Optimal laser-control of double quantum dots

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Coherent single-electron control in a realistic semiconductor double quantum dot is studied theoretically. Using optimal-control theory we show that the energy spectrum of a two-dimensional double quantum dot has a fully controllable transition line. We find that optimized picosecond laser pulses generate population transfer at significantly higher fidelities (>0.99) than conventional sinusoidal pulses. Finally we design a robust and fast charge switch driven by optimal pulses that are within reach of terahertz laser technology.

Double quantum dots (DQDs), i.e., coupled two-dimensional (2D) electron traps, have been under recent and extensive studies both experimentally1,2 and theoretically.3,4,5 The main interest in DQDs arises from their potential for solid-state quantum computation that could be achieved in principle by rapidly switching voltages of electrostatic gates. The gates permit to tune at will the system geometry and hence the electronic properties of DQDs. Coherent manipulation of a single charge6 and coupled spins7,8 has already been achieved, and recently a coherence time of ~200 ns was obtained for a well isolated silicon DQD.9 Theoretical studies on single-electron transport inside the DQD driven by linear switches and linearly polarized continuous waves (CWs) were reported very recently.10 In the latter case the transport is rather sensitive to possible anharmonicity of the potential and limited to uncoupled dots far apart from each other. Electron control in DQDs has been studied also using genetic algorithms as well as rotating-wave and resonant approximations leading to a reduction to a three-level system. To the best of our knowledge, however, a general N-level control scheme by using direct external electric fields has not been introduced for 2D-DQDs until now.

In this paper we discuss the controllability criteria for single-electron states of DQDs by means of external laser pulses. We show that at certain interdot distances some of the single-electron states allow population transfer from the ground state to those states. We apply quantum optimal-control theory (OCT) which yields the optimal laser pulses for predefined transitions. We obtain high occupations (>99%) of the target states in a realistic DQD in a few picoseconds, which is well in the coherent regime. If the initial and final states are chosen to have full localization of the electron in one or the other dot, this scheme enables rapid and controlled transport which is not sensitive to the interdot distance or to the inevitable anharmonicities in the confining potential.

In the static 2D Hamiltonian, \( \hat{H}_0 = -\left( \partial_x^2 + \partial_y^2 \right)/2 + V_c(x, y) \), the external potential describing the DQD is, in its most common form, given by

\[
V_c(x, y) = \frac{\omega_0^2}{2} \min \left[ (x - \frac{d}{2})^2 + y^2, (x + \frac{d}{2})^2 + y^2 \right],
\]

where \( d \) is the distance between the potential minima, and \( \omega_0 = 0.5 \) is the confinement strength with a typical value for DQDs. We apply the effective-mass approximation for electrons moving in GaAs and set the effective mass to \( m^* = 0.067m_e \) and the dielectric constant to \( \kappa = 12.7\varepsilon_0 \). The energies, lengths, and times are given in effective atomic units (a.u.): \( \text{Ha}^* = (m^*/\kappa^2)\text{Ha} \approx 11.30\text{ meV} \), \( a_0^* = (m^*/\kappa)a_0 \approx 10.03\text{ nm} \), and \( u_0^* = \hbar/\text{Ha}^* \approx 58.23\text{ fs} \), respectively.

In Fig. 1 we show the lowest energy levels as a function of \( d \) (left panel) as well as densities of six lowest

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FIG. 1: (color online). Left panel: Lowest eigenenergies of a double quantum dot with \( \omega_0 = 0.5 \) as a function of the interdot distance. Black, red (thick), and blue (thin) curves mark the ground state, controllable states, and uncontrollable states, respectively. Right panel: Densities of six lowest eigenstates at \( d = 5 \). The dashed lines mark the nodes of the wave functions.
eigenstates at \( d = 5 \) (right panel). The \( d = 0 \) limit corresponds to the well-known shell structure of a single 2D harmonic oscillator (HO), where the energy levels are \( n \)-fold degenerate at energies \( n\omega_0 \) \((n = 1, 2, \ldots)\). Increasing \( d \) leads to lifting of the degeneracies and generates crossings and avoided crossings between the energy levels. In the weak-coupling limit \( d \rightarrow \infty \) the bundling of the levels at \( n\omega_0 \) is restored. In this limit, the energies are \( 2n \)-fold degenerate corresponding to two (uncoupled) HO's. We label the states in the DQD as \( |\psi_{ij}\rangle = |ij\rangle \), where \( i = 0, 1, \ldots \) denotes the \((i+1)\)th bundle of states at \( d = 0 \), and \( j = 0, 1, \ldots \) denotes the \((j+1)\)th state in each bundle. As visualized in the right panel of Fig. 1 index \( i \) also corresponds to the number of nodes in the wave function. We show below that our labeling yields simple rules for controllable and uncontrollable states as a function of \( d \).

It is a well-known fact in control theory that an infinite-level single HO is not controllable in the dipole approximation.\(^{10}\) This is in contrast with the truncated HO which (in most cases) satisfies the controllability criteria.\(^{11}\) In qualitative arguments, the uncontrollability of a single HO (\( d = 0 \)) in the dipole approximation stems from the equidistant single-electron spacings. Using the above labeling of the states, the nonvanishing dipole-matrix elements \(|ij\rangle \hat{\mu} |kl\rangle\) between the HO states \((d = 0)\) are

\[
|ij\rangle \hat{\mu} |i+1,j+1\rangle = \sqrt{2}(i+1), \quad (2) \\
|ij\rangle \hat{\mu} |i+1,j\rangle = \sqrt{2}(i-j+1), \quad (3)
\]

where \( \hat{\mu} = -e \mathbf{r} \) is the dipole operator. Eq. (2) holds for all values of \( d \), and the corresponding energy-level spacings remain constant. Hence, transitions \( ij \rightarrow (i \pm 1)(j \pm 1) \) remain uncontrollable. On the other hand, the elements given in the LHS of Eq. (3) change as a function of \( d \), as well as the level spacings. The behavior already suggests that transitions \( ij \rightarrow (i \pm 1)j \) become controllable when \( d \) is increased from zero. Our calculations below confirm this prediction. Starting with the ground state \( |00\rangle \), the controllable transition line is then \( |00\rangle \rightarrow |10\rangle \rightarrow |20\rangle \ldots \) (see the red curves in Fig. 1). In the weak-coupling limit \((d \rightarrow \infty)\), however, the LHS of Eq. (3) becomes

\[
\lim_{d \rightarrow \infty} |ij\rangle \hat{\mu} |i+1,j\rangle = \begin{cases} \infty & \text{if } i-j \text{ is even} \\ \sqrt{2(i-j+1)} & \text{if } i-j \text{ is odd} \end{cases} \quad (4)
\]

so that only the trivial transitions between the degenerate gerade and ungerade states are possible. In the large-\( d \) regime, however, breaking the interdot symmetry leads to the possibility of charge transport between the dots (see below).

Next we apply OCT in order to find optimal laser pulses for transitions from the initial state \( |\Phi_1\rangle = |\Psi(t = 0)\rangle \) to the target state \( |\Phi_F\rangle = |\Psi(t = T)\rangle \) in a fixed time interval \( T \). In the OCT formalism we maximize the overlap \(|\langle \Psi(T)|\Phi_F\rangle|^2\) while minimizing the fluence of the laser pulse. The control equations are\(^{12}\)

\[
i\partial_t \Psi(t) = \hat{H} \Psi(t), \quad \Psi(0) = \Phi_1, \quad (5) \\
i\partial_t \chi(t) = \hat{H} \chi(t), \quad \chi(T) = F \langle \Phi_F|\Psi(T)\rangle, \quad (6) \\
\epsilon(t) = -\frac{A(t)}{\alpha} \ln \langle \chi(t)|\hat{\mu} |\Psi(t)\rangle, \quad (7)
\]

where Eq. (5) is the time-dependent Schrödinger equation with \( \hat{H} = \hat{H}_0 - \hat{\mu} \epsilon(t) \), and \( \chi(t) \) is the Lagrange multiplier. The optimal laser pulse \( \epsilon(t) \) is provided at the end of the iterative procedure.\(^{13}\) We point out that the initial pulse (zeroth iteration) is sinusoidal and has both \( x \) and \( y \) components, whereas the converged optimal pulse is always found to be polarized in the \( x \) direction, i.e., \( \epsilon(t) = \epsilon(t) \hat{x} \). In Eq. (7) we choose a sinusoidal pulse envelope \( A(t) = \sin^2(\pi t/T) \), and restrict the pulse intensity by a penalty factor \( \alpha \). Unless stated otherwise, we have fixed \( \alpha = 0.5 \) leading to pulse intensities \( 10^3 \ldots 10^4 \) \( \text{W/cm}^2 \). We apply a rapidly converging numerical scheme\(^{13,14}\) that has been implemented in the octopus code.\(^{15}\)

We consider excitations only from the ground state and set \( |\Phi_1\rangle = |00\rangle \). Figure 2 shows the maximum overlaps \(|\langle \Psi(T)|\Phi_F\rangle|^2\), i.e., maximum occupations of the target states \( |10\rangle \) and \( |20\rangle \) as a function of the interdot distance (note the logarithmic scale). The pulse lengths are fixed to \( T = 50 \) and \( T = 100 \), respectively. When \( d \) is increased, the target-state occupations increase from the HO value \( \lesssim 0.6 \) (see Ref. \([10]\)) exponentially to close to one. As expected, at large interdot distances \((d \gtrsim 8)\), corresponding to the uncoupling of the DQD, the occupations for \( |00\rangle \rightarrow |20\rangle \) decrease back to the HO value marked by a dashed line. On the other hand, the occupation for \( |00\rangle \rightarrow |10\rangle \) increases even further in this case.
is forbidden by the dipole selection rules. However, the intermediate state |10⟩ does not need to get fully populated during the optimized transition process. The higher states are also involved in the process, and in this example the state |30⟩ receives considerable occupation with a maximum of \( \sim 20\% \) at \( t \sim 90 \). The final target-state occupation is 0.998, whereas using two resonant CWs one after the other we could not exceed 0.9 (pulse length fixed to \( T = 100 \)). Generally, in multilevel transitions of this type, the efficiency of OCT is pronounced with respect to CWs due to the multiplication of errors in the latter approach when full population of intermediate states is required before changing the resonant frequency.

The control of electron transport in the DQD requires initialization of the state by localizing the electron in the one of the dots. Namely, the single-electron ground state of the DQD is a gerade state with half of the electron in one well and half in the other (see the lowermost figure in the right panel of Fig. 1). Only in the limit \( d \to \infty \) the localized states become degenerate eigenstates. However, the initial state can be fixed with certainty by applying a constant external field or by adjusting the gates in the DQD device in order to create a potential shift between the two dots. After the initial localization, electron transport into another well can be driven using a linear switch or a CW with the resonant confinement frequency \( \omega_{\text{res}} \). These types of transport on time scales of \( 10^{-16} \) s, close to the required times for SWAP operations in experiments were reported very recently by Forre and co-workers.

Now we show that OCT provides a very fast (switching times of a few picoseconds) and stable alternative to control the electron transport in a DQD. First we break the degeneracy of the ground state by setting the external potential in the (lower) left dot \( V_{\text{left}} = V_{\text{right}} - 0.2 \). Then the ground state \(|0\rangle \rightarrow |L\rangle \) and the first excited state \(|0\rangle \rightarrow |R\rangle \) correspond to electron localization in the (lower) left and (upper) right dot, respectively, provided that \( d \) is sufficiently large. The result of the OCT calculation for transition \(|L\rangle \rightarrow |R\rangle \) is shown in Fig. 3. The pulse length is fixed to \( T = 100 \) (\( \sim 6 \) ps), and the interdot distance is \( d = 6 \) corresponding to relatively large coupling between the dots. The spectrum of the optimized pulse (a) has a large peak at the resonant frequency \( \omega = \omega_0 = 0.5 \) a.u. \( \sim 9 \) THz, and a few smaller peaks at \( \omega \sim 0.2...0.3 \) and \( \omega \sim 1 \). The small peaks correspond to transitions in the higher states which get significantly populated in the transitions. This is visualized in Fig. 3(b) showing the occupations of \(|L\rangle \) and \(|R\rangle \) (solid lines) that sum up only to about 50% in the middle of the transition at \( T \sim 50 \). We also plot the integrated electron densities \( \rho_{\text{left}} \) and \( \rho_{\text{right}} \) (dashed lines) in the (lower) left and (upper) right parts of the DQD, respectively. The quasi-periodic oscillations in the densities indicate that the electron charge transfers in blobs as visualized in the snapshots in Figs. 3(c-h). In this example we find the final occupation \( |\langle \Psi(T)|R\rangle|^2 = 0.985 \). It is worth noting that the final occupations are closer

FIG. 3: (color online). Upper panel: Optimized pulses (x components) for transitions |00⟩ → |10⟩ (a) and |00⟩ → |20⟩ (b). The interdot distances are fixed to \( d = 3 \) and \( 5 \) and the pulse lengths to \( T = 50 \) and \( 100 \), respectively. Lower panel: Occupations of states involved in the transitions.
We tested a linear field and OCT could simultaneously with the electron localization. This immediately suggests that a combination of a linear field and OCT could be ideal in controlling transport in the uncoupled regime. In this work, however, we focus on coupled DQDs which we in fact find the most challenging in terms of electron control in nanoscale applications.

There are three significant advantages in OCT with respect to a linear switch or a resonant CW when generating electron transport in DQDs. First, the optimization procedure is insensitive to the interdot coupling. The CW approach in principle requires an uncoupled system while during the transport. (c-h) Snapshots of the total electron density ρR + ρL. The double quantum dot has d = 6, ω0 = 0.5, and well-depth asymmetry of V0 = 0.2.

to one at larger interdot distances so that the coupling between the dots is weaker. In this regime the optimized pulses may attain a linear slope. This immediately suggests that a combination of a linear field and OCT could be ideal in controlling transport in the uncoupled regime. In this work, however, we focus on coupled DQDs which we in fact find the most challenging in terms of electron control in nanoscale applications.

Finally we point out that in our future work we aim at combining our approach with magnetic-field optimization which could allow us to coherently control the spin state simultaneously with the electron localization.

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