Optimal control of a symmetric double quantum-dot nanostructure: Analytical results

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We study the potential for optimal control of a symmetric double quantum-dot structure interacting with a single pulsed electromagnetic field. We first use the rotating wave and resonant approximations and reduce the dynamics of the system to that of a degenerate three-level Λ-type system. We also formulate the optimal control problem in terms of differential equations that have to be fulfilled by the optimal electromagnetic fields. We then obtain general analytical expressions for the optimal pulse shapes that lead to global maximization of the final population of the target state and of the time-averaged population of the target state in the quantum-dot structure.

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In the past decade it has been realized that ideas from quantum control in multilevel systems[1–3] can be efficiently applied to the control of the dynamics of electrons and spins in semiconductor quantum dots.[4–6] In this area, specific interest has been given to the potential of controlled single-electron transfer in double quantum-dot structures.[7–16]

In particular, Openov[8] studied a system of a symmetric double quantum-dot structure interacting with a rectangular electromagnetic pulse for the controlled electron transfer between the two quantum dots, and applied his findings for the implementation of the NOT quantum gate. Later, Paspalakis *et al.*[10] studied in detail the interaction of electromagnetic pulses with the symmetric double quantum-dot structure described by Openov and applied the methodology of controlled rotation for the manipulation of the quantum state of the system and the creation of single-quantum gates. The effects of asymmetry of the quantum-dot structure on transfer efficiency was also studied by Tsukanov and Openov.[11] In addition, the potential for electron transfer via the conduction band (continuum of states) in the scheme of Openov has been studied by Basharov and Dubovis.[13] Finally, Tsukanov[15] revisited quite recently the same quantum-dot structure as that of Openov and analyzed rigorously the approximations used in the description of the dynamics of the system.

Lately, optimal control schemes[2,3,17] have also been applied for the control of the dynamics of semiconductor quantum-dot structures.[18–22] In this work, we study the potential for optimal control of the symmetric double quantum-dot structure initially proposed by Openov.[8] We present results in the case that the quantum-dot structure interacts with a single pulsed electromagnetic field. We formulate the optimal control problem in terms of differential equations that have to be fulfilled by the optimal electromagnetic fields.[19,23,24] We then obtain general analytical expressions for the optimal pulse shapes that lead to global maximization of the final population of the target state and of the time-averaged population of the target state in the quantum-dot structure. The first can be used in creating the NOT quantum gate,[25,26] while the latter can be used for electron transfer in a double quantum-dot structure.[7,9,18]

We consider a nanostructure composed of two identical quantum dots (*A* and *B* in Fig. 1). Each one, when isolated, possesses only two bound-state energy levels. These localized states are denoted by $|A1\rangle, |A2\rangle$ and by $|B1\rangle, |B2\rangle$ for the *A* and *B* dots, respectively. The lower bound state has energy ε_1 and the upper bound state has energy ε_2. The geometrical characteristics of the dots are chosen such that the lower energy level is deep in the potential barrier and the upper energy level is near the edge of the potential barrier. These features of the energy levels are carried over to the double quantum-dot nanostructure as the quantum dots are taken to be widely separated.

Therefore, the lower pair of energy levels $|A1\rangle$, $|B1\rangle$ are essentially degenerate, as the tunneling of an electron through the potential barrier between these energy levels is very improbable and will be omitted here. However, as the upper energy levels $|A2\rangle$, $|B2\rangle$ are taken to be near the edge of the potential barrier, the electron tunneling probability between these levels is quite high and will be accounted for. These are the assumptions made initially by Openov[8] and also adapted by others later on.[8,10–13,15,16] These assumptions have also been recently used by Ginzburg and Orenstein for producing slow light in a coupled semiconductor quantum well structure.[27]

The Hamiltonian of the double quantum-dot nanostructure, interacting with an external electromagnetic field $E(t)$, is given by[8,10]

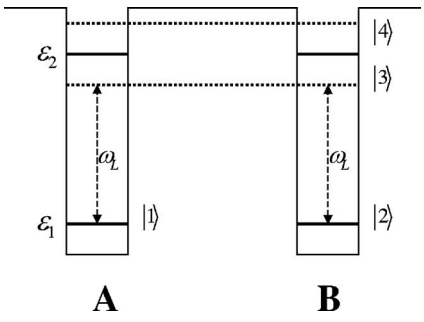

FIG. 1. Schematic diagram of the coupled quantum-dot structure studied. The system posseses two degenerate localized lower levels ($|1\rangle$ and $|2\rangle$) and two delocalized upper levels ($|3\rangle$ and $|4\rangle$). The lower states are coupled on-resonant to the excited state $|3\rangle$ by an external electromagnetic field.

$$\hat{H} = \varepsilon_1(|A1\rangle\langle A1| + |B1\rangle\langle B1|) + \varepsilon_2(|A2\rangle\langle A2| + |B2\rangle\langle B2|) - U(|A2\rangle\langle B2| + |B2\rangle\langle A2|) + E(t)\mu(|A1\rangle\langle A2| + |B1\rangle\langle B2| + \text{H.c.}), \quad (1)$$

where μ is the electron dipole moment for the transition $|a1\rangle \leftrightarrow |a2\rangle$ $(a=A,B)$ and U is the electron hopping energy between the two dots for the excited electronic states $|A2\rangle$ and $|B2\rangle$. Hence $2U=\pi\hbar/\tau$, where τ is the tunneling time, i.e., the time needed by the electron to move from one localized state ($|A2\rangle$) to the other localized state ($|B2\rangle$). The applied field is $E(t)=E_0(t)\cos(\omega_L t)$, with ω_L being the angular frequency and $E_0(t)$ being the slowly varying envelope of the field.

Then we transform the Hamiltonian of the system [Eq. (1)] to the interaction picture, where in the matrix representation of the Hamiltonian only the nondiagonal elements are present, with the following transformation:

$$\hat{V}_{int}(t) = \exp\left[-i\left(\frac{\varepsilon_1}{\hbar}(|A1\rangle\langle A1| + |B1\rangle\langle B1|) + \frac{\varepsilon_2}{\hbar}(|A2\rangle\langle A2| + |B2\rangle\langle B2|)\right)t\right]. \quad (2)$$

As we have mentioned above, the upper localized states $|A2\rangle$ and $|B2\rangle$ are coupled through tunneling and give rise to a pair of delocalized states, a symmetric one $(|3\rangle=(|A2\rangle+|B2\rangle)/\sqrt{2})$ and an antisymmetric one $(|4\rangle=(|A2\rangle-|B2\rangle)/\sqrt{2})$. The energies of the delocalized states $|3\rangle$ and $|4\rangle$ are expressed by means of the electron hopping energy as $\varepsilon_+=\varepsilon_2-U$ $(\varepsilon_-=\varepsilon_2+U)$ for the symmetric (antisymmetric) state. For convenience and consistency in our notation, in the rest of this Brief Report we represent the two lower localized states by $|1\rangle=|A1\rangle$ and $|2\rangle=|B1\rangle$.

We then concentrate our study on the exact resonant excitation case, i.e., the case where the angular frequency $(\hbar\omega_L)$ is equal to the energy difference between the localized states and the symmetric excited state $(\varepsilon_+-\varepsilon_1)$. A very important parameter describing the field-matter interaction strength is the Rabi frequency $\mu E_0(t)/\hbar$. When the maximum Rabi frequency is much smaller than the angular frequency of the applied field, a simplified expression for the Hamiltonian of the system is obtained by eliminating fast oscillating terms. In this approximation called the rotating-wave approximation, valid for specific values of the applied field parameters, the Hamiltonian reads

$$\hat{H} = \frac{1}{2\sqrt{2}}[\mu E_0(t)|1\rangle\langle 3| + \mu E_0(t)|2\rangle\langle 3| + \mu E_0(t)e^{-i2Ut/\hbar}|1\rangle\langle 4| - \mu E_0(t)e^{-i2Ut/\hbar}|2\rangle\langle 4| + \text{H.c.}]. \quad (3)$$

This Hamiltonian can be simplified further by assuming the resonant approximation, which, as shown in Refs. 8 and 15, is a very good approximation for the exact resonance case. In this case, the transitions $|1\rangle(|2\rangle) \leftrightarrow |4\rangle$ can be ignored and the simplified Hamiltonian reads

$$\hat{H}' = \frac{1}{2\sqrt{2}}[\mu E_0(t)|1\rangle\langle 3| + \mu E_0(t)|2\rangle\langle 3| + \text{H.c.}]. \quad (4)$$

Under these approximations, the dynamics of the system reduces to that of a degenerate three-level Λ-type system that it is driven at exact resonance by a single laser field. The latter Hamiltonian will be the starting point for the implementation of the quantum control scheme.

We are initially interested in the determination of the optimal shape and value of $E_0(t)$ in the time interval $[0,T]$ that leads to the maximization of the time-averaged population of state $|2\rangle$, i.e., the quantity $\frac{1}{T}\int_0^T \rho_{22}(t)dt$, where $\rho_{22}(t)$ is the corresponding density-matrix element for the population of state $|2\rangle$. In the case of exact resonant excitation, $\rho_{22}(t)=\sin^4[\theta(t)]$, where $\theta(t)=\mu\int_0^t V(t')dt'$ with $V(t)=E_0(t)/(4\hbar)$.

We use the optimal control methodology of Garcia and co-workers.[19,23,24] The Lagrangian we use is

$$L = \int_0^T A(t)\left[\frac{\partial}{\partial t} + i\hat{Z}(t)\right]\rho(t)dt + \beta\int_0^T L_1 dt. \quad (5)$$

Here, β is a Lagrange multiplier, $A(t)$ is a Lagrange multiplier density, $\hat{Z}(t)$ is a Liouville operator for the three-level system, and $\rho(t)$ is the density-matrix operator. The first term in Eq. (5) ensures that the density matrix satisfies the Liouville equation. The functional density L_1 explicitly includes the description of the optimal control. Following the methodology of Garcia and co-workers,[19,23,24] L_1 is written as

$$L_1 = L_{ob}(\rho) + \lambda V^2(t) + \lambda_1\left[\frac{dV(t)}{dt}\right]^2, \quad (6)$$

where λ, λ_1 are Lagrange multipliers and $L_{ob}(\rho)$ refers to the physical quantity that we wish to maximize during the control time interval. The second term in the right-hand side of Eq. (6) is related to the constraint on the total energy of the control field and the third term is related to a constraint on the minimal experimentally achievable duration of the control pulse.[19,23,24] The latter ensures the exclusion of infinitely narrow or abrupt, steplike solutions.

In our case, $L_{ob}(\rho)=\rho_{22}(t)/T$. In order to have the problem analytically tractable, we will assume that $V(t)$ is slowly varying and omit the last term of Eq. (6). Then,

$$L_1 = \frac{\rho_{22}(t)}{T} + \lambda\frac{\dot{\theta}^2(t)}{\mu^2}. \quad (7)$$

We note that we have omitted the Liouville term of the Lagrange, as we will include the analytical solution for $\rho_{22}(t)$ that has been obtained from the solution of the Liouville equation.[19,23] As $\rho_{22}(t)=\sin^4[\theta(t)]$, Eq. (7) leads to the Euler-Lagrange differential equation

$$\lambda\frac{d^2\theta(t)}{dt^2} - 2\frac{\mu^2}{T}\sin^3[\theta(t)]\cos[\theta(t)] = 0. \quad (8)$$

The boundary conditions for $\theta(t)$ are chosen $\theta(0)=0$ and $\theta(T)=\pi/2$. The first condition makes the Rabi frequency nonzero at $t=0$, but it leads to analytical results for $V(t)$. A time integration of Eq. (8) gives

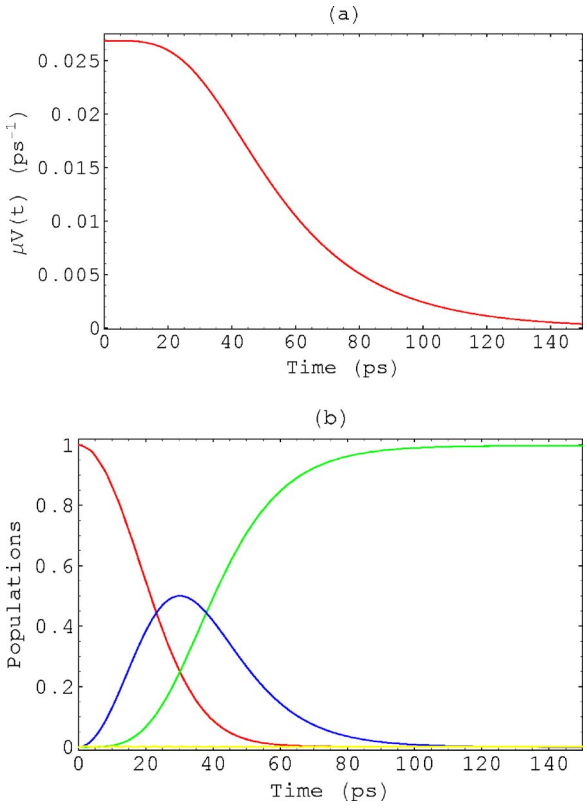

FIG. 2. (Color online) Time evolution of (a) $\mu V(t)$ and (b) of the populations in states $|1\rangle$ (red curve), $|2\rangle$ (green curve), $|3\rangle$ (blue curve), and $|4\rangle$ (yellow curve) with parameters $\varepsilon_1=0.1$ eV, $\varepsilon_2=0.4$ eV, $\hbar U=5\times10^{-4}$ eV, and $\hbar\mu V(0)=\frac{5}{2\sqrt{2}}\times10^{-5}$ eV.

$$L_1-\dot{\theta}\frac{\partial L_1}{\partial\dot{\theta}}=\lambda\frac{\dot{\theta}^2(t)}{\mu^2}+\frac{\sin^4[\theta(t)]}{T}=c, \tag{9}$$

where c is a constant. Applying the boundary conditions, we obtain from Eq. (9) $c=1/T$ and $\lambda=-1/[TV^2(0)]$. Then, Eq. (9) can be rewritten as

$$\int_0^{\theta}\frac{d\theta'}{\sqrt{1-\sin^4\theta'}}=\mu V(0)t. \tag{10}$$

The left-hand side of Eq. (10) is also written as

$$\begin{aligned}\int_1^{\sqrt{2-\cos^2\theta}}&\frac{dy}{\sqrt{y^2-1}(2-y^2)}\\&=-\int_{\pi/2}^{\arcsin(1/\sqrt{2-\cos^2\theta})}\frac{\sin z dz}{1-2\cos^2 z}\\&=\frac{1}{2\sqrt{2}}\ln\left\{\frac{1+\sqrt{2}\cos\left[\arcsin\left(\frac{1}{\sqrt{2-\cos^2\theta}}\right)\right]}{1-\sqrt{2}\cos\left[\arcsin\left(\frac{1}{\sqrt{2-\cos^2\theta}}\right)\right]}\right\},\end{aligned} \tag{11}$$

with $y=\sqrt{2-\cos^2\theta'}$ and $z=\arcsin(1/y)$. Combining the right-hand side of Eq. (10) with the result of Eq. (11), we obtain after some algebra that

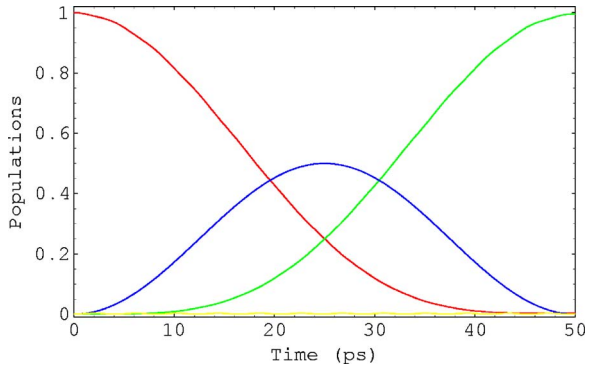

FIG. 3. (Color online) The same as in Fig. 2(b) but for a rectangular pulse that fulfills Eq. (16) and $t_c=50$ ps.

$$\theta(t)=\arccos\sqrt{\frac{8K}{K^2+6K+1}},\quad K(t)=e^{2\sqrt{2}\mu V(0)t}. \tag{12}$$

Therefore,

$$V(t)=\frac{\dot{\theta}}{\mu}=\frac{4[K(t)+1]\sqrt{K(t)}V(0)}{K^2(t)+6K(t)+1}. \tag{13}$$

The form of $\mu V(t)$ from Eq. (13) and the dynamics of the populations for a typical double quantum-dot structure, obtained from the numerical solution of the time-dependent Schrödinger equation using the Hamiltonian of Eq. (1), is shown in Fig. 2. We note that the yellow curve of Fig. 2 shows that the population of state $|4\rangle$ is very small (close to zero) and this confirms the resonant approximation and the validity of the Hamiltonian of Eq. (4).

We are now interested in the analytical determination of the optimal shape and value of $V(t)$ that leads to the maximization of population $\rho_{22}(t)$ at a specific time t_c when one has on-resonant excitation. In order for this to succeed, we will extend the optimal control methodology of Garcia and Grigorenko.[23] In this case,

$$L_1=\rho_{22}(t)\delta(t-t_c)+\lambda\frac{\dot{\theta}^2(t)}{\mu^2}. \tag{14}$$

As $\rho_{22}(t)=\sin^4[\theta(t)]$, Eq. (13) leads to the Euler-Lagrange differential equation

$$\lambda\frac{d^2\theta(t)}{dt^2}-2\mu^2\sin^3[\theta(t)]\cos[\theta(t)]\delta(t-t_c)=0. \tag{15}$$

In this case, too, the boundary conditions for $\theta(t)$ are chosen $\theta(0)=0$ and $\theta(T)=\pi/2$.

Treating the δ function properly, we solve Eq. (14) and obtain the optimal form of $V(t)$ to be

$$V(t)=\frac{\pi}{2\mu t_c}. \tag{16}$$

We note that the optimal form of $V(t)$ is the same as the one obtained from the analytical solution of the problem in the

case of a rectangular pulse excitation.[8,10] This is similar to the optimal pulse form obtained for the case of two-level system excitation.[23] An example of complete population transfer in the same double quantum-dot system as before is shown in Fig. 3.

Using the optimal control methodology of Garcia and coworkers, which has been applied so far only to two-level systems[19,23] and quasi-two-level systems,[24] we obtain general analytical expressions for the optimal pulse shapes that lead to global maximization of the final population of a target state and of the time-averaged population of the target state in a specific double quantum-dot structure.

These results can also be applied in other systems and processes that can be described by the Hamiltonian of Eq. (6). Such processes are, for example, the enantiomeric conversion of chiral molecules and enantiomeric purification of racemic mixtures,[3,28–30] the creation of single-quantum gates (the NOT gate, for example), in microwave-driven three-level superconductor quantum interference device quantum bits,[31–33] and the creation of ultrafast all-optical spin switching in magnetic structures.[34]

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