## Paper VIII

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# Coherent Single-Electron Transport between Coupled Quantum Dots 

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#### Abstract

We propose a method for a fully coherent transport of single electrons between the ground states of two anharmonic coupled quantum dots. The transition is achieved as a result of an intrinsic interplay between an external applied radio-frequency field and the interdot tunnel coupling between the single dot states. We have developed a 4-level model for the system, and full quantitative agreement with the exact solution of the timedependent Schrödinger equation is obtained for a wide range of field parameters. The analytical model has the advantage that it can be used as guidance in the actual design of such systems.


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The ability to fabricate and operate single or few-electron solid state quantum devices of nanometer sizes will have great impact on future technology. Quantum dots are one example of such devices that have numerous potential applications in biology, chemistry and physics. They constitute one of the most potent systems for full experimental control at the quantum level [1]. Two (or more) quantum dots may be interconnected to form so-called 'artifi cial molecules' [2]. These systems have proved to be promising candidates for a quantum bit or 'qubit', the basic component of a quantum computer [3]. The ability to create and maintain coherence for a suffi ciently long time is one of the main obstacles on the way to a physical implementation of a solid state quantum computer. Recently, coherence times of about 200 ns were observed in a double quantum dot system [4].

The possibility to address and manipulate single charge states in the quantum dot is a prerequisite for an effi cient operation of solid state quantum devices. Coupled quantum dots have been the subject of extensive experimental and theoretical studies [5-10]. Several schemes for controlled transport of single electrons between such two-dimensional quantum dots have been experimentally demonstrated $[4,10]$, and experimental methods to determine the interdot tunnel coupling both for ground and excited state have been developed [10, 11]. New techniques for coherent manipulation of charge transport in quantum dot arrays [12] and asymmetric double quantum dots [13] have been proposed.

In this Letter we present a realistic and robust method to transfer a single electron with unit probability between the (quasi stationary) ground states of two coupled twodimensional quantum dots. The initial coupling between the two ground states is so small that they remain stationary for times many orders of magnitude longer than the manipulation time. The driving force is an external microwave fi eld which is in resonance with the transition between the ground state and an excited quasi stationary state in each respective well. The actual transition between the wells is accomplished by tunneling between the two coupled excited states rather than between the ground states. Under certain conditions, only four quantum states in the double well are involved in the dynamics (see Fig. 1). We have developed an analytical model for the coherent transition that coincides with exact ab initio cal-
culations for a wide range of fi eld parameters. The model has general validity and could in principle be applied to other coupled systems like e.g. coupled Cooper-pair qubits in a Josephson circuit [14]. The switching is robust in the sense that the actual shape of the microwave pulse is not crucial for the effi ciency of the gate, and the method is applicable to almost any symmetric anharmonic double well potential. The parameters of the gate may be optimized such that a fully coherent charge transfer can take place within only a fraction of the natural decoherence time in the dots [4]. Our starting point is the two-dimensional double well confi ning potential,

$$
\begin{align*}
W(x, y)= & \frac{1}{2} m^{*} \frac{\omega_{0}^{2}}{D^{2}}\left[(x-D / 2)^{2}(x+D / 2)^{2}+\right. \\
& \left.\left(y^{4}+2 D|y|^{3}+D^{2} y^{2}\right)\right] \tag{1}
\end{align*}
$$

where $D$ is the interdot distance, and $\omega_{0}$ defi nes the strength of the potential barrier. In this Letter we, apply reduced atomic units (a.u.*) throughout, in order to maintain generality of the results. In these units $\hbar=m^{*}=e=1$, where $m^{*}$ is the effective mass of the electron. For a GaAs material $m^{*}=$ $0.067 m_{e}$, with $m_{e}$ being the free electron mass. If we set $\hbar \omega_{0}=3 \mathrm{meV}$ the unit of time becomes about 0.2 ps and the unit of length about 20 nm .

The evolution of the system is governed by the timedependent Schrödinger equation,

$$
\begin{equation*}
i \frac{\partial}{\partial t} \Psi=\left\{-\frac{1}{2}\left(\frac{\partial^{2}}{\partial x^{2}}+\frac{\partial^{2}}{\partial y^{2}}\right)+W(x, y)+x E(t)\right\} \Psi \tag{2}
\end{equation*}
$$

where $E(t)$ is the external $\hat{x}$ polarized microwave fi eld. Here, we simply assume that the fi eld takes the form of a constant intensity monochromatic fi eld, i.e. $E(t)=E_{0} \sin (\omega t)$. The Schrödinger equation is solved numerically based on accurate Fourier transform split operator methods [15]. The wave function is initially prepared in the (pseudo) ground state of dot 1. The net population transfer to dot 2 as a function of time is shown for a particular case in Fig. 1, for a moderate value of the interdot separation $(D=7)$. At the instant when this probability becomes 1 after about 1800 time units, the fi eld is switched off. At that time practically all the population is left in the ground and 1 st excited states in dot 2 , with only a very small interference from the 2nd excited state. After the fi eld


FIG. 1: The probability for electron transport from dot 1 to dot 2 versus time for a double quantum dot with $D=7$ and $\omega_{0}=1$. The microwave field is resonant with the first excited state in each dot, i.e. $\omega=0.906 \omega_{0}$, and the intensity of the field is $E_{0}=0.05$. In this particular example the field is turned off at an instant $(t \sim 1800$ time units) when the population is in a superposition of the ground state and the first (and second) excited state in dot 2. The Rabi-like oscillations in the population are due to tunneling between the two 1 st excited states in dot 1 and 2 , and the overall decrease indicates tunneling between the quasi stationary ground states of each dot. The fast oscillations superimposed on the longer oscillations stem from the small fraction of the total population that is left in the 2nd excited state after the field is turned off.
is turned off, the population will oscillate in a Rabi-like manner between the respective quasi stationary states in dot 1 and 2 due to the tunnel coupling between them. The signatures of these Rabi oscillations are displayed in Fig. 1. The overall decay of the population stems from the tunneling between the two ground states in dot 1 and 2, respectively, and shows that the "lifetime" of these states is only a factor 10 longer than the total transition time. Therefore, in the rest of this Letter, we set $D=10$ in order to keep the ground states stationary for times many orders of magnitude longer than the manipulation time.

The particular example given in Fig. 1 reveals that the whole dynamics is essentially restricted to four quantum levels, i.e. to two states in each dot. These observations inspire a model given in a basis consisting of two states with their wave functions essentially contained within each of the dots. The energy of both states lies below the interdot barrier. We label the states $|g i\rangle$ for the ground states and $|e i\rangle$ for the excited states where $i=1,2$ indicates the dot (see Fig. 2). The microwave frequency $\omega$ is in resonance with the energy separation $\varepsilon$ between the states. Due to the anharmonicity of the potential, we assume that the other excited states can be neglected in the model for moderate fi eld intensities and for not too long interaction times. Now, with the basis defi ned in Fig. 2, the Schrödinger equation reduces to a set of four coupled equations, $i \dot{\mathbf{c}}=H \mathbf{c}$, where $\mathbf{c}=$


FIG. 2: The double well potential, Eq. 1, in the $x$-direction for $D=$ 10 and $\omega_{0}=1$ with the single dot wave functions corresponding to the ground state and the third excited state. The tunnel coupling between the two excited states and the ground states of the two dots are given by $V_{e}$ and $V_{g}$, respectively.
$(\langle g 1 \mid \Psi\rangle,\langle e 1 \mid \Psi\rangle,\langle e 2 \mid \Psi\rangle,\langle g 2 \mid \Psi\rangle)$, and the Hamiltonian

$$
H=\left(\begin{array}{cccc}
-\frac{\varepsilon}{2} & d \sin (\omega t) & 0 & V_{g}  \tag{3}\\
d \sin \omega t & \frac{\varepsilon}{2} & V_{e} & 0 \\
0 & V_{e} & \frac{\varepsilon}{2} & d \sin (\omega t) \\
V_{g} & 0 & d \sin (\omega t) & -\frac{\varepsilon}{2}
\end{array}\right)
$$

The coupling between the lower and the upper states are induced by the microwave fi eld, and $d=E_{0}\langle g 1|(x+D / 2)|e 1\rangle$. The constant coupling $V_{e}\left(V_{g}\right)$ is given by the Rabi frequency of the oscillations between the excited states (ground states). Typically, the tunnel coupling $V_{g} \ll V_{e}$, and $V_{g}$ can be neglected for $D>7$.

The 4 -state system may be decoupled to two 2-level systems by defi ning a new basis set given by the sum (gerade) and difference (ungerade), respectively, of corresponding singlewell states. In the adiabatic representation, this transformation casts the Hamiltonian into the decoupled form,

$$
H_{A}=\left(\begin{array}{cc}
H_{+} & \mathbf{0}  \tag{4}\\
\mathbf{0} & H_{-}
\end{array}\right)
$$

where

$$
H_{ \pm}=\left(\begin{array}{cc}
-\zeta_{ \pm} \pm \frac{V_{e}+V_{g}}{2} & i \frac{d \omega V_{ \pm} \cos (\omega t)}{2\left(d^{2} \sin ^{2}(\omega t)+V_{ \pm}^{2}\right)}  \tag{5}\\
-i \frac{d \omega V_{ \pm} \cos (\omega t)}{2\left(d^{2} \sin ^{2}(\omega t)+V_{ \pm}^{2}\right)} & \zeta_{ \pm} \pm \frac{V_{e}+V_{g}}{2}
\end{array}\right) .
$$

Here, $\zeta_{ \pm}(t) \equiv \sqrt{d^{2} \sin ^{2}(\omega t)+V_{ \pm}^{2}}$ and $V_{ \pm} \equiv\left[\varepsilon \pm\left(V_{e}-V_{g}\right)\right] / 2$. For high fi eld strengths, i.e. when $\left(d / V_{ \pm}\right)^{2} \gg 1 / 2$, each of these sub-systems coincides with the well known LandauZener model $[16,17]$. However, here we consider only weak fi elds, and the probability of transition at resonance by absorption or emission of single photons becomes [17, 18]

$$
p_{ \pm}=\left(\frac{\pi d}{4 V_{ \pm}}\right)^{2}
$$

which is valid for $\left(d / V_{ \pm}\right)^{2} \ll 1$. In the adiabatic basis, the evolution of each sub-system over a half cycle of the fi eld is given by the propagator

$$
S_{ \pm}=\left(\begin{array}{cc}
\sqrt{1-p_{ \pm}} e^{i \gamma_{ \pm}} & \sqrt{p_{ \pm}}  \tag{6}\\
-\sqrt{p_{ \pm}} & \sqrt{1-p_{ \pm}} e^{-i \gamma_{ \pm}}
\end{array}\right) .
$$

The phase shifts $\gamma_{ \pm}$arise as a consequence of the frequency being slightly off resonance. This, in turn, is due to the lifting of the degeneracy of the system induced by the tunnel couplings $V_{e}$ and $V_{g}$. The shifts are $\gamma_{ \pm}=$ $\frac{2}{\omega}\left[\sqrt{d^{2}+V_{ \pm}^{2}} E\left(\frac{d}{\sqrt{d^{2}+V_{ \pm}^{2}}}\right)-\sqrt{d^{2}+\frac{\varepsilon^{2}}{4}} E\left(\frac{d}{\sqrt{d^{2}+\frac{\varepsilon^{2}}{4}}}\right)\right]$, where $E(k)$ is the complete elliptic integral of the second kind [19].

The total propagator after $N$ half fi eld-cycles is found by exponentiating the $S_{ \pm}$-matrices by $N$, multiplying them with the phases $\exp \left( \pm i\left(V_{e}+V_{g}\right) / 2 t\right)$, respectively, and putting all together in a 4 by 4 matrix:

$$
\mathcal{U}=\left(\begin{array}{cc}
e^{-i\left(V_{e}+V_{g}\right) / 2 t} S_{+}^{N} & \mathbf{0}  \tag{7}\\
\mathbf{0} & e^{i\left(V_{e}+V_{g}\right) / 2 t} S_{-}^{N}
\end{array}\right)
$$

Then, the probability of the $g 1 \rightarrow g 2$ transition is found as $|\langle g 2| \mathcal{U}| g 1\rangle\left.\right|^{2}$. Finally, the result may be written as

$$
\begin{equation*}
P(g 1 \rightarrow g 2)=\frac{1}{4}\left(X_{+}+X_{-}-2 \sqrt{X_{+} X_{-}} \cos \theta\right) \tag{8}
\end{equation*}
$$

with

$$
\begin{align*}
X_{ \pm}= & 1-\frac{4 r_{ \pm} \sin ^{2}\left(N \phi_{ \pm}\right)}{\left(1+r_{ \pm}\right)^{2}} \\
r_{ \pm}= & \frac{1}{p_{ \pm}}\left[1-\left(1-p_{ \pm}\right) \cos \left(2 \gamma_{ \pm}\right)+\right. \\
& \left.2 \sin \gamma_{ \pm} \sqrt{1-p_{ \pm}-\left(1-p_{ \pm}\right)^{2} \cos ^{2} \gamma_{ \pm}}\right] \\
\phi_{ \pm}= & \cos ^{-1}\left(\sqrt{1-p_{ \pm}} \cos \gamma_{ \pm}\right) \\
\theta= & \left(V_{e}+V_{g}\right) t+\tan ^{-1}\left[\frac{r_{-}-1}{r_{-}+1} \tan \left(N \phi_{-}\right)\right]- \\
& \tan ^{-1}\left[\frac{r_{+}-1}{r_{+}+1} \tan \left(N \phi_{+}\right)\right] . \tag{9}
\end{align*}
$$

Figure 3 shows the probability of populating the ground state of dot 2 when starting out in the ground state of dot 1 for three different fi eld strengths, namely $E_{0}=0.01,0.05$ and 0.1 , respectively. The solution of the time-dependent Schrödinger equation is shown along with the prediction of the model, Eq. (8). In all cases, the $a b$ initio calculations demonstrate almost complete transfer. We see that for the two lower fi eld strengths, the coincidence with the model is practically complete, whereas discrepancies are seen for $E_{0}=0.1$. This is due to the breakdown of the 4-level approximation, i.e. for higher fi eld strengths more than four states are involved in the dynamics.

In Fig. 4 snapshots of the wave function at different times during the process corresponding to Fig. 3 (intermediate) are
shown. We clearly see that the intermediate states $|e 1\rangle$ and $|e 2\rangle$ are populated during the interaction.

Concerning the transport time, we fi nd that for the more intense microwave fields, it is about the double of the tunneling time between the excited states, $\tau=\pi / 2 V_{e}$, which accords fairly well with intuition. For the weaker fi elds, however, the transport time is mainly determined by the characteristic Rabi-flopping frequency between the ground and excited states. These observations are confi rmed in the model. Since the tunnel coupling $V_{e}$ (and $V_{g}$ ) is weak, $V_{e} / \varepsilon \simeq 0$, Eq. (8) simplifi es to

$$
\begin{equation*}
P(g 1 \rightarrow g 2)=\frac{1}{2}\left(1-\frac{4 r_{+} \sin ^{2}(N \phi)}{\left(1+r_{+}\right)^{2}}\right)(1-\cos \theta) \tag{10}
\end{equation*}
$$

Then, the condition for transport may be formulated as

$$
\begin{equation*}
N \phi \simeq 0(\bmod \pi) \quad \text { and } \quad \theta \simeq \pi(\bmod 2 \pi) \tag{11}
\end{equation*}
$$

As the fi eld strength increases, the trigonometric terms of Eq. (9) become less important, and the second criterion is fulfi lled for $t \simeq \pi / V_{e}=2 \tau$. In this limit, $N \phi$ varies more rapidly than $\theta$, so that the first criterion does not modify the transport time much. Also for weaker fi elds, this criterion is less signifi cant since the sine term in Eq. (10) vanishes in this limit. However, the importance of the trigonometric terms in Eq. (9) can not be neglected, resulting in a transport time much longer than $2 \tau$.

In conclusion, we have presented a realistic method for coherent transfer of a single electron between the ground states of two coupled quantum dots. The transition takes place on the picosecond time scale, which is far below recently achieved coherence times in corresponding systems. We have developed an analytical model for the dynamics that can be used to optimize the parameters of the system in order to achieve the desired fi delity and operation time of the gate. We have demonstrated that the coherent charge transport between the wells can become an almost $100 \%$ revesibel process, which is an important property of a working two-qubit gate in a quantum computer.

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FIG. 3: (Color online). Probability of finding the electron in the ground state of dot 2 as a function of the number of field cycles for $E_{0}=0.01$ (upper), $E_{0}=0.05$ (intermediate), and $E_{0}=0.1$ (lower), with $\omega_{0}=1$ and $\omega=\varepsilon=1.78 \omega_{0}$. The wave function was initially prepared in the ground state of dot 1 . The full (blue) curves stem from $a b$ initio calculations, and the dashed (red) curves are the predictions of the model, Eq. 8.
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FIG. 4: (Color online). Snapshot of the electronic probability density for $E_{0}=0.05$ and $D=10$ at 7 instants, after 0 (upper), 95,150 , $179,210,265$, and 358 (lower) oscillations of the field. The times are indicated with ' $*$ ' in Fig. 3 (intermediate). The axis ranges are from $x=-8$ to $x=8$ and $y=-2$ to $y=2$.
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