Interacting Two-Electron Model of a Coherent Quantum-Dot Single-Electron Turnstile

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We show how coherent single-electron turnstile action in a picosecond time scale can be achieved with high probability in a triple-well semiconductor structure by means of an applied time-dependent, long-wavelength electric field. We demonstrate the turnstile behavior by studying the exact temporal evolution of two electrons, including their Coulomb interaction, and considering both triplet and singlet states.

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A single-electron turnstile is a device where one electron is transferred at a controlled rate between two reservoirs [1]. Typically, the electron tunnels through an intermediate quantum dot region, which, thanks to the Coulomb blockade, regulates the passage of electrons. Such a device has recently been demonstrated [2]. Those turnstiles operated at megahertz frequencies, which are low compared to the relaxation rates in those systems, and therefore the transfer process of individual electrons was incoherent. Experiments to create a semiconductor-based single-electron turnstile operating at terahertz frequencies are currently under way [3]. In this case, one enters the coherent transport regime [4,5], and the classical picture of a point electron being either in the source or in the sink is not adequate: the electron is described by a wave packet which can be spread over the whole structure and we can describe the location of the electron only through probabilities.

In this Letter we study a possible coherent turnstile device operating in a picosecond time scale. Our approach is to study a structure with two interacting electrons in it, and to calculate the exact time evolution of the two-electron wave function under an external, long-wavelength field applied to induce the single-electron transport. We consider a quasi-one-dimensional structure consisting of three quantum wells. The central well is smaller than the other two and will be called the quantum dot. The two larger lateral wells will be referred to as the source (the well where both electrons are located initially) and the sink (the destination of the electrons). These finite "source" and "sink" are not meant to realistically mimic infinite reservoirs; as we will see below, the electron dynamics and the turnstile performance depend on their sizes. Instead, our purpose is to treat the dynamics of the injection process into the dot exactly, e.g., to avoid using an approximate transfer Hamiltonian. This simple model gives us some insight into how the Coulomb interaction and exchange, combined with an appropriate time-dependent field, affect the success of the turnstile. The results also provide a benchmark against which one can test approximate schemes [e.g., time-dependent Hartree or Hartree-Fock (HF), or multiple configuration HF], which will have to be used for more complex models.

A general two-electron quantum-mechanical state can be expanded in a basis set consisting of products of spatial and spin states. The two-electron spin states are the usual triplet and singlet. To ensure the antisymmetry the spatial states corresponding to the triplet and singlet must be antisymmetric and symmetric, respectively. In this paper we assume that there is no spin dynamics. Therefore, the spatial part of the wave function conserves its symmetry.

We consider a quasi-one-dimensional quantum structure, whose size in the longitudinal dimension (z) is much larger than its size L in the transversal dimensions (x, y). The triple quantum well potential in which the electrons move (the "source-dot-sink" structure), $V(z)$, is shown in Fig. 1(a). Because of the narrow lateral confinement, the characteristic energies of the lateral motion are high compared to the energies associated with the longitudinal motion; therefore we can assume that the transverse excited states do not participate in the dynamics. Therefore the

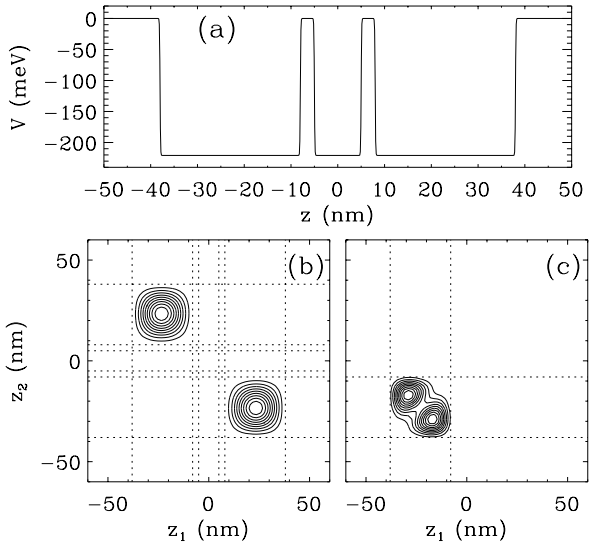

FIG. 1. (a) Potential energy of the triple-well, or source-dot-sink, semiconductor structure. Interacting two-electron ground-state wave function of (b) the complete structure shown in (a), and (c) the auxiliary left-well structure. The dotted lines show the edges of the wells. Both ground states are symmetric under particle exchange.

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two-electron wave function is written as

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, t) = \phi(x_1)\phi(y_1)\phi(x_2)\phi(y_2)\Phi(z_1, z_2, t). \quad (1)$$

We note that $\Psi(\mathbf{r}_1, \mathbf{r}_2, t)$ has the same symmetry as $\Phi(z_1, z_2, t)$ under the exchange of the electrons, since the (x, y)-dependent part is symmetric. The time-dependent Schrödinger equation becomes

$$i\hbar \frac{\partial \Phi}{\partial t} = \left[-\frac{\hbar^2}{2m^*}\left(\frac{\partial^2}{\partial z_1^2} + \frac{\partial^2}{\partial z_1^2}\right) + V(z_1) + V(z_2) + V_{1D}(|z_1 - z_2|) - e(z_1 + z_2)E(t) \right]\Phi, \quad (2)$$

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

$$V_{1D}(|z_1 - z_2|) = \int_0^L dx_1\, dy_1\, dx_2\, dy_2 \times \frac{e^2\phi^2(x_1)\phi^2(y_1)\phi^2(x_2)\phi^2(y_2)}{\epsilon|\mathbf{r}_1 - \mathbf{r}_2|}. \quad (3)$$

The type of quantum structure that we consider can be made with semiconductor alloys, and we use in our calculations the effective mass m^* and dielectric constant ϵ of GaAs.

We search for turnstile action as follows: we assume that initially both electrons are localized in the left well, and solve the time-dependent Schrödinger equation (2) with different external fields $E(t)$ which are used to cause the passage of only one electron to the right well.

All calculations are performed by using the configuration interaction (CI) method [6] which represents the two-electron wave function as

$$\Phi(z_1, z_2, t) = \sum_{i,j} c_{ij}(t)\{\varphi_i(z_1)\varphi_j(z_2) \pm \varphi_j(z_1)\varphi_i(z_2)\}, \quad (4)$$

where $\varphi_i(z)$ are eigenstates of $P_z^2/2m^* + V(z)$. The $+$ $(-)$ sign corresponds to the singlet (triplet). The number of terms in (4) is increased until convergence is achieved. The expansion (4) is substituted in the Schrödinger equation (2) and the coefficients $c_{ij}(t)$ are calculated numerically employing the fourth-order Runge-Kutta method.

As the initial state, we take the ground state of an auxiliary single-well structure that has only the left well of the complete structure shown in Fig. 1(a). We calculate its ground state by diagonalization of the interacting two-electron Hamiltonian, and using $V(z)$ for the auxiliary structure. We find—as expected—that the ground state is the singlet. The ground state of the auxiliary single-well structure [Fig. 1(c)] is not a stationary state of the complete structure. However, it has a very long lifetime in the complete structure compared to the duration of our simulations, which makes it a convenient choice as an initial state localized in the left well.

The probability that one electron is in the left well and the other one is in the right well is given by

$$P_{\mathrm{RL}}(t) = 2\int_L dz_1 \int_R dz_2\, |\Phi(z_1, z_2, t)|^2. \quad (5)$$

The ideal turnstile action can be defined as attaining $P_{\mathrm{RL}}(t) = 1$ at some time t, from the initial $P_{\mathrm{RL}}(t = 0) = 0$. To reach this goal we tried a number of different functional forms for the time dependence of $E(t)$. The simplest $E(t)$ that can be applied is a constant bias field $E(t) = E_0$. Figure 2(a) shows the maximum value of P_{RL}, $P_{\mathrm{RL}}^{\max}$, as a function of E_0, achieved during a simulation of 3.3 ps of duration. $P_{\mathrm{RL}}^{\max}$ shows a dependence on the bias field reminiscent of a resonant tunneling transmission. We mention that longer or shorter simulation times produce slightly different results, as expected due to the complex time evolution of the two-electron wave function. Since our interest here is in exploring turnstile action in times as short as possible (to minimize the effects of phonon scattering), we work mostly within a window of a few picoseconds. We emphasize, however, that our results are not modified significantly within time intervals of at least 20 ps. As an additional check, we also did an analogous calculation recording the first local maximum of P_{RL} versus E_0, with results qualitatively similar to those of Fig. 2(a). The highest value of $P_{\mathrm{RL}}^{\max}$ achieved in Fig. 2(a) is 0.86 (at $E_0 \approx 5$ kV/cm). This means that with a constant field we can achieve a "success rate" of at most 86% for turnstile action. We mention that if the field $E(t)$ is switched on slowly up to a constant value, rather than abruptly as we

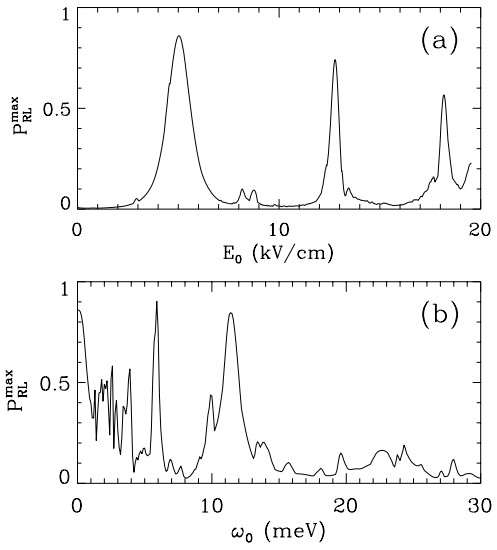

FIG. 2. Maximum probability that one electron is in the right well while the other electron is in the left well versus (a) amplitude of a dc electric field; (b) frequency of an oscillatory electric field of amplitude $E_0 = 5$ kV/cm. The initial state is shown in Fig. 1(c).

have shown here, slightly higher values of $P_{\mathrm{RL}}^{\max}$ can be achieved, up to roughly 0.9. This value depends on the speed of the switching-on of the field.

We have tested several variations of the original structure in the simulation with a constant field, in an attempt to improve the performance of the turnstile. One variation consisted of enlarging the right well (the sink), to reduce the effect of the reflection of the electrons at the right-hand-side end of the structure, thereby increasing the time the electron will spend in the right well. The size of the enlarged sink was 500 Å instead of the original 300 Å; the highest $P_{\mathrm{RL}}^{\max}$ obtained was ≈ 0.84. Enlarging only the left well (the source) to 600 Å produced a highest $P_{\mathrm{RL}}^{\max} \approx 0.52$, and enlarging both source and sink to 600 Å gave a highest $P_{\mathrm{RL}}^{\max} \approx 0.3$. As we can see, a larger sink by itself does not enhance the turnstile performance, and a larger source seems to have in general a negative effect. Another variation consisted of reducing the lateral size L of the structure to make it more strictly one dimensional, which strengthens the quasi-one-dimensional Coulomb repulsion [Eq. (3)] and should, in principle, facilitate the separation of the two electrons. We took $L = 20$ Å (all other results reported in this Letter are for $L = 50$ Å). Again, the result for this modified structure was not substantially better than for the original one: the highest $P_{\mathrm{RL}}^{\max} \approx 0.87$.

We have also investigated a number of double-well structures (without the central dot) and found that results similar to the one presented in Fig. 2(a) can be obtained. With a barrier width of 50 Å, a high P_{RL} probability of 0.92 is obtained for a field value of $E_0 = 7$ kV/cm at a time of 3 ps. One difficulty with the double-well potentials is that the initial state (localized in the left well) is more unstable than in the original structure and tunnels through the barrier even in the absence of the applied field. This effect can of course be reduced by increasing the barrier width, but this in turn affects the tunneling rate and inhibits the turnstile action. In contrast, this problem does not arise in the triple-well structure, because the central dot is effective in suppressing tunneling when the initial state is off-resonance with the dot, and provides a resonant tunneling pathway when the appropriate voltage is applied. An additional advantage of the triple-well structure is that the central dot can be gated individually, and thereby its potential can be used for better control. In the rest of this Letter we concentrate on the triple-well structure, and will report complete results for double wells in a separate publication.

In Fig. 3 we plot (dashed line) the probability P_{RL} as a function of time for the value of E_0 that gives the highest $P_{\mathrm{RL}}^{\max}$ seen in Fig. 2(a). We note that P_{RL} reaches its first and highest local maximum in less than 1 ps, indicating the typical time scale for tunneling through the central dot. We next explore the effect of changing the applied field to another constant value at the time when $P_{\mathrm{RL}}^{\max}$ is obtained. We find two interesting results, shown in Fig. 3: (i) the high value of P_{RL} can be maintained for long

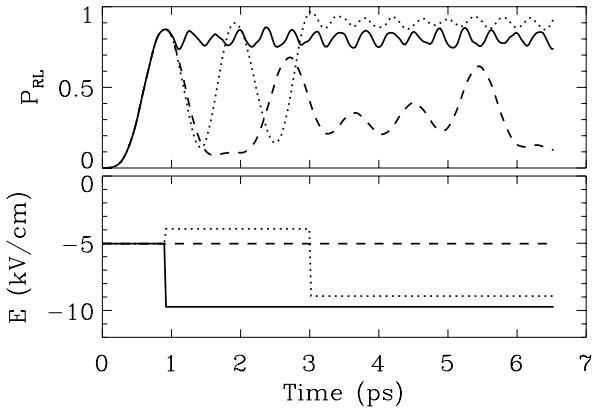

FIG. 3. Top: time evolution of the probability that one electron is in the right well while the other electron is in the left well. Bottom: corresponding applied electric fields. Dashed line: constant field $E_0 = 5$ kV/cm, which gives the highest $P_{\mathrm{RL}}^{\max}$ shown in Fig. 2(a). Solid line: the field after ≈ 0.9 ps is chosen to "lock" the high value of P_{RL} attained at that time. Dotted line: the field between ≈ 0.9 and ≈ 3 ps brings P_{RL} to its highest value, ≈ 0.97, and the field after ≈ 3 ps maintains approximately that value.

times (solid line), and (ii) an even higher value of P_{RL} ($= 0.97$) can be obtained at some later time (dotted line). These results are obtained for specific ranges of values of the new E_0. Interestingly, the high value of $P_{\mathrm{RL}} = 0.97$ can also be "locked" in time to a large extent by changing again the constant bias to a suitable value when the maximum occurs, as shown by the dotted lines. The small oscillations in P_{RL} after its high value is stabilized (after 0.9 ps for the solid line and after 3 ps for the dotted line) could not be eliminated by chosing other field values. They represent a quantum beat between a few two-particle eigenstates of the structure with the applied field, excited coherently by switching the field suddenly on (a detailed analysis of this effect will be presented elsewhere). The results shown in Fig. 3 are the closest we have come to ideal turnstile action, with the added desirable feature that the tunneling of only one electron through the central dot can be followed by a sustained separation of the two electrons by simply changing the value of the constant external field.

Besides piecewise-constant fields, we considered strong oscillatory terahertz fields of different frequencies (produced, for example, by a free-electron laser). In Fig. 2(b) we show the maximum P_{RL} as a function of frequency for the field $E(t) = E_0 \cos(\omega_0 t + \delta)$, with $E_0 = 5$ kV/cm and $\delta = 0$. We note that high "success rates" close to 90% can be achieved for certain frequencies, similar to those obtained with constant fields. Introducing a phase $\delta = \pi/2$ changes the result at low but not at high frequencies, when the period of the field is short compared to the typical tunneling time of 1 ps.

Figure 4 illustrates the effect of the Coulomb interaction and of the symmetry of the two-electron spatial wave

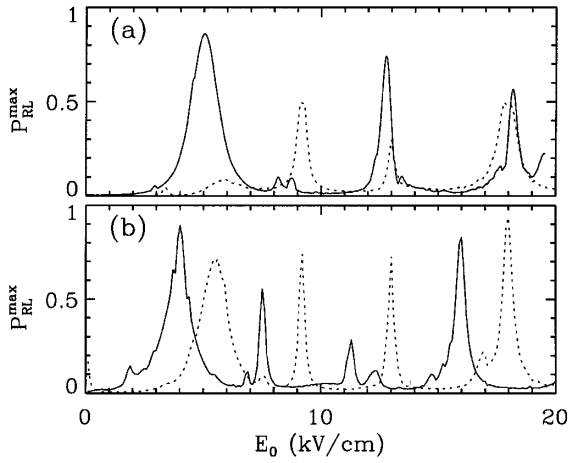

FIG. 4. Maximum P_{RL} versus applied dc electric field. (a) Symmetric and (b) antisymmetric spatial wave function. Solid lines: with Coulomb interaction. Dotted lines: without Coulomb interaction.

function. We plot the maximum P_{RL} as a function of the amplitude E_0 of a constant field switched-on at $t = 0$ [as in Fig. 2(a)], for symmetric and antisymmetric spatial wave functions, with and without Coulomb interaction. The initial states are, as before, the ground states of the auxiliary left-well structure, correspondingly symmetric or antisymmetric, and interacting or noninteracting. The simulations have a duration of $\sim$3.3 ps. In general, the removal of Coulomb repulsion does not change the qualitative nature of the results, but it affects the position and strength of the transmission peaks. The tendency is, as expected, that the resonances with Coulomb repulsion happen at lower fields than without interaction, for both types of wave functions, since the repulsion favors the separation of the electrons. For symmetric wave functions, the strength of the first peak is much larger with than without Coulomb repulsion. This difference is also present for antisymmetric wave functions, but it is less marked, since Pauli exclusion helps the separation of the two electrons in the absence of Coulomb interaction. For distinguishable noninteracting electrons we found that the probability P_{RL} remains low at all times compared to the peak values seen in Fig. 4, which underlines the importance of treating the electrons in the turnstile as a quantum many-body system of indistinguishable particles.

The Coulomb interaction causes what we term a dynamic Coulomb blockade effect in the central dot, evidenced by the fact that the probability of both electrons being in the dot at the same time is negligible when the Coulomb interaction is included, but not when the interaction is switched off. Although this joint probability remains very small at all times, it is, however, not strictly zero. In this sense the dynamic Coulomb blockade effect differs from the usual semiclassical Coulomb blockade. In the latter a full electron is either in the dot (blockade) or outside (no blockade); in the former the wave packet representing the electrons can be spread all over the structure, a fact that affects the Coulomb interaction, and hence the blockade. In this case, the charging energy, defined as the energetic cost for the small time-dependent amplitude to find both electrons in the dot, is described by the full Coulomb interaction (3), and not by a phenomenological capacitive charging energy.

In conclusion, we studied theoretically the time evolution of two interacting electrons in a triple-well structure, to explore the possibility of creating a coherent single-electron turnstile controlled by an external uniform electric field. We found that it is possible to achieve the passage of a single electron through the quantum dot with a high probability by using simple constant and sinusoidal fields, and that it is possible to create and maintain the spatial separation of the electrons by using piecewise-constant fields. We also document the existence of a dynamic, fully quantum-mechanical version of the Coulomb blockade effect in which the joint probability for both electrons being in the dot region is negligible due to their Coulomb repulsion.

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