

## Controlled energy-selected electron capture and release in double quantum dots

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Highly accurate quantum electron dynamics calculations demonstrate that energy can be efficiently transferred between quantum dots. Specifically, in a double quantum dot an incoming electron is captured by one dot and the excess energy is transferred to the neighboring dot and used to remove an electron from this dot. This process is due to long-range electron correlation and shown to be operative at rather large distances between the dots. The efficiency of the process is greatly enhanced by preparing the double quantum dot such that the incoming electron is initially captured by a two-electron resonance state of the system. In contrast to atoms and molecules in nature, double quantum dots can be manipulated to achieve this enhancement. This mechanism leads to a surprisingly narrow distribution of the energy of the electron removed in the process which is explained by resonance theory. We argue that the process could be exploited in practice.

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Quantum dots (QDs) are often referred to as artificial atoms<sup>1</sup> and double quantum dots (DQDs) are the extension to molecules of this analogy.<sup>2</sup> The initial notion for the name came from the quantized levels and transitions of carriers inside nanosized semiconductor structures<sup>3</sup> that resemble those found in atoms. A wealth of other phenomena also present in atoms have found their counterpart in QDs<sup>2,4–7</sup> together with new phenomena handed down from the semiconductor nature of QDs,<sup>8–11</sup> many of which endowed new technological applications to be cast into reality. In this work we concentrate on energy transfer between two QDs driven by long-range electron correlation and mediated by the capture of an electron.

Electron capture in single QDs is an extensively studied topic<sup>12–14</sup> due to its relevance in the development of technological applications. The capture efficiency and its time scale depend substantially on temperature, carrier density, material, and geometry of the QDs.<sup>13–15</sup> The capture and the later relaxation dynamics occur through diverse physical processes such as electron-phonon interactions,<sup>13,14,16,17</sup> multiple exciton generation,<sup>12</sup> and Auger relaxation,<sup>15</sup> all of which can be assessed using pump-probe schemes.<sup>10,12–14,17</sup> Capture by optical phonon emission has been investigated in single<sup>16,18,19</sup> as well as in double QDs.<sup>18</sup> So far, electronically induced interdot capture processes have not been considered at all. In the present work we use numerically exact quantum dynamics to show that electron capture by one QD in a DQD becomes possible by energy transfer to the neighboring QD due to long-range electron correlation. Originally, such processes were predicted to operate between atoms<sup>20,21</sup> where electron capture by one atom occurs while another electron is emitted from an atom in its environment and called interatomic electronic Coulombic capture (ICEC), a name which we would like to adopt also for QDs. For completeness we mention that energy transfer between quantum wells has been studied in a different context; see, e.g., Refs. 22 and 23.

For explicit demonstration we study a system composed of two different QDs which we call the left and right QD and which are described by the model potentials discussed below. Let the left potential well support a one-electron level  $L_0$  and the right one,  $R_0$ . Although included in the calculation, the tunneling between  $L_0$  and  $R_0$  is vanishingly small due to the long interdot distance. As described in Fig. 1, an electron is

initially in the right QD and an electron with momentum  $p_i$  is incoming from the left of the DQD. This electron is captured into the  $L_0$  ground state of the left QD while the excess energy is transferred to the right QD emitting the electron from the  $R_0$  ground state of this QD. According to energy conservation<sup>21</sup>

$$E_{R_0} + \varepsilon_i = E_{L_0} + \varepsilon_f \quad (1)$$

the momentum of the outgoing electron is  $p_f = \sqrt{p_i^2 + 2m^*(E_{R_0} - E_{L_0})}$ , where  $\varepsilon_{i,f} = p_{i,f}^2/2m^*$  and  $m^*$  is the electron effective mass in atomic units. The emitted electron can have a higher or lower momentum than the initial electron, depending on the relation between the bound-state energies  $E_{R_0}$  and  $E_{L_0}$ .

Below, we will first discuss the model potentials of the two QDs and then prove numerically that ICEC takes place. The findings will actually make clear that the process is, in principle, possible for two-site systems with a broad range of binding potentials. Subsequently we investigate how to manipulate DQDs in order to make the probability of ICEC large. This will lead to a slightly more complex physical situation with an interesting energy transfer.

The model potential for the DQDs is based on the effective mass approximation<sup>24,25</sup> and allows us to describe accurately the motion of two electrons inside the nanostructured semiconductor. Thus, it offers straightforward observability of how electron correlation can lead to ICEC. In the specific DQD model adopted from a previous study<sup>26</sup> the dots are represented by two Gaussian wells aligned in the  $z$  direction. In the  $x$  and  $y$  direction we assume a strong harmonic confinement which could be attributed either to depleting gates<sup>8</sup> or to the structure of the semiconductor.<sup>4</sup> The system Hamiltonian is

$$H(\mathbf{r}_1, \mathbf{r}_2) = h(\mathbf{r}_1) + h(\mathbf{r}_2) + \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|}, \quad (2)$$

where

$$h(\mathbf{r}_i) = -\frac{1}{2m^*} \nabla_i^2 + V_c(x_i, y_i) + V_l(z_i) \quad (3)$$

is a one-electron Hamiltonian and

$$V_c(x_i, y_i) = \frac{1}{2} m^* \omega^2 (x_i + y_i)^2, \quad (4)$$

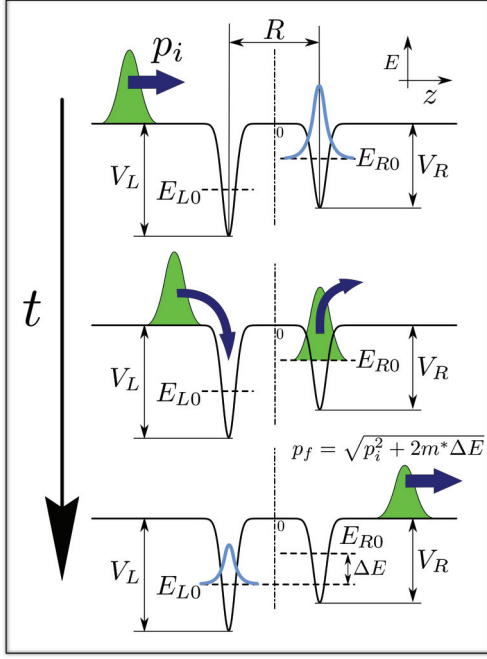


FIG. 1. (Color online) Schematic view of ICEC in a model potential for a DQD. The capture of the incoming electron by the left QD is mediated by its correlation with the electron initially bound to the right QD. After energy transfer, the electron on the right is excited into the continuum and becomes an outgoing electron.

$$V_L(z_i) = -V_L e^{-b_L(z_i+R/2)^2} - V_R e^{-b_R(z_i-R/2)^2} \quad (5)$$

are the transversal confinement and longitudinal open potentials, respectively.  $R$  is the distance between the QDs,  $b_{L,R}$  the sizes of the left and right QD, and  $V_{L,R}$  are their depths. Due to the strong confinement ( $\omega = 1.0$  a.u.  $> V_{L,R}$ ) the relevant excitations are only in the  $z$  direction into the levels  $L_n$  ( $R_n$ ),  $n = 0, 1, \dots$ , of the left (right) QD with energies  $E_{L_n}$  ( $E_{R_n}$ ). For simplicity, we limit ourselves here to triplet configurations, but mention that we do have calculations on singlet configurations which show similar behavior.

The dynamical evolution of the system was obtained by solving the time-dependent Schrödinger equation employing the multiconfiguration time-dependent Hartree (MCTDH) approach.<sup>27,28</sup> The triplet wave function

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, t) = \sum_{i,j} A_{ij}(t) \phi_i(\mathbf{r}_1, t) \phi_j(\mathbf{r}_2, t) \quad (6)$$

was expanded in time-dependent single-particle functions  $\phi_i(\mathbf{r}, t)$  (SPFs) and coefficients  $A_{ij}(t)$  that fulfill the anti-symmetry condition  $A_{ij}(t) = -A_{ji}(t)$ . The SPFs  $\phi_i$  were expanded in one-dimensional basis functions for each of the Cartesian coordinates ( $x, y, z$ ) in a DVR-grid representation (discrete variable representation) with harmonic oscillator DVRs for  $x$  and  $y$ , and a sine DVR for the  $z$  coordinate. The MCTDH equations of motion for coefficients and SPFs were efficiently solved using the approach implemented in the MCTDH-Heidelberg package.<sup>27,29</sup> A complex absorbing potential (CAP) of order 2 was placed in the  $z$  coordinate to absorb the outgoing electron before it reaches the end of the grid. We placed CAPs at different positions and confirmed

that the results discussed below are not affected by the CAP. The Coulomb potential was regularized to prevent divergences at  $\mathbf{r}_1 = \mathbf{r}_2$ ,  $1/r_{12} \rightarrow 1/\sqrt{r_{12}^2 + a^2}$  with  $a = 0.01$ , and then transformed into sums of products using the POTFIT<sup>29</sup> algorithm of MCTDH. The convergence of numerical results was ensured.

Let us discuss the results. We first investigate what happens if only the right QD is present. The result is depicted in Fig. 2(a) (setup A). The parameters  $V_R = 0.6$  a.u. and  $b_R = 1.0$  a.u. used give a single bound state with an energy of  $E_{R_0} = -0.246$  a.u. (we set the origin of the energy scale to  $2\hbar\omega = 2$  a.u. throughout the study). The incoming wave packet (WP<sub>*i*</sub>) was represented by an energy-normalized Gaussian peaked around  $\varepsilon_{WP_i} = 0.056$  a.u. with energy width  $\Delta E_{WP_i} \approx 0.033$  a.u. and spatial width  $\Delta x_{WP_i} = 10.0$  a.u. The ionization of the bound electron by the incoming one and the excitation to higher states in the transversal directions are energetically forbidden for these parameters.

The dynamics of the scattering process is visualized in Fig. 2(a) by the longitudinal electronic density  $\rho(z, t) = \int d\mathbf{r}' \int dx \int dy |\Psi(\mathbf{r}, \mathbf{r}', t)|^2$  as a function of  $z$  and  $t$ . It is clearly seen that the incoming electron is completely reflected while the other electron remains bound in the right QD.

We now add the left QD at a distance  $R = 10.0$  a.u. and show that ICEC takes place in the DQD according to the scheme in Fig. 1. We choose the potential well of the left QD somewhat deeper ( $V_L = 0.8$  a.u.,  $b_{L,R} = 1.0$  a.u.) than that of the right QD while leaving the parameters of the latter unchanged (setup B). This choice leads to two non-overlapping bound one-electron states,  $L_0$  and  $R_0$ , with energies  $E_{L_0} = -0.377$  a.u. and  $E_{R_0} = -0.246$  a.u.

The spatially resolved time evolution of  $\rho(z, t)$  in Fig. 2(b) clearly shows emission of electronic density to the right of the DQD starting at  $t \approx 400$  a.u. The slope of the final wave packet (WP<sub>*f*</sub>) trajectory traveling to the right changed compared to that of the incoming WP<sub>*i*</sub> indicating that the emitted electron has acquired momentum during the process. From the slope we estimate an average momentum  $p_f^{(\text{plot})} \approx 0.63 \pm 0.02$  a.u. which is in full agreement with energy conservation in ICEC [see Eq. (1)], where  $\Delta E = E_{R_0} - E_{L_0} = 0.131$  a.u. gives  $p_f = 0.612$  a.u. We also computed examples for  $\Delta E < 0$  that showed, accordingly, the emission of decelerated electrons to the right.

Obviously, ICEC takes place in the DQD. To have a quantitative measure, we computed the reaction probability (RP). The RP is a function of the energy of the incoming electron and tells us the probability with which an incoming electron with a given energy is caught in the left well and simultaneously an electron is emitted to the right from the right well. Of course, the energy of the emitted electron is regulated by Eq. (1). Technically this is done by computing the energy-dependent absorbed flux into the right CAP after normalization with the distribution of the incoming wave packet WP<sub>*i*</sub>.<sup>27,29</sup> Due to this normalization, the RP is independent of WP<sub>*i*</sub> which makes it an absolute measure. The RP corresponding to  $\rho(z, t)$  depicted in Fig. 2(b) is shown at the right-hand side of the panel. It peaks at an energy of about  $\varepsilon_i = 0.12$  a.u. where it acquires a value of 0.5%. It is seen that ICEC in QDs is selective in energy. The peak in the RP appears close to the total energy  $E_T = \varepsilon_i + E_{R_0}$  which fits to the energy transferred

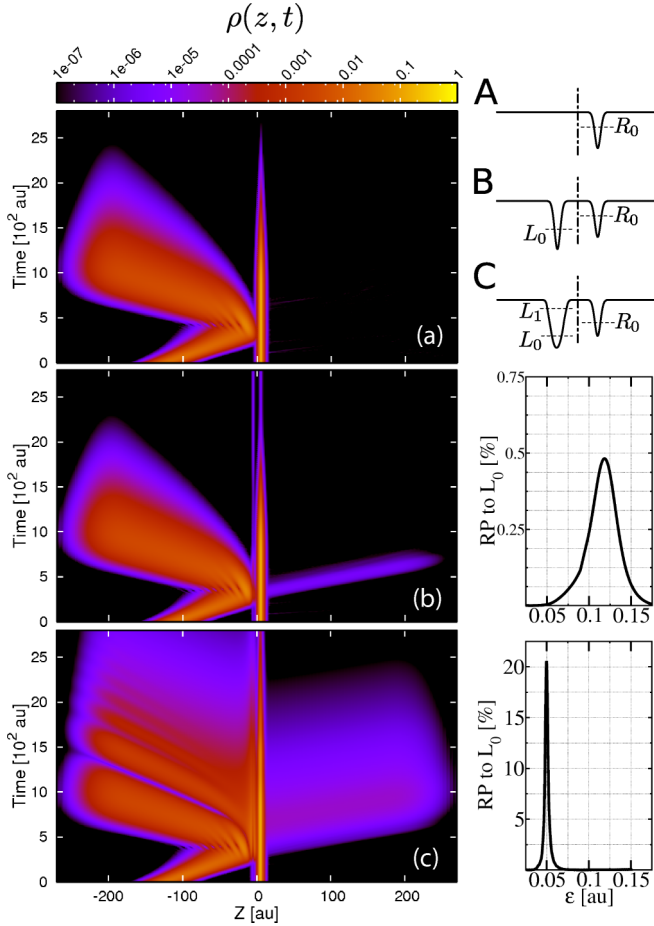


FIG. 2. (Color online) Evolution of the electronic density (left panels) and reaction probabilities (RP) (right panels) for three different setups shown in the upper right corner. The incoming wave packet ( $WP_i$ ) approaches from the left to the DQD centered at  $z = 0$  a.u. which is initially occupied by an electron in the right QD ( $R_0$  state). Both  $WP_i$  and  $R_0$  are the same in all three cases. The complex absorbing potentials (CAPs) are placed at  $z = \pm 170$  a.u. (a) The left QD is missing and no emission to the right is observed. (b) The left QD has a single one-electron state  $L_0$ . Emission of the electron initially in  $R_0$  through ICEC takes place. The emitted packet acquires momentum according to the energy conservation, Eq. (1), and is faster than the incoming packet in this case. (c) The left QD supports two one-electron states and the DQD exhibits a two-electron  $|L_1 R_0\rangle$  resonance state which is populated and decays, strongly enhancing the RP of the ICEC channel. The RP shows a Breit-Wigner shape.

to the QD system by ICEC:  $E_T^{\text{peak}} = E_{L_0} - E_{R_0}$ . Considering that the capture of a freely moving electron is a rather intricate process in general,<sup>13,14,30</sup> a probability of 0.5% is rather high. On the other hand, it is still a rather low value if ICEC is to be utilized in practical applications.

How does one enhance the reaction probability of ICEC substantially? To answer this relevant question we make use of the physics of resonance states. To that end we widen the potential well of the left QD by choosing  $V_L = 0.71$  and  $b_L = 0.3$  a.u. such that this dot displays a bound excited one-electron state  $L_1$  in addition to its ground state  $L_0$  [see upper right corner of Fig. 2 (setup C)]. The energies in this case are  $E_{L_1} = -0.048$  and  $E_{L_0} = -0.441$  a.u. The incoming

electron properties were kept unchanged and we notice that the energy of  $WP_i$  is insufficient to open the ICEC channel to the  $L_1$  state even if we take into account the energy width of this wave packet. The ICEC channel to the  $L_0$  state is, of course, still open. However, due to the lower energy of  $L_0$ , the RP of ICEC directly populating that level is even lower than that in case B.

The results of the propagation in setup C are shown in Fig. 2(c). It is eye catching that the electron density emitted to the right is now much larger than in case B. The RP to the right [right-hand side of Fig. 2(c)] is now amplified and peaks at 20% at the energy  $\varepsilon_i = 0.05$  a.u. of the incoming electron. Compared to case B, this is an amplification by a factor of 40. We remind the reader that the RP is independent of the incoming wave packet used. There is another very interesting property of the RP which can be relevant for practical applications, namely that the RP is very narrow in energy, much narrower than in case B.

Let us briefly discuss the density plot in Fig. 2(c) which also shows several unusual features. From the plot the momentum gives  $p_f^{(\text{plot})} \approx 0.70 \pm 0.02$  a.u. in agreement with  $p_f = 0.70$  a.u., which follows from Eq. (1). In sharp contrast to case B, the  $WP_f$  is not created in a relatively sharp instant of time [compare Figs. 2(b) and 2(c) at the site of the DQD,  $z = 0$ ] but rather continuously with an exponential decay in time which gives a hint about the mechanism of amplification which will be discussed below. The emitted electron density to the left side becomes more complex compared to Fig. 2(b) and shows signatures of interference which we attribute to the superposition between the reflection of the incoming wave packet  $WP_i$  and electrons emitted to the left in the same energy range.

The substantial amplification of electron capture by the left QD and the other features mentioned above can be well understood by realizing the interplay of two effects: first, the appearance of a resonant state and second that this state efficiently decays to the ICEC channel.

Due to the additional one-electron level  $L_1$ , the DQD of setup C accommodates a *two-electron* resonance  $|L_1 R_0\rangle$ , which has one electron on each of the QDs. Such states have been shown to decay fast by energy transfer to  $|L_0\rangle$  plus an outgoing electron via interatomic Coulombic decay (ICD).<sup>26,31–35</sup> The resulting story is then that if the incoming electron is in the energy range of the two-electron resonance state, it has a higher probability to be caught in this state than capturing of one electron and emitting another electron. This state can decay by ICD thus strongly amplifying the RP of the ICEC channel.

Let us discuss how this picture explains our observations in Fig. 2(c). The energy of the  $|L_1 R_0\rangle$  can be estimated for large interdot distances  $R$  as  $E_{L_1 R_0} \approx E_{R_0} + E_{L_1} + 1/R$ . In order to be substantially populated by the scattering process, this two-electron energy should correspond to the total energy  $E_T = \varepsilon_i + E_{R_0}$ . For the parameters used,  $E_{L_1 R_0} \approx 0.052 + E_{R_0}$  a.u., which is indeed very close to the peak of the RP which is at  $\varepsilon_i = 0.05$  a.u. The exponential decay in time observed above for the continuous emission of electrons to the right can be attributed to the lifetime of the  $|L_1 R_0\rangle$  resonance populated by the incoming electron.



Decay rates (inverse lifetimes) in QDs can be computed using different methods.<sup>26,31,36</sup> Here, we employed imaginary-time propagation to arrive at the resonant state of setup C and then the state is let to evolve in real time to measure the total decay rate.<sup>26</sup> The decay rate obtained for case C is  $\Gamma_C = 39 \pm 2 \times 10^{-4}$  a.u. For consistency we have also fitted a Breit-Wigner peak shape<sup>37</sup> to the RP on the right-hand side of Fig. 2(c) and obtained  $\Gamma_C^{(RP)} = 38 \pm 1 \times 10^{-4}$  a.u. which is in perfect agreement with the results from the propagations. Finally, we mention for completeness that the resonance after being populated by the incoming electron can also decay by emitting elastically the electron to the left resembling that of a shape resonance:<sup>37</sup>  $e^- + |R_0\rangle \rightarrow |L_1 R_0\rangle \rightarrow |R_0\rangle + e^-$ . This electron is responsible for the interference effects mentioned above. Our calculations show, however, that this depopulation channel is minor in comparison to the ICEC channel.

Having proven that ICEC takes place, we now transfer the parameters to realistic semiconductor QDs. The quasi one-dimensional shape used in the model is applicable to experimentally achievable DQDs, for example QDs embedded in nanowires<sup>4</sup> or electrostatically defined dots.<sup>8</sup> The process is driven by long-range Coulomb interactions, so we expect ICEC to be also applicable to other QDs geometries such as self-assembled vertically stacked dots.<sup>10,11,14,17</sup> We convert the atomic units of setups B and C into units of GaAs QDs using the effective mass approximation.<sup>26</sup> Then  $R^{GaAs} \approx 98$  nm,  $\Delta E^{GaAs}(B) = 1.55$  meV,  $\Delta E^{GaAs}(C) = 2.30$  meV, and  $\Delta E_{L_1 R_0}^{GaAs}(C) = 0.61$  meV, and for  $WP_i$  we have  $\varepsilon_{WP_i} = 0.66$  meV and  $\Delta E_{WP_i} \approx 0.4$  meV. These energies are well in the range of intraband level spacings of QDs in nanowires<sup>4,6</sup> and of intrashell levels in self-assembled QDs.<sup>17</sup> The time scale depicted in Fig. 2 is 160 ps for GaAs QDs. As seen in the figure, ICEC emission occurs for case B on a surprisingly short time scale of 10 ps. This is much faster than the reported capture

times of 100 ps for free carriers in bulk GaAs into InAs/GaAs QDs in single-layer samples measured at room temperature.<sup>38</sup> Notice that electron capture by emission of optical phonons is ineffective in our case where the phonon energy is much larger than the electronic transition.<sup>16,18</sup> The lifetime of the  $|L_1 R_0\rangle$  resonance in case C is 14.3 ps and thus also short. This is important because the decay of this resonance may compete with relaxation via phonons. The times for ICEC are, however, faster than reported intraband decay times due to acoustic phonon emission for InGaAs/GaAs QDs.<sup>17</sup> It is relevant to mention that the width of the RP peak in Fig. 2(c) is only 0.046 meV.

In summary, fully correlated electron dynamics was used to show that long-distance energy transfer between the quantum dots of a DQD is possible due to long-range electron correlation. The transfer is achieved by a fundamental electronically induced process where capture of an electron in one QD induces a release of another electron from a distant quantum dot. This fundamental process turns out to be particularly fast and can overcome other important capture mechanisms such as acoustic phonon emission. The presence of a two-electron resonance in the DQD results in a substantial enhancement of the energy transfer and leads to a well defined and narrow energy distribution of the emitted electron. The ICEC mechanisms in DQDs are not only interesting from the point of view of basic physics, but could, in principle, also be exploited to implement devices which generate nearly monochromatic low energy electrons in a given direction. We think that the implementation can be based on currently available nanowires, particularly those with long free-electron lifetimes.

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