

## Coherent Control of Interacting Electrons in Quantum Dots via Navigation in the Energy Spectrum

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Quantum control of the wave function of two interacting electrons confined in quasi-one-dimensional double-well semiconductor structures is demonstrated. The control strategies are based on the knowledge of the energy spectrum as a function of an external uniform electric field. When two low-lying levels have an avoided crossing, our system behaves dynamically to a large extent as a two-level system. This characteristic is exploited to implement coherent control strategies based on slow (adiabatic passage) and rapid (diabatic Landau-Zener transition) changes of the external field. We apply this method to reach desired target states that lie far in the spectrum from the initial state.

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The control of quantum systems is a fundamental challenge in physical chemistry, nanoscience, and quantum information processing [1,2]. Quantum control is the manipulation of the temporal evolution of a system in order to obtain a desired target state or value of a certain physical observable. From the experimental point of view, the techniques of quantum control are highly developed in the area of magnetic resonance, and more recently great progress has been made in quantum chemistry thanks to the development of ultrafast laser pulses [3].

Coherent control in semiconductor quantum dots has become an active field of research in the past 15 years. Early works on electron localization in double-well systems spurred intense theoretical activity. In a seminal Letter, Grossmann *et al.* [4] showed that, by applying an appropriate ac electric field, the tunneling of the electron between the wells could be coherently destroyed, thereby maintaining an existing localization in one of the wells. Shortly after, Bavli and Metiu [5] found ways to, starting from the delocalized ground state, localize the electron wave function and then to preserve the localization with a precisely tailored time-dependent electric field. A large body of literature followed these pioneering works. A decade later, the first steps in the theoretical exploration of localization and control of two interacting electrons in quantum dots were made [6–8]. Whereas Zhang and Zhao studied a model two-level system, Tamborenea and Metiu studied a more realistic multilevel system inspired by quasi-one-dimensional semiconductor nanorods. The study of two-electron localization and control in double dots has remained active ever since [9–13].

In this Letter, we propose an efficient method to control the wave function of two interacting electrons confined in quasi-one-dimensional nanorods [8,14]. The control method is based on the knowledge of the energy spectrum as a function of an external uniform electric field. The method requires that the system behaves locally—near avoided level crossings—as the Landau-Zener (LZ) two-

level model [15]. This fact is exploited to navigate the spectrum using slow (adiabatic) and rapid (diabatic) changes of the external control parameter. Although this characteristic may seem rather restrictive, it is, in fact, a general property of systems with interaction between its energy levels. The level repulsion must not be too strong, though, so that the spacing at the avoided crossings remains smaller than the mean level spacing.

Let us consider a quasi-one-dimensional double quantum dot with two interacting electrons in it in the presence of a spatially uniform electric field [8]. Denoting by  $z$  the longitudinal coordinate, the Hamiltonian of the two electrons reads

$$H \equiv -\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial z_1^2} + \frac{\partial^2}{\partial z_2^2} \right) + V(z_1) + V(z_2) + V_C(|z_1 - z_2|) - e(z_1 + z_2)E(t), \quad (1)$$

where  $m$  is the effective electron mass in the semiconductor material,  $V_C$  is the Coulomb interaction between the electrons,  $V$  is the confining potential, and  $E(t)$  is an external time-dependent electric field. The confining potential is a double quantum well with a well width of 28 nm and an interwell barrier of 4 nm and is 220 meV deep (a typical depth for a GaAs-AlGaAs quantum well). We mention that the control results that we report here are robust with respect to the fine-tuning of the parameters of the structure. We normally assume that the initial state is the ground state, which is a singlet. Since the Hamiltonian is spin-independent, the total spin is conserved, and the spatial wave function remains symmetric under particle exchange at all times.

We first consider the case of a constant electric field, to be considered at this point as a parameter in the Hamiltonian. In Fig. 1, we show the spectrum of eigenenergies of the Hamiltonian of Eq. (1) versus electric field. The energies  $\epsilon_i(E)$  and eigenstates  $\phi_i(E, z_1, z_2)$  are obtained by numerical diagonalization. We have used as a

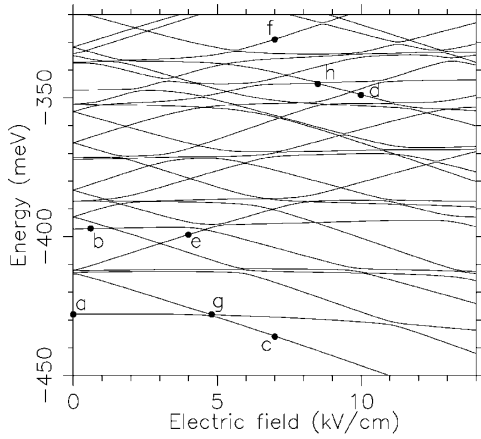


FIG. 1. Energy spectrum of our system as a function of the external uniform electric field.

basis set the symmetric combinations of the 12 lowest single-particle eigenfunctions. Thus, our basis of the two-particle Hilbert space has  $12 \cdot (12 + 1) / 2 = 78$  states. We can see in Fig. 1 that the spectrum is composed of nearly straight lines [16]. A closer look reveals that all level crossings are avoided, giving rise to adiabatic curves that never cross each other. The fact that all crossings are avoided ones is due to the electron-electron interaction, which couples the energy levels of the noninteracting system [17].

The straight lines of the spectrum are distributed in three clearly distinguishable groups: those with negative, zero, and positive slope. In each group, the slopes are very similar, and, far from the avoided crossings, the wave functions have a distinct kind of localization, as follows [see Figs. 1 and 2(a)–2(f)]: (i) For zero slope, the electrons are delocalized, that is, each electron is in a different dot [Figs. 2(a) and 2(b)]; (ii) for negative slopes, both electrons are in the left dot [Figs. 2(c) and 2(d)]; and (iii) for positive slopes, both electrons are in the right dot [Figs. 2(e) and 2(f)]. Along a given straight line, the eigenstates do not change much; thus, each line has associated a characteristic shape of the wave function. Near an avoided crossing, states with different types of localization mix. These mixed states do not have a well-defined localization type. As an example, in Figs. 2(g) and 2(h) we show the eigenstates at the avoided crossings between the first two levels at  $E = 4.81$  kV/cm and between levels 21 and 22 at  $E = 8.48$  kV/cm, respectively.

Our goal is to find a method to control the wave function. The previous discussion about the spectrum and the characteristics of the wave functions at and far from the avoided crossings suggests a possible control strategy. For example, starting at state (a) in Fig. 1 and varying slowly (adiabatically) the electric field, we reach state (c), which has a different type of localization (see Fig. 2). On the other hand, if we vary the parameter  $E$  quickly, the final state will have the same localization as the initial one (see below,

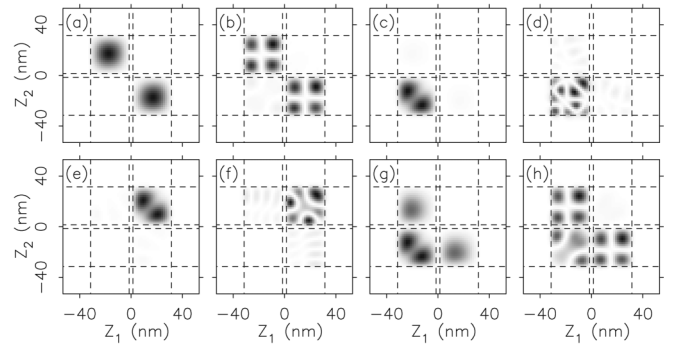


FIG. 2. Spatial wave functions  $\phi_i(E, z_1, z_2)$  corresponding to labels (a)–(h) in Fig. 1. States (a) and (b) have one electron in each well, wave functions (c) and (d) are localized in the left well, and wave functions (e) and (f) have both electrons in the right well. States (a)–(f) are far from avoided crossings and therefore have well-defined localization properties. This is not the case for eigenstates (g) and (h), which are at avoided crossings.

Fig. 3). These types of transitions will be the building blocks of our control strategy. The exact meaning of slow and fast in this context is given by the LZ model [15].

The LZ theory treats a rather simple and generic situation of a two-level avoided crossing. The LZ Hamiltonian in the diabatic basis  $\{|+\rangle, |-\rangle\}$  is

$$H = \begin{bmatrix} \varepsilon_+(\lambda) & \varepsilon \\ \varepsilon & \varepsilon_-(\lambda) \end{bmatrix}, \quad (2)$$

where  $\varepsilon$  is a constant, while the diagonal  $\varepsilon_{\pm}(\lambda) = E_0 + \alpha_{\pm}\lambda$  are linear functions of the parameter  $\lambda$ . It is assumed that the parameter  $\lambda$  varies linearly with time. It can be shown that the probability of remaining in state  $|+\rangle$  is given by  $P_+ = \exp[-2\pi\varepsilon^2/\hbar(\alpha_+ - \alpha_-)\lambda]$ , where  $\dot{\lambda}$  is the rate of variation of the parameter. Conversely,  $P_- = 1 - P_+$ . By selecting the rate of change of the parameter  $\lambda$ , we can control the final state of the system. For slow variations of  $\lambda$  ( $\dot{\lambda} \ll \varepsilon^2/\hbar$ ), the system follows the adiabatic curve passing from the initial diabatic state to the other one. In the opposite case, when  $\dot{\lambda} \gg \varepsilon^2/\hbar$ , the evolution takes place on the diabatic curve, and the state remains as the initial one. It can be shown that near an avoided crossing our system can be treated as a two-level LZ model [18]. We compared the evolution of the two-level LZ Hamiltonian [Eq. (2)] to that of the complete Hamiltonian [Eq. (1)] for many rates of variation of the parameter (electric field), and we found very close agreement. The numerical solution of the time-dependent Schrödinger equation was obtained using the usual fourth-order Runge-Kutta method [6,8]. We use a time step of 0.1 fs, which ensures that the precision of all of the reported probabilities and overlaps is better than 0.4%.

The adiabatic transition from state (a) to (c) [see Figs. 1, 2(a), and 2(c)] is an extremely simple solution to the problem of localization in a realistic double quantum dot

[7–9]. In fact, more complex and interesting control problems can be tackled. Namely, by suitable combinations of rapid (diabatic) and slow (adiabatic) changes of the electric field, it is possible to travel over the spectrum connecting distant pairs of states. That is, we can not only control the distribution of electrons in the dots (localization and delocalization) but we are also able to choose finer details of the final state, such as, for example, its nodal domains.

We now show a complex navigation through the spectrum in which the system is taken from the ground state to a specific high-energy state. In this case, the target is state (b) in Fig. 2 (see also Fig. 1), which shares the localization type with the ground state (they are both delocalized) but has a more complex nodal structure. This process is depicted in Fig. 3. We want to reach the excited state by means of diabatic and adiabatic transitions. The intended navigation path is displayed with arrows in the spectrum of Fig. 3(a). The small arrows indicate slow variations of the control electric field whose objective is to follow the adiabatic states (i.e., the eigenfunctions of the Hamiltonian at the successive values of the electric field). The long arrows denote diabatic transitions at the avoided crossings. Here we use instantaneous jumps of the electric field, but we have checked that rise times of the order of 0.1 ps do not change significantly our results. The time dependence of the electric field is shown in Fig. 3(b). In order to know in detail how the evolution of the wave function proceeds, we show in Figs. 3(c) and 3(d) different aspects of the time-dependent wave function. In Fig. 3(c), we compute the time-dependent localization probabilities  $P_{LL}$  that the two electrons are in the left well and  $P_{RL}$  that they are in different wells. Figure 3(d) gives the absolute value of

the overlap of the evolving state with the energy eigenstate  $\phi_i(E)$ , and Fig. 3(e) displays the spatial wave function at the various times indicated in Fig. 3(d).

Let us discuss in detail the behavior of the evolving wave function. We start from the ground state with zero electric field and move adiabatically up to a field of 3.5 kV/cm, as shown in Fig. 3(a). This process takes 100 ps [see Fig. 3(b)]. Note in Fig. 3(d) that the overlap with the adiabatic eigenstate  $\phi_1$  is approximately 1. After that, the field is quickly increased [the first jump of the electric field in Fig. 3(b), at  $t = 100$  ps] so that the system goes through the first avoided crossing. At this avoided crossing, the overlap between the evolving state and the adiabatic eigenstates begins to decay, from almost 1 to close to 0.97. For example, at time  $t_1 = 190$  ps, the wave function still resembles the ground state [see Fig. 3(e)] but displays a degree of mixture with localized states, as evidenced by the finite probability in the lower-left quadrant. Afterwards, we move slowly until  $t_3 = 300$  ps, passing adiabatically the second avoided crossing at  $E = 11.2$  kV/cm. The mixed nature of the wave function at the avoided crossing (at  $t_2 = 243$  ps) can be seen in Fig. 3(e). After the crossing, at  $t_3$ , the wave function is highly localized on the left dot [see Fig. 3(e)]. At this point, we still have ahead of us a long way to the desired final state, most of it along a spectral “line” of negative slope. Although it would be tempting to make a sudden change of the control parameter to its final value, that strategy is not satisfactory. It is best to proceed slowly far from the avoided crossings and rapidly around them. This procedure has the advantage of allowing our state to adjust to the gradual changes of the adiabatic states in the regions

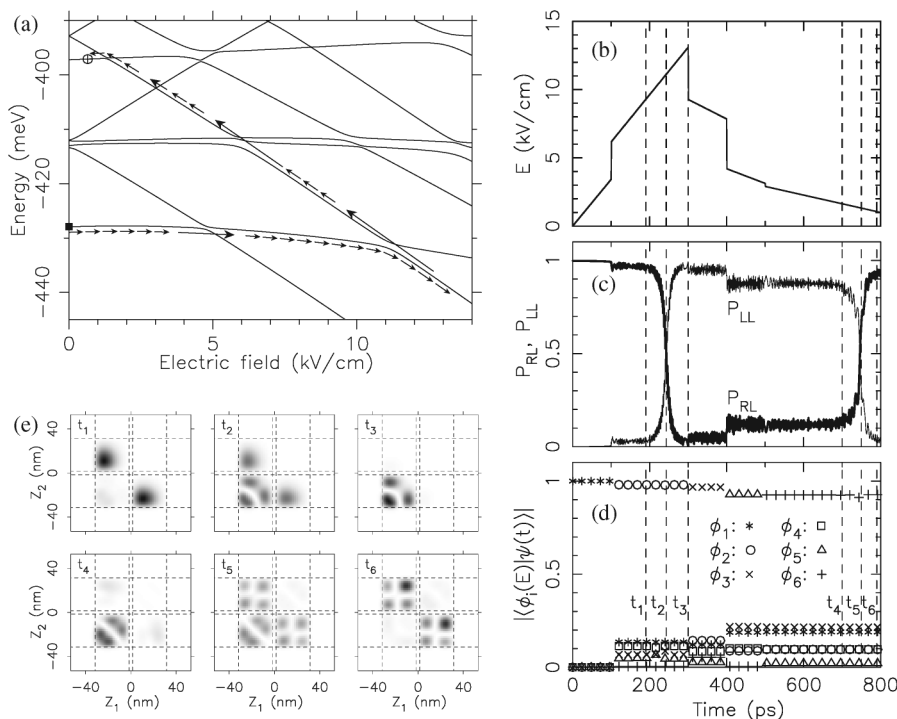


FIG. 3. (a) Schematic diagram of the intended path followed by the state. Short (long) arrows indicate slow (fast) variations of the electric field. The initial state is marked as  $\blacksquare$  and the target state as  $\oplus$ . (b) External electric field (the control parameter) as a function of time. (c) Probabilities that the two electrons are in the same (left) well ( $P_{LL}$ ) and in different wells ( $P_{RL}$ ). (d) Absolute value of the overlap of the evolving state with the energy eigenstate  $\phi_i(E)$ . (e) Spatial wave functions at various times indicated in (d).

between crossings. These gradual changes do not entail changes in the type of localization but rather displacements of the probability density within the quadrants which are already populated. In the remainder of the path, we cross three avoided crossings diabatically and the last one slowly. The latter, being very narrow, turned out to be the hardest one to pass adiabatically. This passage took 300 ps, as seen in Fig. 3(b). In this avoided crossing, the wave function goes from a strong localization in the left dot [wave function at  $t_4$  in Fig. 3(e)] to a clear delocalization in the final state. We remark that the overlap of the final state with the desired state, at  $t_6 = 800$  ps, is 0.93 [see Fig. 3(d)].

Before concluding, it is worth comparing the present control method with others found in the literature. In Ref. [8], a different localization scheme was proposed for the system studied here. In that work, the electron localization is obtained, starting from the ground state at zero electric field, with a piecewise constant electric field. The time scales involved, of a few picoseconds, which are experimentally accessible, are the same in the two approaches. However, the present method has the advantage of being more robust since it does not require the fine-tuning of the field jumps, and, furthermore, it gives higher probabilities of reaching the target state. Moreover, in Ref. [8], the controlled state is a superposition of only the two lowest-energy eigenstates, while in our proposed method a much more general navigation of the spectrum is naturally possible, allowing one to connect very distant states. More recently, an efficient method of control was proposed and applied to the creation of entangled states in spin systems [19]. The method is based on the navigation of the energy spectrum, expressed as a function of an external control parameter, which is varied always adiabatically. A key element of the controlled system of that study is that the interaction, which controls the nature of the level crossings, can be switched off at will. This additional control tool is clearly not generic. Here we propose a control method based on similar general ideas but which is more general in the sense that the interaction among levels does not need to be controlled. Finally, we mention that nonadiabatic LZ transitions have been applied to control single-electron transport [20], and adiabatic passage has been used to control localization and suppression of tunneling [21].

In summary, we have proposed an efficient method to control the wave function of a two-electron quantum dot system. This method is based on slow and fast variations of a control parameter which in our study is given by an external electric field that couples to the electrons through the dipole Hamiltonian. The success of this method relies on the condition that the interaction between neighboring levels be well described by the two-level LZ model. Although this may seem a severe limitation to the applicability of the method, this condition is quite generally satisfied. For example, it has been recently shown in the

paradigmatic stadium billiard that the transitions between neighboring levels are of the LZ type when the billiard boundary is deformed [22]. We have shown that with this method an effective control of the wave function can be achieved, even for rather ambitious control goals. While the technology to produce the required ramped electric fields, controllable in the picosecond time scale with enough flexibility may not be currently available, we expect that our proposal will further motivate their experimental development.

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