Localization and entanglement of two interacting electrons in a quantum-dot molecule

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The localization of two interacting electrons in a coupled-quantum-dots semiconductor structure is demonstrated through numerical calculations of the time evolution of the two-electron wave function including the Coulomb interaction between the electrons. The transition from the ground state to a localized state is induced by an external, time-dependent, uniform electric field. It is found that while an appropriate constant field can localize both electrons in one of the wells, oscillatory fields can induce roughly equal probabilities for both electrons to be localized in either well, generating an interesting type of localized and entangled state. We also show that shifting the field suddenly to an appropriate constant value can maintain perfect localization in time for both types of localization.

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Coherent control of quantum systems is at the heart of promising disciplines like femtochemistry and quantum information processing. A basic operation of quantum control, namely, the localization of a single electron in coupled quantum wells, has been extensively studied in the last decade. In two early publications, conditions to maintain existing localization with an AC field and to create and maintain localization with a semi-infinite AC field were identified. Thereafter, localization in two-level systems, multilevel systems, induced by ultrashort laser pulses, in dissipative environments, in molecular systems, in trapped Bose-Einstein condensates, by means of circularly polarized fields, with bichromatic fields, including the effect of Coulomb charging energy, and with quantized electromagnetic fields, has been studied.

When two or more interacting particles are present the possibility of entanglement of the many-body wave function arises. Entanglement is an essential ingredient in any scheme of quantum information processing like quantum cryptography and quantum computation, and therefore it is a problem of great current interest to find or design systems where entanglement can be manipulated.

In the case of a single-electron, two-level system consisting of the lowest symmetric and antisymmetric states of the double well potential, perfect localization can be achieved with a strong periodic electric field that causes the two Floquet quasi-energies to be degenerate. This scheme is not applicable to the two-electron system, because it requires a pair of states whose superposition results in a localized state, a condition that is not met in this system. An alternative and trivial way of inducing localization in a two-electron double-well system is to adiabatically tilt the potential with a slowly increasing electric field. Trying to localize the electrons on a short time scale is more difficult: switching the field on rapidly excites higher electronic states causing a coherent motion from one well to another. In this Letter we examine this regime of very fast localization.

We investigate the localization and entanglement of two interacting electrons in a system of coupled quantum dots, induced by spatially uniform electric fields with a simple time dependence. Systems of coupled quantum dots, sometimes referred to as quantum-dot molecules or artificial molecules, have been actively investigated in the last five years, both experimentally and theoretically. Our main findings are as follows: (i) A constant electric field can bring the two electrons from their ground state (highly delocalized) to a state of high degree of localization in one of the dots, at a certain time; (ii) At that time, a step in the field to another constant value can maintain the localization essentially indefinitely; (iii) An oscillatory field produces a different type of localization, where both electrons are likely to be found together in either dot with roughly equal probabilities. This type of localization is a purely many-body phenomenon, and arises due to the Coulomb interaction between the electrons, which causes entanglement of the two-body wave function; (iv) The entangled/localized states can also be maintained in time by changing from the oscillatory field to an appropriate constant field. In all cases, localization takes place in a time scale of a few picoseconds.

Our system is a quasi one-dimensional, double-quantum-dot structure with two electrons in it. The transversal size of the dots is taken to be $L = 50\,\text{Å}$, and the double-well potential in the longitudinal direction, $V(z)$, is shown in Fig. 1(a). The energies associated with the transverse dimensions are, due to the narrow lateral confinement, high compared to those of the longitudinal motion. Therefore, the lateral degrees of freedom do not participate in the dynamics and the two-electron wave function can be written as (we discuss below the spin part of the wave function)

$$
\Psi(r_1, r_2, t) = \phi(x_1)\phi(y_1)\phi(x_2)\phi(y_2)\Phi(z_1, z_2, t).$$

(1)

where $\phi(x) = \sqrt{2/L}\sin(\pi x/L)$. The time-dependent Schrödinger equation becomes

$$
i\hbar \frac{\partial \phi}{\partial t} = \left[-\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_{1D}(|z_1 - z_2|) - e(z_1 + z_2)E(t)\right]\Phi,

(2)

where $E(t)$ is an external time-dependent electric field, and $m^*$ is the effective mass. $V_{1D}$ is the Coulomb interaction given by

$$V_{1D}(|z_1 - z_2|) = \int_0^L dx_1 dy_1 dx_2 dy_2 \int_0^L dz_1 dz_2 \int_0^L dz_3 dz_4 V_1(z_1, z_2, z_3, z_4).$$
We use the effective mass $m^*$ and dielectric constant $\epsilon$ of GaAs.

In all our calculations the ground state is the initial state. The spin part of the ground state of the two interacting electrons is the singlet state $\Psi^\text{LL}$ and correspondingly (the fermionic wave function is antisymmetric) the spatial part of the wave function is symmetric under particle exchange. We calculate the spatial part of the ground state by numerical diagonalization of the energy eigenvalue problem of the interacting electrons. A plot of the ground state is shown in Fig. 1(b) as a function of the $z$-coordinates of the two electrons. Since the Hamiltonian of the system including the external electric field is spin independent, the spin wave function is the singlet at all times. Therefore, the evolving spatial wave function remains symmetric (under particle exchange) at all times. We emphasize that the absence of triplet states in the expansion of the wave function (Eq. (4) below) is not an approximation, but a consequence of our choice of initial state and the lack of spin dependence in the Hamiltonian.

\[
\frac{e^2 \phi^2(x_1) \phi^2(y_1) \phi^2(x_2) \phi^2(y_2)}{\epsilon |\mathbf{r}_1 - \mathbf{r}_2|}.
\]

(3)

we find the lowest value of $P_{LL}(t) + P_{RR}(t)$, that both electrons are in the right dot, and $P_{LL}(t)$, that both electrons are in the left dot. Since the probability of ionization is kept small at all times $P_{RL}(t) + P_{RR}(t) + P_{LL}(t) \approx 1$.

For the ground state, shown in Fig. 1(b), $P_{RL} \approx 0.9988$ and $P_{RR} = P_{LL} \approx 0.0006$. That is to say that in the ground state the two electrons have a very small probability to be found in the same well, which is expected due to their Coulomb repulsion. In the rest of this Letter we explore the question of whether an external electric field (time dependent but spatially uniform) can induce localization of the two electrons on a very fast (picosecond) time scale.

We start the search for localization with the simplest case, a constant electric field, $E(t) = E_0$. Before $t = 0$ the system is in the ground state, and at $t = 0$ the field $E_0$ is switched-on suddenly. We compute the evolution of the two-electron wave function as well as the probability $P_{RL}(t)$ during a simulation interval of 9 ps. For each field $E_0$ we find the lowest value of $P_{RL}$ that occurs within that time interval, and we plot the result as a function of $E_0$ in Fig. 2(a). The minimal $P_{RL}$ shows a few peaks but for only one value of $E_0$ ($E_0 = -5.18$ kV/cm) does it drop below 0.1. To take a closer look at the peak with strongest localization, we calculate the three probabilities $P_{RL}$, $P_{RR}$, and $P_{LL}$ for that field, and plot them versus time in Fig. 3(a). In this case, $P_{RL}$ and $P_{RR}$ show an oscillatory behavior, while $P_{LL}$ remains negligible at all times. Physically, the two electrons oscillate between a state in which they are highly localized in the right well and another state which is completely delocalized.

In Fig. 3(b) we illustrate two operations of control of the wave function that can be performed with piecewise-constant electric fields. First, the thick-line curve of $P_{RL}(t)$ in Fig. 3(b) (produced by the electric field shown by a thick line in Fig. 3(c)) indicates that the low value of $P_{RL}$ obtained earlier (at $t \approx 3$ ps in Fig. 3(a)) can be
maintained permanently by switching the field to another special value. The field value that locks $P_{RL}$ at its minimum was found through a systematic search. The second operation consists of un-locking the localization and resuming oscillations similar to those produced by the initial constant field. The timing of this second switching is found to be immaterial. The new field value is not arbitrary; in this case it is such that the oscillation resumes at the expense of $P_{RL}$. This feature was observed for all the AC fields ($\omega_{0R}$ and $E_{0R}$) we looked at. Physically, the localization with an AC field is that both electrons are (with high probability) together in one of the wells, with roughly equal probabilities to be found in either well. The two electrons are here in quantum states that are both localized (to a large extent) and entangled. We mention that all the states occupied by the two interacting electrons in our simulations are entangled, in the usual sense that they are not factorizable into single-particle states. We use the label “localized/entangled” for the low $P_{RL}$ states of Fig. 4(a) to emphasize that, in these states, while each individual electron is delocalized (it can be found in either dot with roughly 50% probability), the two electrons are correlated and very likely to be found in the same dot.

We saw above that an appropriate constant electric field can localize to a large extent both electrons in a well of choice at certain times, and the localization can be locked by switching the field to another appropriate value. We will see next that the nature of the localization is different when oscillatory fields are applied. We consider a sinusoidal field of the form $E(t) = E_0 \cos \omega_0 t$ (we discuss below the effect of a slow switching-on.) Fig. 2(b) shows a contour plot of the minimum probability $P_{RL}$ achieved in a simulation interval of 9 ps, as a function of $E_0$ and $\omega_0$. Darker areas correspond to lower values of $P_{RL}$, i.e., to stronger localization. The most prominent feature in this plot is the existence of a number of “resonant” frequencies, which lead to localization for wide ranges of $E_0$. The lowest value of $P_{RL}$, 0.027, is obtained for $E_0 = 5$ kV/cm and $\omega_0 = 5.6$ meV. Other combinations of $E_0$ and $\omega_0$ also yield values of $P_{RL}$ below 0.1. We computed $P_{RL}(t)$, $P_{RR}(t)$ and $P_{LL}(t)$ for the frequencies that lead to strong localization and for different values of $E_0$, and in Fig. 4(a) we show the result for the case of strongest localization. Fig. 4(b) shows the corresponding field. We notice that the localization, or reduction of $P_{RL}$, results in an increase of both $P_{RR}$ and $P_{LL}$, as opposed to the case of a constant field, where only $P_{RR}$ increased at the expense of $P_{LL}$. This feature was observed for all the AC fields ($\omega_{0S}$ and $E_{0S}$) we looked at. Physically, the localization with an AC field is that both electrons are (with high probability) together in one of the wells, with roughly equal probabilities to be found in either well. The two electrons are here in quantum states that are both localized (to a large extent) and entangled. We mention that all the states occupied by the two interacting electrons in our simulations are entangled, in the usual sense that they are not factorizable into single-particle states. We use the label “localized/entangled” for the low $P_{RL}$ states of Fig. 4(a) to emphasize that, in these states, while each individual electron is delocalized (it can be found in either dot with roughly 50% probability), the two electrons are correlated and very likely to be found in the same dot.

FIG. 2. Minimum probability $P_{RL}$ obtained during a time interval of 9 ps after switching on the external field. (a) For a constant field of amplitude $E_0$. (b) For a sinusoidal field of amplitude $E_0$ and frequency $\omega_0$. Darker areas correspond to lower values of $P_{RL}$, and therefore to stronger localization.

A sudden switching-on of the field introduces high frequencies and therefore population of higher lying excited
states, which results in a rugged evolution of $P_{RL}, P_{RR}$ and $P_{LL}$. A smoother evolution of these probabilities (Fig. 4(c)) is produced by the field plotted in Fig. 4(d), which is switched on more slowly.

![Graph of probabilities](image)

**FIG. 4.** (a) Probabilities that the two electrons are in the different combinations of wells, for the oscillatory electric field shown in (b). Dashed line: $P_{RL}$, solid line: $P_{RR}$, dotted line: $P_{LL}$; (b) $E(t) = E_0 \cos \omega_0(t - t_0)$, switched on suddenly at $t_0 = 10$ ps. $E_0 = 5$ kV/cm and $\omega_0 = 5.6$ meV, which gives the lowest value of $P_{RL}$. (c) Same as in (a) for the field with slow switching-on shown in (d); (d) $E(t) = E_0 \exp[(t - t_0)^2/\lambda^2] \cos \omega_0(t - t_0)$, with $\lambda = 5$ ps. and $t_0 = 10$ ps. $E_0$ and $\omega_0$ as in (b). (e) Various probabilities for the field with slow switching-on and sudden shift to constant value, used to lock in the localized/entangled state; (f) Field that produces the probabilities shown in (e).

Once the two electrons are in the localized/entangled state obtained at $t \approx 13.5$ ps in Fig. 4(c), they can be forced to stay localized by suddenly shifting the field to an appropriate constant value. In Fig. 4(c) we show this effect, along with the electric field that produces it (shown in (f)). The control of entangled quantum states in solid state systems is of great current interest. Loss and Sukhorukov studied entanglement in coupled quantum dots involving the spin degree of freedom. Here we have identified a possibly complementary method that creates localization with entanglement in the spatial wave function of two electrons in coupled quantum dots.

In summary, we have found ways to create rapidly and to maintain localization in a two-electron coupled-quantum dots system with uniform electric fields with a simple time dependence. While a constant electric field creates pure localization of both electrons in one well, oscillatory fields induce entangled states that exhibit localization in either dot with roughly equal probabilities. This localization-with-entanglement is a purely many-body phenomenon brought about by the Coulomb interaction between the electrons, and the method we propose to create it is potentially useful in future applications of the physics of entangled states in solid state systems.

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