raising and lowering operators for pigment α, respectively, and ε_α is the corresponding excitation energy. The $H_{\rm I}$ is the interaction Hamiltonian

$$H_{\rm I} = \sum_{\alpha=1,\beta>\alpha}^{3} g_{\alpha\beta}(\sigma_\alpha^\dagger \sigma_\beta^- + \sigma_\beta^\dagger \sigma_\alpha^-), \tag{2}$$

where $g_{\alpha\beta}$ is the coupling strength between α and β. We describe the dynamics of the system by using a master equation and solve it by using the quantum trajectory method.[26,27] The master equation of the system is

$$\frac{{\rm d}\rho}{{\rm d}t} = -i[H,\rho] + \frac{1}{2}\sum_{\alpha=1}^{3}(2A_\alpha \rho A_\alpha^\dagger - A_\alpha^\dagger A_\alpha \rho - \rho A_\alpha^\dagger A_\alpha), \tag{3}$$

where the jump operators are defined as $A_\alpha = \sqrt{2\gamma}\sigma_\alpha^-$ for the donor pigments with $\alpha = 1,2$, which account for the energy dissipation, and $A_3 = \sqrt{2\kappa}\sigma_3^-$ is associated with the charge separation of the acceptor pigment.

We now assume that all the pigments are in state ρ_0 at the initial time $t_0 = 0$, where only the two donor pigments are coherently excited, and ρ_0 may be either pure or mixed. To determine the state of the total system at a later time t, provided that no jump has occurred during the time from t_0 to t, we need to solve the nonunitary Schrodinger equation ${\rm d}\bar{\rho}_{\rm c}/{\rm d}t = -{\rm i}[H_{\rm c}, \bar{\rho}_{\rm c}]$, where $H_{\rm c}$ is the non-Hermitian Hamiltonian given by

$$H_{\rm c} = H - \frac{\rm i}{2}\sum_{\alpha=1}^{3} A_\alpha^\dagger A_\alpha, \tag{4}$$

$\bar{\rho}_{\rm c}$ is the unnormalized conditional density operator which accounts for the past state of the system until a jump happens, i.e., if no jump has occurred during the time from t_0 to t, the normalized conditional density operator at time t is given by

$$\rho_{\rm c}(t) = \frac{\bar{\rho}_{\rm c}(t)}{{\rm Tr}\bar{\rho}_{\rm c}(t)}. \tag{5}$$

The evolution governed by the nonunitary Schrodinger equation is randomly interrupted by one of the jumps, and the probability for jump A_α occurring during the interval $[t_0, t_0+\Delta t)$ is given by $\langle A_\alpha^\dagger A_\alpha\rangle \Delta t$. The density operator $\rho(t)$ is obtained by performing an ensemble average over the different conditioned density operators at time t. If a jump occurs, no matter whether the excitation of the donor pigments dissipates to the environment or the charge separation is induced by the acceptor pigment, the system will collapse to the ground state $|0\rangle$, therefore the ensemble average of the density matrix at time t is performed over two possible realizations: ground state $|0\rangle$ (jump) and conditional states $\rho_{\rm c}$ (no-jump), yielding the statistical mixture

$$\rho(t) = P_{\text{no-j}}\rho_{\rm c} + P_{\rm j}|0\rangle\langle 0|, \tag{6}$$

where $P_{\text{no-j}}$ represents the probability that no jump occurs, which can be calculated by the nonunitary Schrodinger equation. Therefore, the probability that a jump occurs in the interval $[t, t+\Delta t)$ is given by

$$\begin{aligned} P_{\rm c}(t) &= \frac{{\rm d}P_{\rm j}}{{\rm d}t}\Delta t = \frac{{\rm d}(\langle 0|\rho(t)|0\rangle)}{{\rm d}t}\Delta t \\ &= 2\Delta t\gamma \sum_{\alpha=1}^{2}\langle\alpha|\rho_{\rm c}|\alpha\rangle + 2\Delta t\kappa\langle 3|\rho_{\rm c}|3\rangle \\ &= w_1\Delta t + w_2\Delta t, \end{aligned} \tag{7}$$

where $w_2 = 2\kappa\langle 3|\rho_{\rm c}|3\rangle$ denotes the probability density that the excitation of the acceptor pigment is leaked to a reaction center. We calculate the efficiency of excitation transfer at time t by integrating all the contribution of $w_2\,{\rm d}t$ before time t. It is given by

$$\eta(t) = \int_{t_0}^{t} w_2(t')\,{\rm d}t'. \tag{8}$$

If we assume that the system is in a pure state at the initial time, then the conditioned density operator is written as $\rho_{\rm c} = |\psi_{\rm c}(t)\rangle\langle\psi_{\rm c}(t)|$, where the evolution of $|\psi_{\rm c}(t)\rangle$ satisfies the Schrodinger equation ${\rm d}|\psi_{\rm c}(t)\rangle/{\rm d}t = -{\rm i}H_{\rm c}|\psi_{\rm c}(t)\rangle$. By assuming $|\psi_{\rm c}(t)\rangle = \sum_{\alpha=1}^{3} x_\alpha(t)|\alpha\rangle$ and solving a set of equations of $x_\alpha(t)$, we will easily obtain the exact form of $|\psi_{\rm c}(t)\rangle$.

3. Review of measures of classical correlation and quantum correlation

In order to show our main results, we will review quantum concurrence, quantum discord, Von Neumann entropy, and quantum mutual information in this section. The effects of classical correlation and quantum correlation in the three-quasi-spin-pigment system will be investigated in the next section.

3.1. Entanglement of formation

Quantum systems are correlated in ways different from the classical objects, entangled states are nonclassical because they cannot be prepared only with the help of local operations and classical communications.[28] The entanglement of formation is proposed to quantify the resources required to create an entangled state.[29,30] Suppose that two parties A and B share a quantum state ρ^{AB}, we can always get an ensemble of pure states $\{|\psi_i\rangle\}$ with probabilities p_i

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|. \tag{9}$$

The entanglement of each pure state $|\psi_i\rangle$ is defined in the following form:

$$E(\psi_i) = -\mathrm{Tr}(\rho_{\mathrm{A}_i}\log_2\rho_{\mathrm{A}_i}) = -\mathrm{Tr}(\rho_{\mathrm{B}_i}\log_2\rho_{\mathrm{B}_i}), \tag{10}$$

where ρ_{A_i} and ρ_{B_i} are the reduced density matrices of $|\psi_i\rangle\langle\psi_i|$ over subsystems B and A, respectively. The complete ensemble of pure states usually has many groups. In all these ensembles, there exists one kind of decomposition whose average of entanglement is the smallest compared to those of the others. The entanglement of formation of state ρ can be defined as

$$E(\rho) = \min \sum_i p_i E(\psi_i). \tag{11}$$

The above entanglement of formation can be expressed as a direct function of ρ in a pair of qubits system.[28] For a general state ρ of the two qubits (pure or mixed state), we can get the spin-flipped state through the spin-flip transformation

$$\tilde{\rho} = (\sigma_y \otimes \sigma_y)\rho^*(\sigma_y \otimes \sigma_y), \tag{12}$$

where ρ^* is the complex conjugate of ρ, and σ_y is the standard time reversal operator. For the system of spin-$\frac{1}{2}$ particles, it associates to the matrix

$$\sigma_y = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}.$$

The entanglement of formation is rewritten as

$$E(\psi_i) = E(C(\psi_i)), \tag{13}$$

where $C(\psi_i) = |\langle\psi_i|\tilde{\psi}_i\rangle|$, which is the concurrence. Here the function $E(C)$ is given by

$$E(C) = h\Big(\frac{1+\sqrt{1-C^2}}{2}\Big), \tag{14}$$

and $h(x) = -x\log_2 x - (1-x)\log_2(1-x)$. The $E(C)$ has the same monotonicity with the concurrence from 0 to 1. So it is convenient to take the concurrence as a measure of entanglement[28]

$$C(\rho) = \max\{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\}, \tag{15}$$

λ_i's are the eigenvalues of the Hermitian matrix $R = \sqrt{\sqrt{\rho}\tilde{\rho}\sqrt{\rho}}$, and they are non-negative real numbers. We will use the concurrence to measure the entanglement of the system considered in this work.

3.2. Quantum discord

The quantum discord is another measure of quantum correlation, which is different from the entanglement of formation and can capture all the correlations in a quantum state.[31] We first review the measure of mutual information before giving the measure of quantum discord. In the classical information theory,[32] the classical correlation between any two variables can be measured by the mutual information

$$J_{\mathrm{c}}(A:B) = H(A) - H(A|B), \tag{16}$$

where $H(X) = -\sum_i p_i \log_2 p_i$ is the Shannon entropy used to quantify the information in a sequential variable $X = \{x_i\}$ with associated probability distribution $\{p_i\}$. The conditional entropy is defined as

$$H(A|B) = -\sum_{a,b} p_{ab}\log_2 p_{a|b} = H(AB) - H(B), \tag{17}$$

which represents a weighted average of the entropies of A given value B. Here $p_{a|b} = p_{ab}/p_b$. Based on the above notation, an equivalent expression is proposed to be

$$I_{\mathrm{c}}(A:B) = H(A) + H(B) - H(AB), \tag{18}$$

which is called the classical mutual information. The I_{c} can be promoted to the quantum mutual information. In the bipartite system, the quantum mutual information is defined as

$$I_q(\rho_{\mathrm{A:B}}) = S(\rho_{\mathrm{A}}) + S(\rho_{\mathrm{B}}) - S(\rho_{\mathrm{AB}}), \tag{19}$$

where $S(X) = -\mathrm{Tr}(X\log_2 X)$ is the Von Neumann entropy of system X ($X = \rho_{\mathrm{A}}$, ρ_{B}, ρ_{AB}). It can be used to measure the total correlation of bipartite. The above equation is directly modeled on the form of the classical mutual information I_{c}. Here $S(\rho_{\mathrm{A}})$ ($S(\rho_{\mathrm{B}})$) describes the uncertainty of independent subsystem A (B), while $S(\rho_{\mathrm{AB}})$ denotes the uncertainty of the combined system AB. Note that the measures have to be operated in the Hilbert space $H_{\mathrm{A}} \otimes H_{\mathrm{B}}$, which is different from the classical theory. The definition of conditional entropy (17) is measuring dependence. Now we introduce projectors $\{\Pi_j^{\mathrm{B}}\}$ performed locally on B. We can get the states of system A through the operations of B

$$\rho_j^{\mathrm{A}} = \mathrm{Tr}_{\mathrm{B}}(\{\Pi_j^{\mathrm{B}}\rho_{\mathrm{AB}}\Pi_j^{\mathrm{B}}\})/q_j, \tag{20}$$

where $q_j = \mathrm{Tr}_{\mathrm{AB}}(\{\Pi_j^{\mathrm{B}}\rho_{\mathrm{AB}}\Pi_j^{\mathrm{B}}\})$. The conditional entropy of $S_{\{\Pi_i^{\mathrm{B}}\}}(\rho_{\mathrm{A|B}})$ is a weighted average of $S(\rho_j^{\mathrm{A}})$

$$S_{\{\Pi_i^{\mathrm{B}}\}}(\rho_{\mathrm{A|B}}) = \sum_j q_j S(\rho_j^{\mathrm{A}}), \tag{21}$$

where q_j is the distribution of probability. The mutual information J_{c} can be extended to the quantum realm, that is

$$J_{\mathrm{q}}(\rho_{\mathrm{A:B}}) = S(\rho_{\mathrm{A}}) - S_{\{\Pi_i^{\mathrm{B}}\}}(\rho_{\mathrm{A|B}}), \tag{22}$$

where J_{q} depends on the choice of $\{\Pi_j^{\mathrm{B}}\}$, thus the minimum difference between I_{q} and J_{q} is defined as the quantum discord

$$D(\rho_{\mathrm{A:B}}) = \min_{\{\Pi_i^{\mathrm{B}}\}} [I_{\mathrm{q}}(\rho_{\mathrm{A:B}}) - J_{\mathrm{q}}(\rho_{\mathrm{A:B}})], \tag{23}$$

or equivalently

$$D(\rho_{A:B}) = I_q(\rho_{A:B}) - \max_{\{\Pi_i^B\}}[J_q(\rho_{A:B})]. \quad (24)$$

The second term is defined as the classical correlation. Let $I_c(\rho_{AB})$ replace $\max_{\{\Pi_i^B\}}[J_q(\rho_{A:B})]$, we have

$$I_c(\rho_{AB}) = I_q(\rho_{A:B}) - D(\rho_{A:B}). \quad (25)$$

In a quantum state, there are quantum information and classical information. The conditional entropy $S_{\{\Pi_i^B\}}(\rho_{A|B})$ contains the measurement of B, the quantum discord is unequal usually under the interchange between A and B. In this case, we need to adopt the two side measurements for these correlations.

4. Discussion

In this section, we will discuss the dependence of the efficiency of excitation energy transfer on the initial correlated condition of the donor pigments, and investigate the dynamics of bipartite correlations of the trimer. Two cases will be considered, in which the initial states of the donor pigments are pure and mixed, respectively.

In the first case, we assume that the initial trimer is prepared in the pure state $|\psi_0\rangle = x_{10}|1\rangle + x_{20}|2\rangle$, where $|x_{10}|^2 + |x_{20}|^2 = 1$. By using the definition in the above section, we can get the explicit form of the initial concurrence of the two donor pigments, i.e., $C(|\psi_0\rangle_{12}) = 2|x_{10}||x_{20}|$, and other correlation measures, i.e., $I_q(|\psi_0\rangle_{12}) = 2I_c(|\psi_0\rangle_{12}) = 2Q_D(|\psi_0\rangle_{12}) = -2\sum_{i=1}^{2}|x_{i0}|^2\log_2|x_{i0}|^2$. Through solving the Schrodinger equation of the pure initial states and assuming $g_{12} = g_{21}$ and $g_{13} = g_{23}$, we obtain the evolving parameters of $|\psi_c(t)\rangle$, i.e.,

$$x_i(t) = e^{-(ig_{12}+\gamma)t}\left[x_{i0} - ig_{13}(x_{10}+x_{20})\int_0^t f(t')e^{-(ig_{12}+\gamma)t'}dt'\right]$$

for $i = 1, 2$, and $x_3(t) = f(t)(x_{10}+x_{20})$, where

$$f(t) = -2ig_{13}e^{-(ig_{12}+\gamma+\kappa)t/2}\sin(\Omega t/2)/\Omega,$$
$$\Omega = \sqrt{8g_{13}^2 - (\gamma-\kappa+ig_{12})^2}.$$

Based on these results, the explicit form of the efficiency of energy transfer is given by

$$\eta = \frac{16\kappa g_{13}^2(\kappa+\gamma)(1+2|x_{10}||x_{20}|)}{|\Omega|^2} \times\left[\frac{1}{(\Omega^*-\Omega)^2+4(\kappa+\gamma)^2} - \frac{1}{(\Omega^*+\Omega)^2+4(\kappa+\gamma)^2}\right] \quad (26)$$

when time approaches to infinity. From the above results, we can easily find that η increases linearly with $C(|\psi_0\rangle_{12})$, i.e., the efficiency of energy transfer directly depends on the concurrence of the initial pure states of the donor pigments. We also need to emphasize that the rate γ of energy dissipation may be helpful for η, which implies that the effects coming from the environment may enhance the energy transfer. We can also obtain the dynamic form of the bipartite correlations of the system. The concurrence of various bi-partitions of the system is $C(\rho_{ij}(t)) = 2\sqrt{|x_i(t)|^2|x_j(t)|^2}$, where $\rho_{ij}(t) = \mathrm{Tr}_k\{\rho(t)\}$ is the reduced density matrix with $i,\ j,\ k = 1,\ 2,\ 3$ and $i,\ j \neq k$. The quantum discord, the classical correlation, and the total correlation of the system are given by

$$Q_D(\rho_{ij}(t)) = \left(|x_i(t)|^2 + |x_j(t)|^2\right)\log_2\left(|x_i(t)|^2 + |x_j(t)|^2\right) - \left[|x_i(t)|^2\log_2(|x_i(t)|^2) + |x_j(t)|^2\log_2(|x_j(t)|^2)\right],$$
$$I_c(\rho_{ij}(t)) = -\left[|x_i(t)|^2\log_2(|x_i(t)|^2) + |x_j(t)|^2\log_2(|x_j(t)|^2)\right],$$
$$I_q(\rho_{ij}(t)) = \left(|x_i(t)|^2 + |x_j(t)|^2\right)\log_2\left(|x_i(t)|^2 + |x_j(t)|^2\right) - 2\left[|x_i(t)|^2\log_2(|x_i(t)|^2) + |x_j(t)|^2\log_2(|x_j(t)|^2)\right].$$

In the second case, the initial system is in a mixed state

$$\rho_0 = x_0|1\rangle\langle 1| + (1-x_0)|2\rangle\langle 2| + y_0|1\rangle\langle 2| + y_0^*|2\rangle\langle 1|, \quad (27)$$

where the non-negative definition of a physical density matrix requires that $x_0 \in [0, 1]$ and $1 - 4x_0(1-x_0) + 4|y_0|^2 \gg 0$.

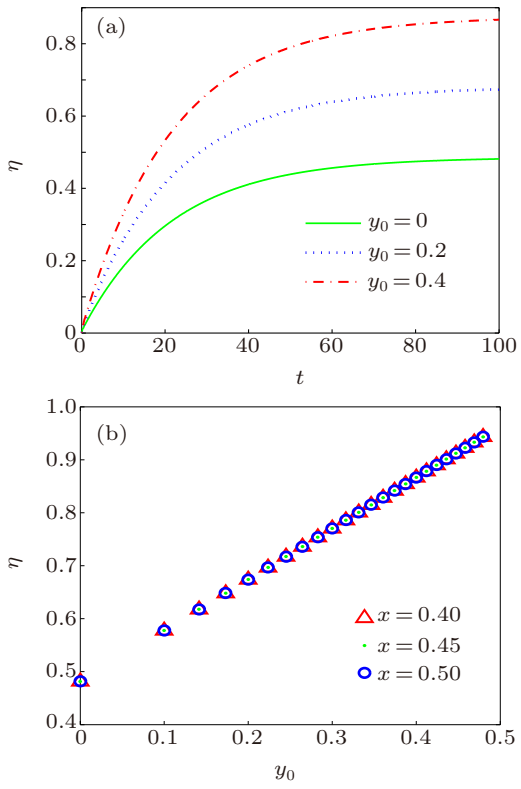


Fig. 1. (color online) (a) Efficiency $\eta(t)$ versus time t, (b) efficiency η at a certain large time versus initial parameter y_0.

In the following numerical results, we set $\varepsilon_1 = \varepsilon_2 = 1.2911 \times 10^4$ cm^{-1}, $\varepsilon_3 = 1.2748 \times 10^4$ cm^{-1}, $\gamma = 1$ ns^{-1}, $\kappa = 4$ ps^{-1}, $g_{13} = 1$ mev, $g_{12} = 5.91 \times 10^2$ cm^{-1}. In Fig. 1(a), we plot the efficiency $\eta(t)$ versus time t with different initial parameter y_0. We find from Fig. 1(a) that the efficiency increases with time and approaches to the saturation when the time becomes larger. The saturate values depend on the initial parameters. Figure 1(b) shows that the saturate efficiency is in proportion to y_0 but has no connection with population parameter x_0. The $y_0 \neq 0$ means that the two donor pigments are correlated, thus it is concluded that the energy transfer efficiency

depends on the initial correlation of the donor pigments even though the initial states are mixed. In Fig. 2, the saturate values of efficiency versus concurrence, quantum discord, classical correlation, and total correlation of the initial donor pigments are shown. We find that $\eta(t \to \infty)$ not only increases linearly with the initial concurrence of the donor pigments, which is similar to the case of pure initial states, but also increases with the quantum discord of the donor pigments. However, $\eta(t \to \infty)$ is independent of the initial classical correlation of the donor pigments, which is different from the case of pure initial states.

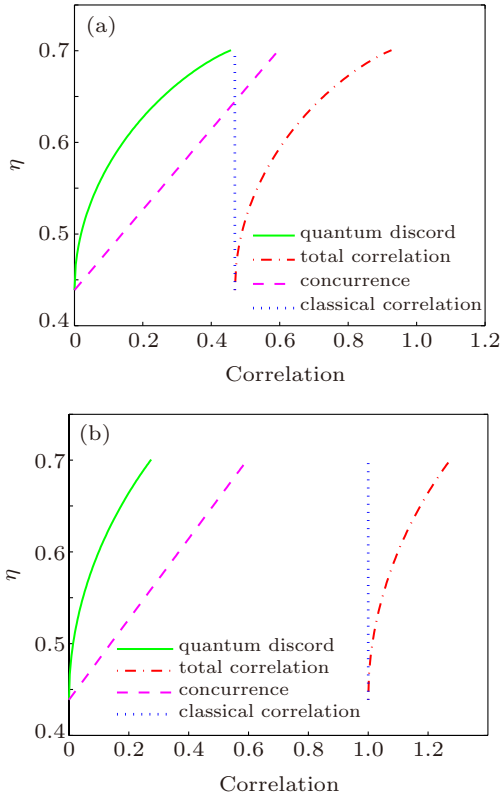


Fig. 2. (color online) Efficiency $\eta(t \to \infty)$ versus the initial concurrence, quantum discord, and classical correlation of the donor pigments, with (a) $x_0 = 0.1$ and (b) $x_0 = 0.5$.

In the following, we will show the dynamics of four different kinds of correlations between two donor pigments. In Fig. 3, concurrence, quantum discord, classical correlation, and total correlation of two donor pigments versus time t with different initial conditions are plotted. We set $y_0 = 0.0$, $y_0 = 0.2$, $y_0 = 0.45$, and $y_0 = 0.5$ in Figs. 3(a)–3(d), respectively. In Fig. 3(a), corresponding to the maximum mixed state of the initial donor pigments, we find that the concurrence and the quantum discord start from zero and increase with time, and on the contrary, the classical correlation decreases with time. All correlations approach to saturation finally. In Figs. 3(b) and 3(c), the initial concurrence and the initial quantum discord of the

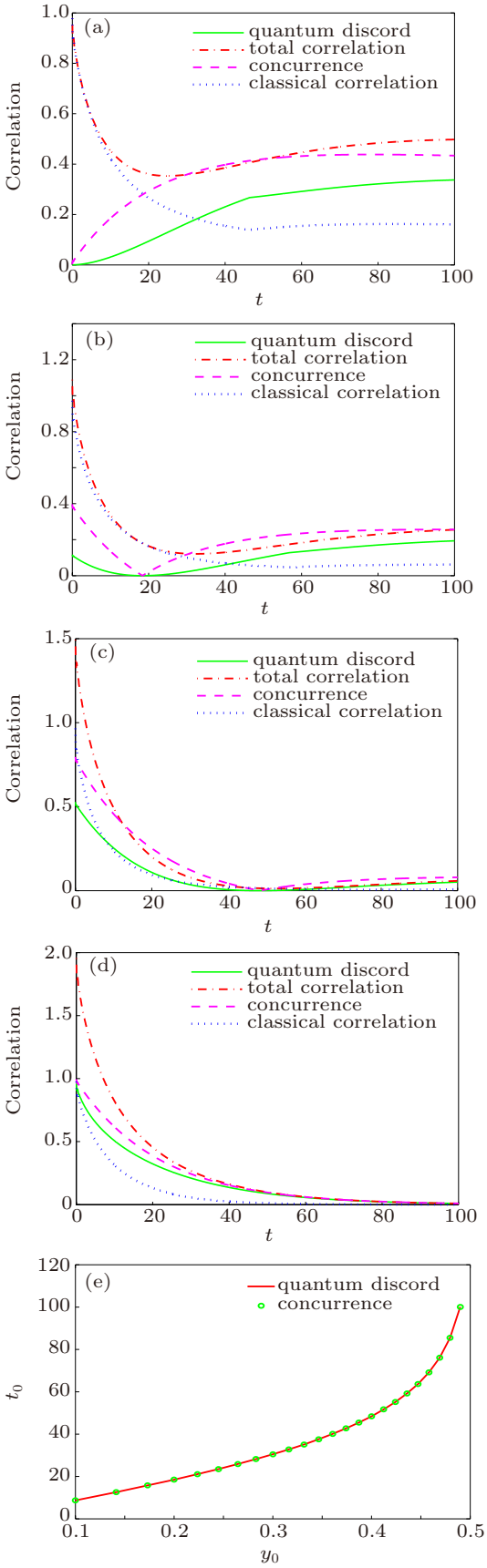


Fig. 3. (color online) Concurrence, quantum discord, classical correlation, and total correlation between the two donor pigments versus time t, with (a) $y_0 = 0.0$, (b) $y_0 = 0.2$, (c) $y_0 = 0.45$, and (d) $y_0 = 0.5$. (e) The sudden death time of concurrence and quantum discord versus initial value y_0.

donor pigments are not zero, and the two correlations decrease with time first and then increase after a sudden death.[33] In Fig. 3(d), corresponding to the pure initial state of the donor pigments, we find that all correlations decrease to zero with time. The time at which the sudden death occurs increases with y_0 as shown in Fig. 3(e). The sudden death time quickly becomes very large when y_0 approaches to 0.5, which is also shown in Fig. 3(d). From the above figures, we find that the dynamics of correlations in the case of pure initial state are very different from those in the cases of mixed initial states. The reason is that the present system is only a dissipation one, no dephasing effects have been considered for the system.

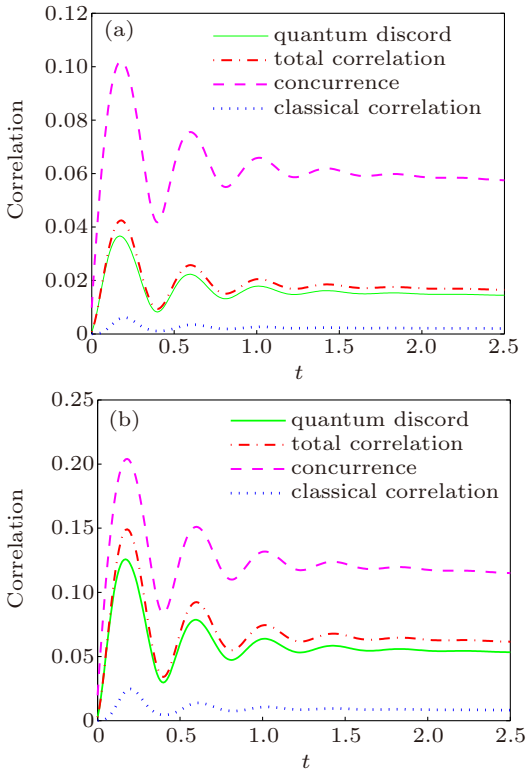


Fig. 4. (color online) Concurrence, quantum discord, classical correlation, and total correlation between one donor pigment and one acceptor pigment versus time t, where (a) $y_0 = 0$, (b) $y_0 = 0.5$.

In Fig. 4, we plot the dynamics of various correlations of one of the donor pigments and the acceptor pigment. We set $y_0 = 0$ and $y_0 = 0.5$ in Figs. 4(a) and 4(b), respectively. In both cases, we find that all the correlation measures start from zero and approach to the saturation finally, the concurrence is always larger than the other three measures, and the classical correlation nearly disappears. In our model, as we have mentioned above, the evolution of the quantum states is restricted to the zero- and one-excitation subspaces. It means that once the excitation is transferred from the donor pigments to the acceptor pigment, the correlation between one donor pigment and the acceptor pigment, mainly in the quantum form, is produced and evolves.[34] Because of the reversibility of quantum evolution, this effect can also be fed back to the quantum correlations between the two donor pigments. This is why the quantum correlations between two donor pigments are more active than the classical correlation, as shown in Figs. 3(a)–3(d).

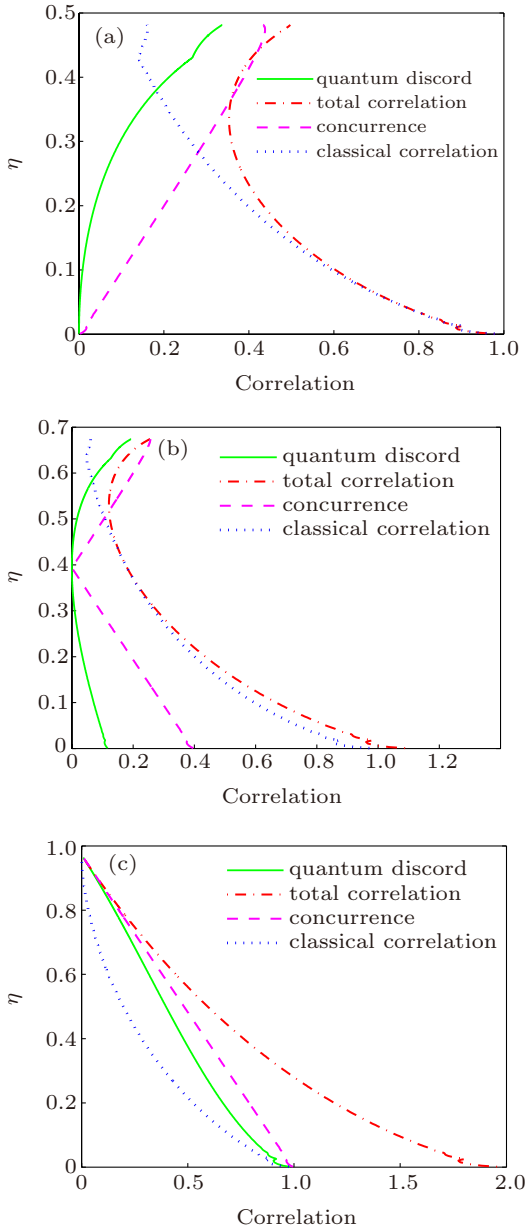


Fig. 5. (color online) Efficiency $\eta(t)$ versus the dynamics of various correlations of two donor pigments, where (a) $y_0 = 0$, (b) $y_0 = 0.2$, and (c) $y_0 = 0.5$.

Finally, we plot the efficiency of excitation transfer $\eta(t)$ versus the dynamics of various correlations of two donor pigments in Fig. 5. We find very different relations of η with quantum correlation and classical correlation. In all cases with different y_0, the classical correlation is always decreasing with increasing η; does this mean that the excitation transfer needs to consume the classical correlation of the donor pigments? However, there are no fixed relations between η and quantum correlations, they change with the same trend when the initial donor system is in the maximum mixed state (Fig. 5(a)), but

have a contrary trend when the initial donor system is in the pure state (Fig. 5(c)).

5. Conclusions

In summary, we have studied theoretically the excitation energy transfer and the correlation dynamics of a three-quasi-spin-pigment system. In our model, we have emphasized the excitation dissipation of the environment but ignored the effects of dephasing. We have investigated the efficiency of excitation transfer depending on two kinds of correlations, initial correlation and dynamics correlation of the donor system that includes two pigments. We found that the efficiency depends on the initial concurrence and the quantum discord of the donor pigments, but is independent of the initial classical correlation. We also found that the dynamics of efficiency and the classical correlation of the donor pigments have contrary change tendencies, and the concurrence, quantum discord, and total correlation of the donor pigments have similar properties to the classical correlation for the efficiency only when the initial donor pigments are in a pure state. We have also studied the dynamics of the four kinds of bipartite correlations among the trimer pigments. We found that the phenomena of sudden death of concurrence and quantum discord of the donor pigments occur if the initial quantum correlation is neither zero or maximum.

Appendix A

In this appendix, we give the explicit forms of various correlations of state (27). The concurrence is

$$C(\rho_0) = 2\sqrt{|y_0|^2},$$

the classical correlation is

$$\begin{aligned} &I_{\rm c}(\rho_0)\\ &= \max\Big\{\Big[\lambda_1\log_2\frac{\lambda_1}{q_1}+\lambda_2\log_2\frac{\lambda_2}{q_1}+\beta_1\log_2\frac{\beta_1}{q_2}+\beta_2\log_2\frac{\beta_2}{q_2}\Big]\\ &\quad -[(1-x_0)\log_2(1-x_0)+x_0\log_2 x_0]\Big\}, \end{aligned}$$

and the total correlation is given by

$$\begin{aligned} I_{\rm q}(\rho_0) \;=\; & -2[(1-x_0)\log_2(1-x_0)+x_0\log_2 x_0]\\ & +\frac{1+\sqrt{1-4[x_0(1-x_0)-|y_0|^2]}}{2}\\ & \times\log_2\frac{1+\sqrt{1-4[x_0(1-x_0)-|y_0|^2]}}{2}\\ & +\frac{1-\sqrt{1-4[x_0(1-x_0)-|y_0|^2]}}{2}\\ & \times\log_2\frac{1-\sqrt{1-4[x_0(1-x_0)-|y_0|^2]}}{2}, \end{aligned}$$

the quantum discord is obtained by

$$Q_{\rm D}(\rho_0) = I_{\rm q}(\rho_0) - I_{\rm c}(\rho_0),$$

where we set

$$\begin{aligned} \frac{\lambda_1}{q_1} &= \frac{1}{2}+\frac{\sqrt{(x_0-\sin^2\theta)^2+|y_0|^2\sin^2 2\theta}}{2(x_0\cos^2\theta+(1-x_0)\sin^2\theta)},\\ \frac{\lambda_2}{q_1} &= \frac{1}{2}-\frac{\sqrt{(x_0-\sin^2\theta)^2+|y_0|^2\sin^2 2\theta}}{2(x_0\cos^2\theta+(1-x_0)\sin^2\theta)},\\ \frac{\beta_1}{q_2} &= \frac{1}{2}+\frac{\sqrt{(x_0-\cos^2\theta)^2+|y_0|^2\sin^2 2\theta}}{2(x_0\sin^2\theta+(1-x_0)\cos^2\theta)},\\ \frac{\beta_2}{q_2} &= \frac{1}{2}-\frac{\sqrt{(x_0-\cos^2\theta)^2+|y_0|^2\sin^2 2\theta}}{2(x_0\sin^2\theta+(1-x_0)\cos^2\theta)},\\ \lambda_{1,2} &= \left[x_0\cos^2\theta+(1-x_0)\sin^2\theta\right]/2\\ &\quad \pm\sqrt{(x_0-\sin^2\theta)^2+|y_0|^2\sin^2 2\theta}/2,\\ \beta_{1,2} &= \left[x_0\sin^2\theta+(1-x_0)\cos^2\theta\right]/2\\ &\quad \pm\sqrt{(x_0-\cos^2\theta)^2+|y_0|^2\sin^2 2\theta}/2. \end{aligned}$$

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