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To cite this article: Diego S Acosta Coden *et al* 2019 *Phys. Scr.* **94** 025101

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Fast optical control of a coded qubit in a triple quantum dot

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Received 31 July 2018, revised 27 November 2018

Accepted for publication 10 December 2018

Published 2 January 2019



Abstract

In this work, we study strategies for the optical control, within the dipole approximation, of a qubit encoded in the total intrinsic angular momentum states of three electrons confined in a triple quantum dot. The system is modeled using effective confining potentials, and its electronic structure is calculated using the configuration interaction method. Optimal control theory (OCT) was applied to design low-fluence time-dependent electric fields controlling the qubit in times shorter than a nanosecond. The resulting pulses produce transitions between the qubit states for experimentally available field amplitudes with high fidelity. Moreover, studying the dominant frequencies present in the OCT pulses, we show that the switching between the qubit states can also be achieved with simpler combinations of sinusoidal driving fields that produce transitions to intermediate states. The limitations of an extended Hubbard description for the model and its dynamic behavior are also discussed.

Keywords: quantum dots, optimal control theory, quantum control

(Some figures may appear in colour only in the online journal)

1. Introduction

The multiple requirements that a physical system must fulfill to be considered a worthy qubit have been described extensively. Those candidates based on physical systems whose fabrication and control techniques have been driven by industrial applications are a sensible choice. The semiconductor physics has been exhaustively developed to provide better materials and devices to the electronic industry. Semiconductor nanodevices can be constructed with an ever increasing variety of materials, sizes and shapes [1–3]. Besides, the number of electrons confined in the device can be chosen precisely. All these characteristics result in systems with an scalability and tunability that is lacking in other implementations [4–7], in particular the parameters that

define the optical and electrical properties can be tailored quite precisely [1–3].

Physical properties of semiconductor quantum dots with few electrons confined in it can be selected to meet and satisfy different criteria [1–3, 8, 9]. The controllability, *i.e.* the ability to change the quantum state of the system in a reliable and repetitive way with a very high fidelity is most stringent. In recent years there has been an increasing interest in controlling quantum phenomena in molecular systems and nanodevices [10–18]. The coherent quantum control of electrons in quantum dots exposed to electromagnetic radiation is of great interest, not only in quantum information processing but in many technological applications as charge transport devices [19–21]. Several studies in quantum control of double quantum dots (DQDs) has been performed using gate voltages and optimized laser pulses [22–24]. In addition, the number of quantum control experiments is rapidly rising

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through the improvement of laser pulse shaping and closed-loop learning techniques [22–24].

A qubit state in a few electron quantum dot can be encoded using the electron charge or, as in the case of study of this work, the electron spin. There are a lot of different ways in order to implement a many electron spin qubit. Throughout this work we will analyze the spin manipulation of a three electron spin qubit. There exist different ways of implementing a three-spin qubit [25]. Among the three electron quantum dot devices for quantum information processing we can highlight the exchange-only qubit [26], the spin-charge qubit [27], the hybrid qubit [28–30], the resonant exchange qubit [31, 32], and the always-on exchange-only qubit [33]. These three electron nanodevices can be implemented confining three electrons in either a single quantum dot, DQD, or triple quantum dot (TQD) depending on the objective.

So far, the works dealing with coded qubits [34] based on the spin states of three electrons confined in a TQD have investigated the switching between the two basis states forcing the system with potential gates [35]. The voltage controlled coded qubit was designed by Hawrylak and Korkusinski, see [35], and originally was intended as a three-electron system together with three tunable gated quantum dots. The design allowed a host of different mechanisms to control and steer the three-electrons quantum state for instance, the exchange-only qubit involves the manipulation of the exchange interaction between the electrons. We use the term coded qubit because it does not make reference to any particular control mechanism. The basis states of the coded qubit are two eigenstates with total intrinsic angular momentum $S_z = 1/2$. Switching times on the order of tens or hundreds of nanoseconds are commonly achieved and, since the decoherence mechanisms have characteristics time scales of microseconds, the number of controlled operations that could be performed is relatively low. Regrettably, with gated operations it is not possible to use frequencies beyond hundreds of Gigahertz so sub nanoseconds operations, and consequently larger number of controlled operations, are beyond the reach of gated systems [36]. More recently a similar proposal that uses a time-dependent electric field to drive a molecular magnet promises operation times on the picoseconds order [37]. So, it seems reasonable to explore the manipulation of the coded qubit using as control a time-dependent electric field with a frequency on the Terahertz range to achieve operation times in the order of the picoseconds. Of course, using an electromagnetic field introduce a set of difficulties to overcome. As we will show, there is no need to address the electrons individually, it is just enough that the field strength remains constant along the spatial region that contains the TQD, which will have a characteristic length around 100 nanometers. The dynamical behavior and control of coded qubits based on spin states of three-electron TQD have been analyzed theoretically rather thoroughly, using Hubbard Hamiltonian approximations, or effective Heisenberg Hamiltonians [34, 38, 39]. These approaches were justified since, for a broad range of parameters, the qubit basis states are far away from the other three-electron states. Besides, for the driving frequencies and forcing amplitudes accessible to gate technology, the system shows well-defined Rabi oscillations.

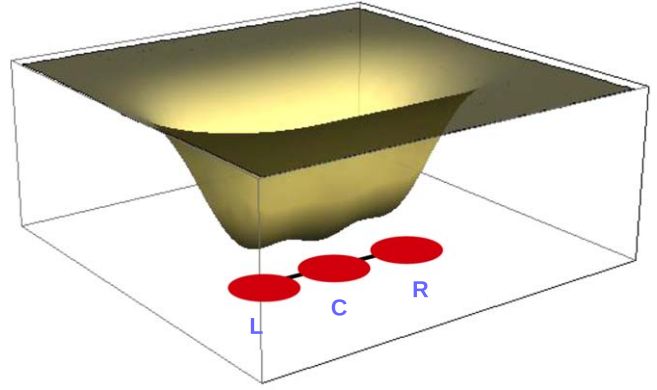


Figure 1. Scheme of the linear arrangement of three quantum dots named as left (L), center (C) and right (R). The red circles in the horizontal x - y plane represent the confinement regions of charge of the two-dimensional electron gas formed in the interface of a typical heterostructure. The confining potential used in this work, consisting in a superposition of a Gaussian well for each one, is depicted above the plane.

Since we will consider frequencies quite different to those applied by metallic gates, neither a simple sinusoidal driving would result in fast Rabi oscillations nor a model that fits the two lowest eigen-energies values would predict accurately the dynamical behavior. It is in scenarios like the one described where optimal control theory (OCT) provides the means to design sequences of composite control pulses.

The aim of this work is to present a detailed analysis of the optical control of three electrons in a two-dimensional TQD by means of optimal control theory. The paper is organized as follows. In section 2 we introduce the model for the two-dimensional three-electron TQD (2A) and briefly describe the method used to calculate its electronic structure (2B). In section 2.3, we describe optimal control equations for the two-dimensional three-electron quantum dot device. In section 3.1 we analyze the electronic structure of the device using different approaches and in section 3.2 we study the operation of the coded qubit by means of OCT. Finally, in section 4, we discuss our most relevant results.

2. Model and methods

2.1. Model of the TQD

We consider a linear triple quantum dot (LTQD) with three electrons. The x axis is chosen along the LTQD such that the dots are centered at positions $\mathbf{R}_n = (x_n, 0)$ ($n = 1, 2, 3$), as shown in the figure 1. The dynamical behavior of the system is governed by a Hamiltonian, $H = H_0 + V(t)$, where

$$H_0 = \sum_{i=1}^3 h(\mathbf{r}_i) + \sum_{i,j=1}^3 V_C(|\mathbf{r}_i - \mathbf{r}_j|), \quad (1)$$

is the time independent Hamiltonian of the three-electron TQD system and $V(t)$ corresponds to the external driving fields that are applied to produce transitions between selected initial and target three-electron states. The one-electron

Hamiltonian is given by

$$h(\mathbf{r}) = -\frac{\hbar^2}{2m^*}\nabla^2 + \sum_{i=L,C,R} W_i(\mathbf{r}) \quad (2)$$

and contains the two-dimensional kinetic energy and the confinement potential energy $W_i(\mathbf{r})$, which in this work is modeled by a Gaussian well

$$W_i(\mathbf{r}) = -W_i \exp\left(-\frac{|\mathbf{r} - \mathbf{R}_i|^2}{2a^2}\right), \quad (3)$$

of depth W_i and range a . In quantum dots electrostatically produced, their size and separation can be both controlled by tunable gate voltages through metallic electrodes deposited on the heterostructure interface. In the model, setting the depths W_i ($i = L, C, R$) of each dot simulates the experimental tuning by the electrostatic plunger gates V_1 , V_2 and V_3 respectively. Usually, the regime of work of the device is characterized by two detuning parameters, $\varepsilon = V_1 - V_3$ and $\varepsilon_m = V_2 - (V_1 + V_3)/2$. $V_C(|\mathbf{r}_i - \mathbf{r}_j|) = e^2/4\pi\epsilon\epsilon_0 r_{ij}$ is the electron-electron Coulomb repulsion; e and m^* are the effective charge and mass of the electrons in the heterostructure, respectively.

Finally,

$$V(t) = -e\mathbf{F}(t) \cdot \sum_i \mathbf{r}_i = -eF(t) \sum_i x_i \quad (4)$$

represents the interaction with an external uniform time-dependent electric field $\mathbf{F}(t)$ along the LTQD and is the Hamiltonian used for controlling the evolution of the system.

The numerical results presented in this work were obtained using as parameters for the quantum dots those of the GaAs compound: effective mass $m^* = 0.067m_e$, effective dielectric constant $\epsilon = 13.1$, Bohr radius $a_B^* = 10$ nm and effective atomic unit of energy 1 Hartree $^* = 10.6$ meV. The confining potentials parameters at zero detuning ($\varepsilon = \varepsilon_m = 0$) were chosen to obtain binding energies and a ground state energy similar as those found in actual quantum dots, and are $W_L = W_R = 53$ meV, $W_C = 51$ meV for the three wells to have the same depth, and $a = 16.3$ nm, with the central dot separated 35 nm from the left and right ones.

As has been said in the Introduction the basis states of the qubit are two eigenstates with total intrinsic angular momentum $S_z = 1/2$. As usual in the literature, we consider the pair of states with lowest energy that satisfy that $S_z = 1/2$, and this eigenstates cannot be calculated exactly.

2.2. Electronic structure

We use the full configuration interaction (CI) method to calculate the stationary three-electron states of the LTQD, in the absence of the time-dependent field and in any subspace with defined S_z , where S_z is the z component of the total spin $\mathbf{S} = \mathbf{S}_1 + \mathbf{S}_2 + \mathbf{S}_3$. We mainly focus in $S_z = 1/2$ since we know that for three-electron system this subspace contains both the ground state and the first excited state with this projection of total spin. Also, because we are interested in the electrical manipulation of the system, the states with different

S_z will not play a role in our study and we will not consider them.

We change to the second-quantization representation of H_0

$$H_0 = \sum_{ij,\sigma} \varepsilon_i c_{i\sigma}^\dagger c_{i\sigma} + \frac{1}{2} \sum_{i,j,k,l} V_{ijkl} c_{i\sigma}^\dagger c_{j\sigma'}^\dagger c_{k\sigma'} c_{l\sigma}, \quad (5)$$

where the second-quantization creation ($c_{i\sigma}^\dagger$) and annihilation ($c_{i\sigma}$) operators are such that $|\varphi_{i\sigma}\rangle = c_{i\sigma}^\dagger |\text{vac}\rangle$, with the one-electron wave functions $\varphi_{i\sigma}$ being solutions of the eigenvalue problem $h\varphi_{i\sigma} = \varepsilon_i \varphi_{i\sigma}$, h is the one-particle Hamiltonian (equation (2)) and σ labels the eigenstates of up or down ($\pm 1/2$) projections of σ_z . Furthermore,

$$V_{ijkl} = \int \varphi_i^*(\mathbf{r}_1) \varphi_j^*(\mathbf{r}_2) \frac{e^2}{4\pi\epsilon\epsilon_0 r_{12}} \varphi_k(\mathbf{r}_2) \varphi_l(\mathbf{r}_1) d\mathbf{r}_1 d\mathbf{r}_2 \quad (6)$$

are the two-particle matrix elements of the Coulomb interaction.

The three-particle eigenstates $|\Psi_n\rangle$ of the subspace $S_z = 1/2$ of H_0 are obtained by exact diagonalization of H_0 in a basis of configurations of antisymetrized products $|\Phi_{ijk}\rangle \equiv c_{i\uparrow}^\dagger c_{j\uparrow}^\dagger c_{k\downarrow}^\dagger |\text{vac}\rangle$ of two spin-up and one spin-down orbitals of h

$$|\Psi_n\rangle = \sum_{ijk} a_{ijk}^{(n)} |\Phi_{ijk}\rangle. \quad (7)$$

The time-dependent Hamiltonian $V(t)$, equation (4),

$$V(t) = \sum_{ij,\sigma} V_{ij} c_{i\sigma}^\dagger c_{j\sigma} = -F(t) \sum_{ij,\sigma} \mu_{ij} c_{i\sigma}^\dagger c_{j\sigma}, \quad (8)$$

with $\mu_{ij} = \langle \varphi_i | ex | \varphi_j \rangle$, induces transitions between the different levels of H_0 although, since H is spin-independent, there are no transitions between subspaces of different total spin S .

The implementation and the accuracy of the CI method depends on the number of one-electron wave functions used in the calculations. Results present along this work were performed using 9 orbitals obtained by direct solution of equation (2) [16, 40]. Nevertheless, the large number of orbital configurations entering in an accurate calculation spoils a simple interpretation of the three-electron LTQD states in terms of configurations of dot occupations.

On the other hand, it has been shown [41, 42] that many quantum dot properties can be described in simple terms with a properly parameterized extended Hubbard approximation to the Hamiltonian (5), namely,

$$\begin{aligned} H_{\text{Hub}} = & \sum_{\langle i,j \rangle, \sigma=\uparrow,\downarrow} \tau_{ij} (d_{i\sigma}^\dagger d_{j\sigma} + \text{h.c.}) \\ & + \sum_{i=1}^N \left[\frac{1}{2} (U - U_C) n_i (n_i - 1) + V_i n_i \right] \\ & + \sum_{\langle i,j \rangle} U_C n_i n_j, \end{aligned} \quad (9)$$

where τ_{ij} are nearest-neighbor hopping parameters, U and U_C are respectively the on-site and intersite repulsion, and V_i is the gate electrostatic potential at dot i ; $d_{i\sigma}^\dagger$ ($d_{i\sigma}$) creates (annihilates) an electron localized at dot i , and $n_i = \sum_{\sigma=\uparrow,\downarrow} d_{i\sigma}^\dagger d_{i\sigma}$ is the occupation of dot i .

The effect of the time-dependent electric field is accounted for by the matrix elements of the one-electron operator

$$V(t) = -\mu F(t) = -F(t) \sum_{ij, \sigma=\uparrow, \downarrow} \mu_{ij} c_{i\sigma}^\dagger c_{j\sigma} \quad (10)$$

between the H_{Hub} eigenstates, where the explicit form of μ in the three-electron configuration basis set is shown in the appendix A.

For the Hubbard model calculations, we shall assume a negligible overlap between one-electron states localized at the dots, so that, the dipole moment operator becomes diagonal and nonvanishing for double occupied configurations only, i.e. $\mu = \text{diag}(0, 0, \lambda, -\lambda, \lambda, -\lambda)$, with $\lambda = \langle \varphi_R | ex | \varphi_R \rangle$. For the sake of comparison to CI calculations with confinement potentials, we chose hopping matrix elements $\tau_{ij} = \tau = 1.0$ meV, Coulomb on-site repulsion $U = 6.4$ meV and intersite repulsion $U_C = 1.6$ meV, so that they become qualitatively comparable to each other.

2.3. Optimal control of the state dynamics

For controlling the qubit, encoded in the two lowest LTQD states Ψ_0 and Ψ_1 , we propose to design a time-dependent electric field $F(t)$ able to drive the state of the system $\Psi(t)$ from $\Psi(0) = \Psi_0$ to $\Psi(T) = \Psi_1$, in a given prescribed time T as short as possible. We assume the time-dependent electric field $F(t)$ to be uniform and applied along the longitudinal direction x of the LTQD. Then, the state $\Psi(t)$ must satisfy the time-dependent Schrödinger equation

$$i \frac{\partial \Psi(t)}{\partial t} = H \Psi(t) = [H_0 - \hat{\mu} F(t)] \Psi(t). \quad (11)$$

OCT provides a systematic method to find the optimal pulse $F_{\text{OCT}}(t)$ that drives the solution of the Schrödinger equation (11), while maximizing the overlap of the final state to a given target state ϕ_F . We briefly outline here the theory and some technical details of the method as applied in this work [43, 44].

The yield of the control process is defined by the following functional

$$J_1[\Psi] = |\langle \Psi(t) | \phi_F \rangle|^2. \quad (12)$$

In order to avoid high energy fields a second functional is introduced

$$J_2[\varepsilon] = -\alpha \left[\int_0^T F^2(t) dt \right], \quad (13)$$

where the fluence is the time-integrated intensity of the field and α is a time-independent Lagrange multiplier. As we already know, the electronic wavefunction has to satisfy the time-dependent Schrödinger equation introducing a third functional

$$J_3[\varepsilon, \Psi, \chi] = -2 \text{Im} \int_0^T \left\langle \chi(t) \left| \frac{\partial}{\partial t} - H(t) \right| \Psi(t) \right\rangle, \quad (14)$$

where we have introduced the time-dependent Lagrange multiplier $\chi(t)$. Finally, the Lagrange functional has the form $J = J_1 + J_2 + J_3$. The Variation of this functional with

respect to $\Psi(t)$, $F(t)$ and $\chi(t)$ allows us to obtain the desired control equations [44]

$$i \frac{\partial \Psi(t)}{\partial t} = H(t) \Psi(t), \quad \Psi(0) = \phi \quad (15)$$

$$i \frac{\partial \chi(t)}{\partial t} = H(t) \chi(t) \quad (16)$$

$$\chi(T) = |\phi_F\rangle \langle \phi_F | \Psi(T) \rangle \quad (17)$$

$$F(t) = -\frac{1}{\alpha} \text{Im} \langle \chi(t) | \hat{\mu} | \Psi(t) \rangle. \quad (18)$$

This set of coupled equations can be solved iteratively. The solution can be obtained using several approaches, for example, using the efficient forward-backward propagation scheme developed in reference [45]. The algorithm starts with propagating $|\phi\rangle$ forward in time, using in the first step a guess of the laser field $F^{(0)}(t)$. At the end of this step we obtain the wavefunction $|\Psi^{(0)}(T)\rangle$, which is used to evaluate $|\chi^{(0)}(T)\rangle = |\phi_F\rangle \langle \phi_F | \Psi^{(0)}(T) \rangle$. The algorithm continues with propagating $|\chi^{(0)}(t)\rangle$ backwards in time. In this step it is clear that we need to know both wave functions ($\Psi^{(0)}$ and $\chi^{(0)}$) at the same time. In this step we obtain a first version of the optimized pulse $F^{(1)}(t)$. We repeat this operation until the convergence of J is achieved. The values of the Lagrange multiplier α are chosen in order to achieve the desired fluences. The numerical integration of the forward and backward time evolution was performed using high precision Runge-Kutta algorithms under various initial guesses (e.g. constant, random, monochromatic and a superposition of two harmonic pulses). The resulting optimal pulse and the time evolution under its driving were found to be robust for all these various starting conditions.

3. Results

3.1. Energy spectra and dipole transition moments

The CI method provides very accurate numerical approximations for both, the eigenvalues and eigenfunctions of systems of interacting electrons, as long as a large enough number of one-electron wave functions are used to perform the calculations. The large number of one electron functions needed to obtain the desired accuracy in the three-electron energies implies in general a large number of configurations, and therefore a representation of the hamiltonian provided by the Hubbard model could allow a more direct and simple interpretation of the relevant configurations on a site basis set, that is, a basis of orbitals localized around a given dot. By using this simple model, the symmetry of total spin, and the projection in the z axis, the number of configurations can be reduced to only six in total. We denote these configuration states as $|i\rangle$, with $i = 0, 1, 2, 3, 4, 5$. This simple model can provide insights of the mechanism involved in the effects of an electric field in the system. Then, in the present section we compare the results of the electronic structure and the response to an electric field obtained with CI calculations and

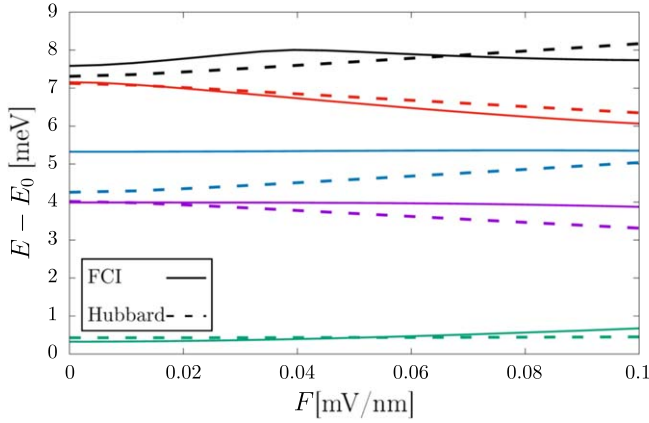


Figure 2. Energy gaps $E_n - E_0$ of the TQD levels referred to the ground state as a function of the electric field F calculated with the CI method (solid lines) and the Hubbard model (dashed lines). As discussed in the text, the Hubbard model describes qualitatively well the gaps, with the exception of $n = 3$. Although the Hubbard model predicts a small energy gap $E_3 - E_2$ smaller than 0.1 meV, the most accurate result given by CI calculations is more than 1 meV.

the Hubbard model presented in the previous section, in order to know in which aspects both approximations describe the results with the same features.

Figure 2 shows the energy levels gaps with respect to the ground state of the LTQD calculated with the CI method and the Hubbard model, as a function of the magnitude of an applied external uniform electric field F . At zero field, the energy levels are roughly grouped as (E_0, E_1) , (E_2, E_3) and (E_4, E_5) with relatively small gaps between them. For the CI calculations we obtain $E_1 - E_0 \simeq 0.23$ meV, $E_3 - E_2 \simeq 1$ meV and $E_5 - E_4 \simeq 0.64$ meV.

The Hubbard model at zero detuning provides a simple picture for this structure. The two lowest lying levels are single occupied; the second and the highest pairs are double occupied dots configurations of higher energies, $U - 2U_C$ and U , respectively, with small gaps between the levels of each pair $\Delta E \sim \tau^2/U$. As shown in the figure, the agreement of the energy gaps is fairly good, with the main qualitative difference between the CI and Hubbard being the gap of the pair (E_2, E_3) , which is underestimated within the approximate model. This discrepancy has consequence on the dynamics of the qubit as we shall discuss in the section below.

The Hubbard model provides insight on the configurations forming the states from CI calculations. At zero external field and vanishing detuning $V_2 = 0$, the six hubbard eigenstates, ordered from the lowest to the highest eigenenergy are approximately given by $|0\rangle$, $|1\rangle$, $\frac{1}{\sqrt{2}}(|2\rangle + |3\rangle)$, $\frac{1}{\sqrt{2}}(|2\rangle - |3\rangle)$, $\frac{1}{\sqrt{2}}(|4\rangle + |5\rangle)$ and $\frac{1}{\sqrt{2}}(|4\rangle - |5\rangle)$.

Application of an external electric field F produces a superposition between the configuration states with one electron by dot with those with two electron by dot, such that $|\Psi_i(F)\rangle = \sum_n c_{in}(F)|n\rangle$, where the coefficients c_{in} stand for contributions of single and double occupied configurations, having magnitudes $c_{in} \sim \mathcal{O}(\tau/U) \ll 1$. Since any one-particle operator involves the hopping of a single electron from a dot to its nearest neighbor, it cannot connect single occupied

states (nor double occupied states) to each other. Thus, this small mixing between single and doubly occupied states allows for dipole transitions among the energy levels. The difference between the Hubbard model and the CI calculations is reflected in the dipole transition moment calculations as shown below.

The switching between the qubit states, denoted by $|\Psi_0\rangle \rightarrow |\Psi_1\rangle$, i.e. the particular time-evolution of the system when it is driven by a time-dependent electric field, shall depend on the magnitude of the transition moments μ_{ij} coupling the lowest-lying states. Figures 3(a) and (b) show the behavior of the dipole transition moments μ_{ij} as functions of the electric field strength F , obtained from the CI method and Hubbard model calculations, respectively. The transitions moments μ_{02} , μ_{23} and μ_{31} , are shown in solid lines, while the other moments are depicted with dashed lines. We use this convention to illustrate two different dynamical mechanisms to switch between the qubit states, namely, a ‘direct’ transfer $|\Psi_0\rangle \rightarrow |\Psi_1\rangle$ and an ‘indirect’ one $|\Psi_0\rangle \rightarrow |\Psi_2\rangle \rightarrow |\Psi_3\rangle \rightarrow |\Psi_1\rangle$.

A direct comparison of the CI and Hubbard results for the transition dipole moments, see figure 3, shows that, in the case of the direct transition moment, they differ roughly in an order of magnitude ($\mu_{01}^{\text{Hubb}} \ll \mu_{01}^{\text{CI}}$) with μ_{01}^{Hubb} being almost independent of F in the range depicted. As shown above, the dipolar moment depends strongly on the small mixing between the single and doubly occupied configurations. Since the CI is obtained with a much more flexible basis set, this small weights are accurately represented, while the Hubbard basis includes only 6 configurations (appendix A).

On the other hand, μ_{01}^{CI} decreases slightly when F increases its value. Interestingly, the CI calculation gives a nearly constant $\mu_{02} \simeq \mu_{31}$ for a wide range of F , behavior that is also approximately shown by the Hubbard results. Nevertheless, also in this case, the μ^{CI} becomes much larger than μ^{Hubb} . The most remarkable difference between both descriptions is the transition μ_{23} , for which the Hubbard calculation overestimates the CI value and becomes strongly dependent on the field.

These results, together with the already mentioned difference in the gap $E_3 - E_2$, illustrate the limitations of the Hubbard model to describe the transitions when doubly occupied configurations are relevant. Therefore, all dynamical processes discussed below, were only performed with magnitudes calculated with the CI method.

Finally, other paths differing from the direct and indirect ones, such as $|\Psi_0\rangle \rightarrow |\Psi_2\rangle \rightarrow |\Psi_1\rangle$ or $|\Psi_0\rangle \rightarrow |\Psi_3\rangle \rightarrow |\Psi_1\rangle$, are ruled out due to a low or vanishing dipole moment between a given pair or states. On the other hand, transitions involving higher excited states, like $|\Psi_0\rangle \rightarrow |\Psi_5\rangle \rightarrow |\Psi_3\rangle \rightarrow |\Psi_1\rangle$ are not found in the OCT solution to be discussed below, possibly because of the requirement of low fluence of the pulse.

3.2. Qubit dynamics

The transition dipole moments calculated with the CI wave functions were used to optimally design fast low-fluence pulses to control the switching between the qubit states

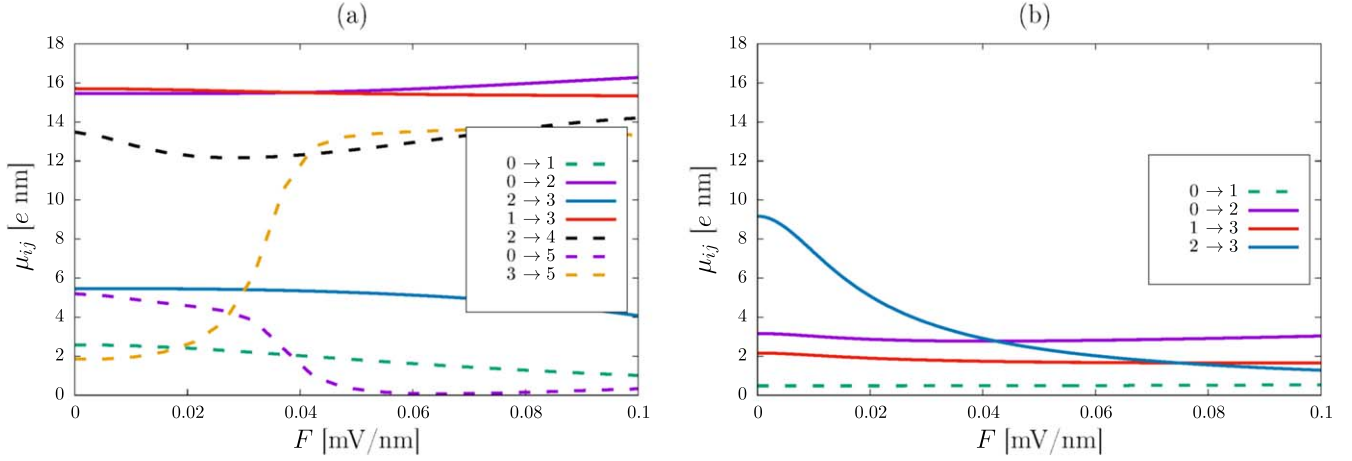


Figure 3. Relevant transition dipole moments between the eigenstates of the (a) CI and (b) Hubbard Hamiltonians as a function of the electric field F . The Hubbard parameters are $\tau = 1$ meV, $U = 6.4$ meV and $U_C = 1.6$ meV. See the text for details. In the figure the unit for the dipole moment is given by e nm, where e is the electron charge.

$\{|\Psi_0\rangle, |\Psi_1\rangle\}$. In other words, the population, defined as $|\langle\Psi|\Psi(t)\rangle|^2$, is transferred from the initial to the target state.

Due to the imposed joint constraints on the pulse length and the low fluence, the resulting pulse is not always able to accomplish a complete population transfer to the target state. Pulses of very short lengths ($T \lesssim 10$ ps) and low fluence, can transfer the initial state with $\lesssim 0.9$ fidelity, which is lesser than the required accuracy for quantum information applications.

When the amplitude of the applied pulse is near the value $F = \pi/\mu_{01}T$ (i.e. small values of the time-independent Lagrange multiplier α , see equation (13)), the OCT method favors monochromatic pulses driving a direct Rabi transition with frequency $\omega_{01} \simeq 540$ GHz. By choosing larger values of α , the amplitude of the resulting pulse becomes smaller, and Rabi transitions are not longer possible for the fixed high yield. Nevertheless, in those cases, there are other solutions, involving transitions to excited states, that can perform the transfer process within the imposed constraints. We shall focus here on these low-amplitude fast pulses able to drive the state with high-yields, although at the expense of using transitions to the low lying excited states, external to the logical computational subspace.

All the calculations presented in the following are in a range of pulse length and fluence for which the tailored pulses reach 99% (or higher) of population transfer.

A typical pulse $F_{\text{OCT}}(t)$ obtained from the OCT optimization, for a pulse length of $T = 60$ ps, is shown in figure 4(a) as a black solid line together with the sequential pulse $F_{\text{seq}}(t)$, equation (19), to be discussed below (red thin line).

A Fourier analysis of $F_{\text{OCT}}(t)$ shows strong contributions from three frequencies: $\omega_{20} = 6.73$ THz, $\omega_{32} = 2.36$ Tz and $\omega_{31} = 8.54$ Tz, corresponding to the energy gaps of the TQD: $\hbar\omega_{20} = 4.18$ meV and $\hbar\omega_{32} = 1.47$ meV and $\hbar\omega_{31} = 5.31$ meV. These results suggest that the dynamics can be viewed as transitions along the paths connecting the initial and target states and having the largest transition dipole moments, i.e. $\Psi_0 \rightarrow \Psi_2 \rightarrow \Psi_3 \rightarrow \Psi_1$.

The behavior of the pulse, as a time-dependent function, can be better understood analyzing the data shown in figure 4(b). It shows a map of the Fourier transform of the slice of $F_{\text{OCT}}(t)$ in a time window $(t, t + \Delta T)$, for $\Delta T = 10$ ps, as a function of the frequency ω and the time. It can be seen that while the lowest frequency ω_{32} is present all along the pulse length T , ω_{20} and ω_{31} are present, roughly, during the first and second halves, respectively. The dynamics of the state populations, figure 4(c), confirms this picture. During the first 10 ps the pulse produces a transfer of population from the state $|\Psi_0\rangle$ to the state $|\Psi_2\rangle$ exclusively; then, while the transferring of population to this state continues, the population transfer $|\Psi_2\rangle \rightarrow |\Psi_3\rangle$ is activated until the state $|\Psi_0\rangle$ becomes completely depleted, at nearly $T/2$. In the second half ($T/2, T$), a similar process increases the population of the target state $|\Psi_1\rangle$ with population that is transferred to it from state $|\Psi_3\rangle$ besides, during this interval, the transferring of population $|\Psi_2\rangle \rightarrow |\Psi_3\rangle$ continues happening until the only significantly populated state is the target one, at time T . Figure 4(d) shows that similar processes occur for a longer pulse with $T = 90$ ps.

From the discussion above, a simpler two-frequencies sequential pulse is proposed for $0 \leq t \leq T$:

$$F_{\text{seq}}(t) = F_1(t)\theta(T/2 - t) + F_2(t)\theta(t - T/2), \quad (19)$$

where $\theta(t)$ is the step function, and

$$F_1(t) = A \cos(\omega_{20}t) + B \cos(\omega_{32}t), \quad (20)$$

$$F_2(t) = A \cos(\omega_{31}t) + B \cos(\omega_{32}t), \quad (21)$$

where the assumptions that the same amplitude A for the transitions $|\Psi_0\rangle \rightarrow |\Psi_2\rangle$ and $|\Psi_3\rangle \rightarrow |\Psi_1\rangle$ in the ranges $(0, T/2)$ and $(T/2, T)$, respectively, and a constant amplitude B for $|\Psi_2\rangle \rightarrow |\Psi_3\rangle$ along the whole range T are made.

The analytic solution of the time-dependent Schrödinger equation for this pulse, within the rotating wave approximation (RWA), is given in appendix B. The resulting pulse for $T = 60$ ps, shown in figure 4(a) with red thin line, resembles to a large extent the optimal pulse. Also the time variations of the occupations when this pulse is applied,

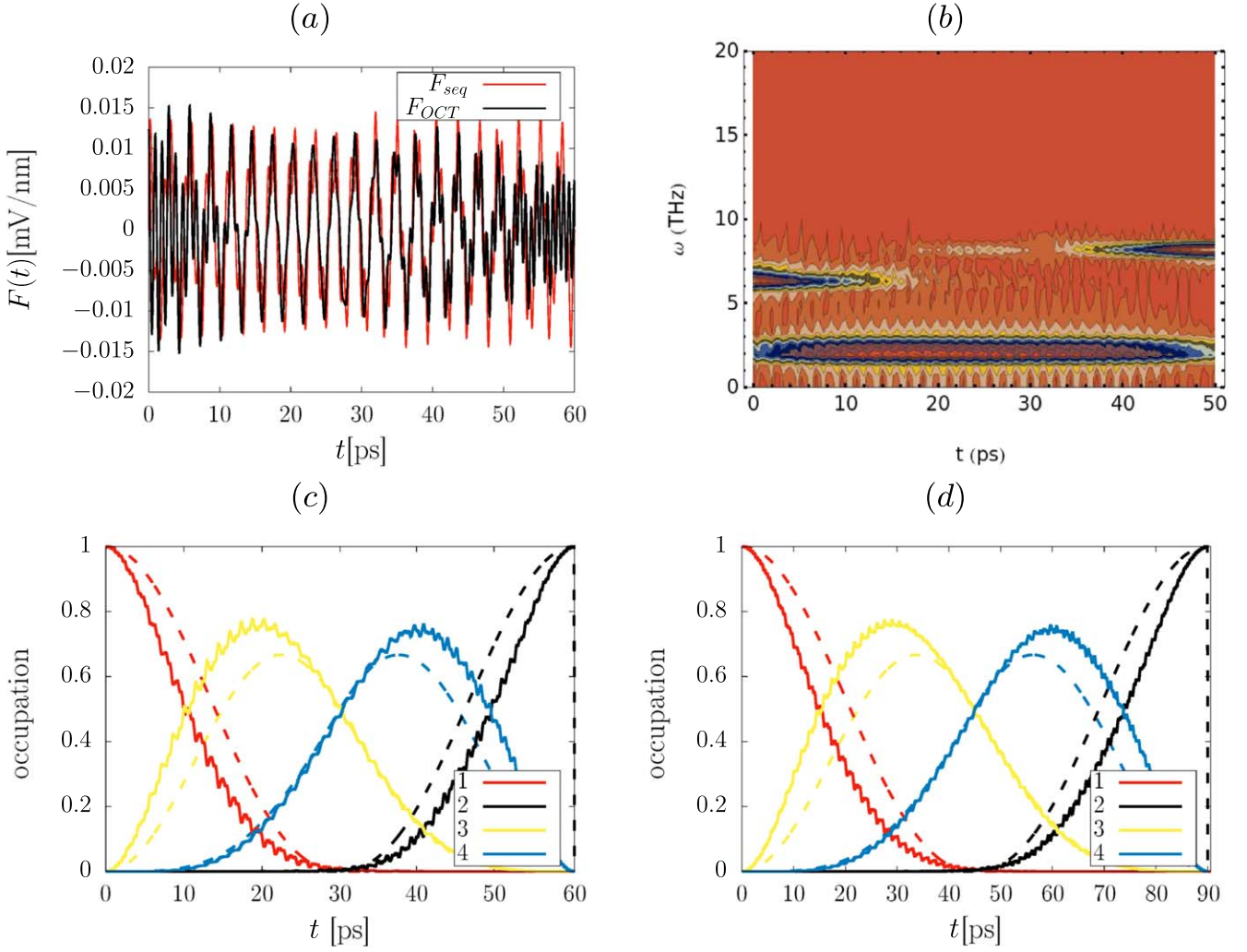


Figure 4. (a) Optimally (OCT) designed and three-level model pulses for $|\Psi_0\rangle \rightarrow |\Psi_1\rangle$ population transfer in $T = 60$ ps. (b) Map of Fourier transform of the OCT pulses $F(t)$ calculated within a time window $(t, t + \Delta t)$ as a function of t and ω , with $\Delta t = 10$ ps. Lower panels: time evolution of the population of the four lowest states resulting from driving the system with the pulses of $T = 60$ (c) and $T = 90$ ps (d).

dashed curves in figures 4(c) and (d), represent a good approximation to those obtained with optimal pulse.

In the usual description of three level systems, the application of $F_{\text{seq}}(t)$ can be considered as two sequential three-level processes, namely, a ladder-transition ($|\Psi_0\rangle \rightarrow |\Psi_2\rangle \rightarrow |\Psi_3\rangle$) with $F_1(t)$, followed by a Λ -process ($|\Psi_2\rangle \rightarrow |\Psi_3\rangle \rightarrow |\Psi_1\rangle$) with $F_2(t)$.

The relationship between the fluence and length of the pulses for high yield transitions $|\Psi_0\rangle \rightarrow |\Psi_1\rangle$ required for quantum information processing was further investigated. Figure 5 shows the locus of high fidelity processes (~ 0.9999) in the plane time-fluence for direct Rabi transitions, OCT designed pulses and sequential pulses. As it can be seen, all of them satisfy an approximate power-law $\rho \sim T^{-\gamma}$ with $\gamma \approx 2$.

The known RWA solution for the two-level process, provides an analytic relation between the fluence and the time length T for a monochromatic Rabi pulse of frequency ω_{10} transferring completely the population from the initial to the

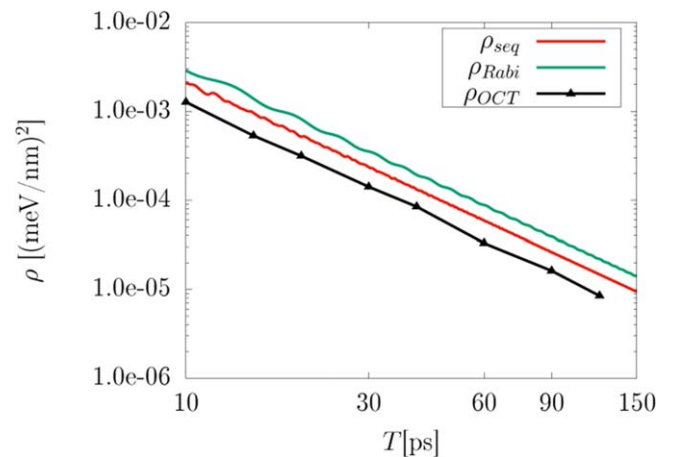


Figure 5. Mean square amplitude of the field for a several OCT designed pulses having $10 \text{ ps} \leq T \leq 150 \text{ ps}$ ρ_{OCT} , as compared with two- (Rabi) ρ_{Rabi} and three-level based models ρ_{seq} (see text for further details).

target state, giving

$$\rho_{\text{Rabi}} = \left(\frac{\pi}{\mu_{01}} \right)^2 \frac{(2T\omega_{01} + \sin(2T\omega_{01}))^2}{4\omega_{01}T^3}. \quad (22)$$

For times T much longer than ω_{10}^{-1} , the second term can be neglected and $\rho \sim T^{-2}$.

We could perform the same analysis for the indirect strategy $|\Psi_0\rangle \rightarrow |\Psi_2\rangle \rightarrow |\Psi_3\rangle \rightarrow |\Psi_1\rangle$.

The conditions for the dynamics of the sequential pulse (19) within the RWA, as given in appendix B, are as follows: the ground state is initially occupied, and at some time τ its population is completely transferred to the second and third excited states. Then these two states are depopulated, and the probability is transferred to the target state initially depopulated. In appendix B it is shown that $\tau = T/2$. The mean square amplitude for this model is given by

$$\rho_{\text{seq}} = \frac{1}{T} \int_0^T F_{\text{seq}}(t)^2 dt. \quad (23)$$

In figure 5 we compare the mean square amplitude as a function of the control time T for the Rabi oscillation (22), the sequential strategy (23), and the OCT results. The OCT results correspond to the lowest fluence in which the target can be reached with a yield of 99.99%. For any given T , the fluence for the Rabi strategy is always larger than the sequential pulse and the OCT protocol, i.e. $\rho_{\text{Rabi}} > \rho_{\text{seq}} > \rho_{\text{OCT}}$. In the figures 4(c) and (d) we show the time evolution of the state probabilities for $T = 60$ and 90 ps obtained with OCT (solid line) and the sequential pulse model (dashed line). Similarity of both strategies shows that the mechanism involved in the OCT dynamics are basically described by $F_{\text{seq}}(t)$. The differences could be reduced by including envelope profiles in the model.

4. Conclusions

In this work, we aimed to design fast pulses for accurate controlling a qubit encoded in the three-electron states of a TQD.

We have shown that driving fields in the optical range can be designed by applying optimal control theory, while still satisfying prescribed sub-nanosecond operation times, employing experimentally available field amplitudes and achieving high fidelity transfer to the target state.

The pulses obtained without a frequency cutoff, have transfer times between the qubit states on the order of tens to hundreds of picoseconds and achieving the fidelity required for quantum information processing. Their frequency spectrum correspond, mainly, to the energy gaps between the qubit states as well as between some of the closer excited states and the qubit states.

If the frequencies present in the pulse spectrum are restricted to be under the THz range, as in experiments with gate voltage control, only direct Rabi transitions between the

qubit states are found. On the other hand, by allowing optical range frequencies to be present in the designed pulse, fast switching process involving intermediate transitions to the closer excited states are obtained.

Since the dynamics of the TQD strongly depends on the precise representation of both the electronic structure and the transition dipole moments, we compared our configuration-interaction calculations to the description provided by the extended Hubbard model, which is frequently used in the literature. Our findings show that, although a proper parametrization of the Hubbard model provide energy levels with a reasonable agreement with those obtained using the CI method, it cannot do the same for the electric dipole transition moments. Since these transition moments are needed to study the switching between the qubit states we conclude that the dynamics predicted using the Hubbard approach is not reliable for designing control strategies involving transitions to excited states such as the analyzed in this work.

Finally, our assumption that the external electric field is uniform is unnecessary, although the net effect of the space modulation of the electric field would be to reduce the switching rate or to give rise to a more complicated pulse sequence.

Acknowledgments

We acknowledge SECYT-UNC, SGCyT-UNNE (PI 17F020) and CONICET (PIP-11220150100327CO, PUE2017-22920170100089CO, PIP-11220130100361CO) for partial financial support. OO wishes to acknowledge the warm hospitality of the Nanophysics Group at FACENA and IMIT-CONICET, Corrientes, where this work was done.

Appendix A. Effective six-level Hubbard model

By choosing the basis $\{|n\rangle\}$ ($n = 0, \dots, 5$) [25], of single occupied $|0\rangle$ and $|1\rangle$ and double occupied configurations $|2\rangle$, $|3\rangle$, $|4\rangle$ and $|5\rangle$,

$$|0\rangle = \frac{1}{\sqrt{2}}(-|\Phi_{123}\rangle + |\Phi_{231}\rangle) \quad (A1)$$

$$|1\rangle = \frac{1}{\sqrt{6}}(|\Phi_{123}\rangle + |\Phi_{231}\rangle) - \sqrt{\frac{2}{3}}|\Phi_{312}\rangle \quad (A2)$$

$$|2\rangle = |\Phi_{311}\rangle \quad (A3)$$

$$|3\rangle = |\Phi_{133}\rangle \quad (A4)$$

$$|4\rangle = |\Phi_{211}\rangle \quad (A5)$$

$$|5\rangle = |\Phi_{233}\rangle, \quad (A6)$$

the effective 6-level Hubbard Hamiltonian takes the form

$$H_{\text{Hub}} = \begin{pmatrix} 0 & 0 & \frac{\tau}{2} & \frac{\tau}{2} & \frac{\tau}{2} & \frac{\tau}{2} \\ 0 & 0 & \frac{\sqrt{3}\tau}{2} & -\frac{\sqrt{3}\tau}{2} & -\frac{\sqrt{3}\tau}{2} & \frac{\sqrt{3}\tau}{2} \\ \frac{\tau}{2} & \frac{\sqrt{3}\tau}{2} & V_1 - V_2 + U - 2U_C & 0 & 0 & 0 \\ \frac{\tau}{2} & -\frac{\sqrt{3}\tau}{2} & 0 & -V_2 + V_3 + U - 2U_C & 0 & 0 \\ \frac{\tau}{2} & -\frac{\sqrt{3}\tau}{2} & 0 & 0 & V_2 - V_3 + U & 0 \\ \frac{\tau}{2} & \frac{\sqrt{3}\tau}{2} & 0 & 0 & 0 & -V_1 + V_2 + U \end{pmatrix}. \quad (\text{A7})$$

The dipole moment in the 3-particle basis $|n\rangle$ becomes

$$\mu = \begin{pmatrix} 0 & 0 & -\frac{\nu}{\sqrt{2}} & \frac{\nu}{\sqrt{2}} & \frac{\nu}{\sqrt{2}} & -\frac{\nu}{\sqrt{2}} \\ 0 & 0 & -\sqrt{\frac{3}{2}}\nu & -\sqrt{\frac{3}{2}}\nu & -\sqrt{\frac{3}{2}}\nu & -\sqrt{\frac{3}{2}}\nu \\ -\frac{\nu}{\sqrt{2}} & -\sqrt{\frac{3}{2}}\nu & \lambda & 0 & 0 & 0 \\ \frac{\nu}{\sqrt{2}} & -\sqrt{\frac{3}{2}}\nu & 0 & -\lambda & 0 & 0 \\ \frac{\nu}{\sqrt{2}} & -\sqrt{\frac{3}{2}}\nu & 0 & 0 & \lambda & 0 \\ -\frac{\nu}{\sqrt{2}} & -\sqrt{\frac{3}{2}}\nu & 0 & 0 & 0 & -\lambda \end{pmatrix} \quad (\text{A8})$$

Assuming $\lambda = \langle \varphi_R | ex | \varphi_R \rangle = -\langle \varphi_L | ex | \varphi_L \rangle$ is the diagonal matrix elements of the dipole moment when evaluated with functions localized at the left (right) dots, and $\nu = \langle \varphi_L | ex | \varphi_C \rangle \sim \mu S_{LC} \ll \lambda$, S_{LC} being the overlap between basis functions located at the left (or right) and center dots. In the approximate model of the LTQD, $\lambda \approx 1$ and $\nu \approx 0$.

Appendix B. RWA solution of Schrödinger equation for the sequential pulse $F_{\text{seq}}(t)$

We present here the time-dependent solution for the dynamics of the LTQD states driven by the pulse $F_{\text{seq}}(t)$, equation (19).

Defining $\Omega_{02} = \mu_{02}A$ and $\Omega_{23} = \mu_{23}B$ and neglecting rapidly oscillating terms (RWA), the Schrödinger equation in the interaction picture, reads

Ladder-process: $\omega_a = \omega_{20}$, $\omega_b = \omega_{32}$

$$i\dot{c}_0(t) = \frac{\omega_{02}}{2}c_2 \quad (\text{B1})$$

$$i\dot{c}_2(t) = \frac{\omega_{02}}{2}c_0 + \frac{\omega_{23}}{2}c_3 \quad (\text{B2})$$

$$i\dot{c}_3(t) = \frac{\omega_{23}}{2}c_2 \quad (\text{B3})$$

Λ -process: $\omega_a = \omega_{31}$, $\omega_b = \omega_{32}$

$$\begin{aligned} i\dot{c}_2(t) &= \frac{\Omega_{23}}{2}c_3 \\ i\dot{c}_3(t) &= \frac{\Omega_{23}}{2}c_2 + \frac{\Omega_{02}}{2}c_1 \\ i\dot{c}_1(t) &= \frac{\Omega_{02}}{2}c_3 \end{aligned} \quad (\text{B4})$$

By imposing the initial and final conditions

$$c_0(0) = 1, \quad c_2(0) = c_3(0) = 0, \quad (\text{B5})$$

$$c_1(T) = 1, \quad c_2(T) = c_3(T) = 0, \quad (\text{B6})$$

the following solutions are obtained

Ladder-process:

$$\begin{aligned} c_0(t) &= \left(\frac{\Omega_{02}}{\Delta}\right)^2 \cos\left(\frac{\Delta}{2}t\right) + \left(\frac{\Omega_{23}}{\Delta}\right)^2 \\ c_2(t) &= -i\left(\frac{\Omega_{23}}{\Delta}\right) \sin\left(\frac{\Delta}{2}t\right) \\ c_3(t) &= \left(\frac{\Omega_{02}\Omega_{23}}{\Delta^2}\right) \left(\cos\left(\frac{\Delta}{2}t\right) - 1\right) \end{aligned} \quad (\text{B7})$$

Λ -process:

$$\begin{aligned} c_1(t) &= \left(\frac{\Omega_{02}}{\Delta}\right)^2 \cos\left(\frac{\Delta}{2}(t-T)\right) + \left(\frac{\Omega_{23}}{\Delta}\right)^2 \\ c_3(t) &= -i\left(\frac{\Omega_{23}}{\Delta}\right) \sin\left(\frac{\Delta}{2}(t-T)\right) \\ c_2(t) &= \left(\frac{\Omega_{02}\Omega_{23}}{\Delta^2}\right) \left(\cos\left(\frac{\Delta}{2}(t-T)\right) - 1\right). \end{aligned} \quad (\text{B8})$$

Taking $\tau = T/2$ the pulse becomes symmetric, as observed in the OCT pulses, and results in a complete depletion of both the initial and target states at $T/2$: $|c_0(T/2)|^2 = 0 = |c_1(T/2)|^2$. The continuity of the solutions at $T/2$ also implies $\Omega_{02} = \sqrt{2}\Omega_{23}$ and

$$T = \frac{4}{\Delta} \arccos\left(-\frac{\Omega_{23}^2}{\Omega_{02}^2}\right), \quad (\text{B9})$$

therefore, $T = 8\pi/3\sqrt{3}\Omega_{23}$.

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