Tunable ground-state degeneracies in double quantum dots

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Abstract

We have studied the effect of electron–electron interactions on planar double quantum dots subjected to an external magnetic field. Contrary to all other earlier works on similar systems, our accurate results for the energy levels and the dipole-allowed transition energies reveal the absence of singlet–triplet crossing (due to electron correlations only) in the case when the dots occupy only two electrons. For a larger number of electrons, we find the expected crossing of the energy levels. The corresponding far-infrared optical absorption spectra show the effect of electronic interactions as well as the underlying symmetries of these systems. The hyper-exponential increase of the exchange energy, as derived in our model, would facilitate the coherent control of the spin states in a double dot, as proposed in recent experiments.

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The physics of the few-electron quantum dot (QD)—the artificial atom [1] has been quite extensively studied during the last decades, and yet our understanding of quantum interactions in these systems are often put to a severe test. With the advent of new techniques in the design and creation of these nanostructured systems a wider horizon of applications has been opened, in particular for quantum computation. Earlier pioneering works [2] have introduced the idea of spin-qubit based quantum gate, especially, the suitability of two-spin operations to perform quantum computations. Here one of the key issues involves the exchange energy that arises due to two neighboring dots that are tunnel coupled. Theoretical analysis of the exchange energy indicates a rather significant feature: In an increasing magnetic field, an antiferromagnetic state changes into a ferromagnetic state. This property has been proposed [3] to be useful as a two-qubit gate device operated by a magnetic field.

The double QD system where the individual dots are either formed by depletion of the two-dimensional electron gas by the gates placed on the surface or by the vertical confinement in a quantum well, has emerged as the most promising candidate for realization of a quantum gate. It has also gained increasing attention due to its possible realization as a spin-qubit based quantum gate. Investigation of the properties of a double QD is therefore important for fundamental understanding as well as for device applications. For a parabolic double QD, several authors [4] have used the numerical technique of exact diagonalization for two electrons. However, the magnitude of the exchange energy was always found to be small. A different choice of the confinement potential, the Gaussian confinement, which is expected to be more realistic has also been reported recently [5].

In this work, we report on a very accurate study of the Gaussian confined double QD (GDQD) containing a few interacting electrons. The exact diagonalization method was employed here to evaluate the energy levels and the dipole-allowed transitions. We found that the oft-reported singlet–triplet crossing (due to correlations) for two electrons is actually absent in our system. This unexpected result indicates that the antiferromagnetic/ferromagnetic switching does not take place here. As a

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consequence, the magnetic field is not the most suitable parameter to be used in a quantum gate design. On the other hand, in a GDQD we find another surprising property of the exchange energy: it shows a rapid variation with the gate voltage. This property is in fact suitable for fabrication of a quantum gate device operated solely by electrostatics.

The single-particle Hamiltonian for a confined electron subjected to a magnetic field parallel to the z-axis can be written as

\[
\mathcal{H}_0 = \frac{1}{2m^*} \left( \mathbf{p} - \frac{e}{c} \mathbf{A} \right)^2 + V_G,
\]

where \( \mathbf{A} = \frac{1}{2} \mathbf{B} (y, x, 0) \) is the vector potential in the symmetric gauge, and \( e = |-e| \). Following the convention adapted in all earlier works \cite{3-7}, we ignore the Zeeman contribution in the rest of the paper. The confining potential \( V_G \) is shaped as a combination of three Gaussians

\[
V_G(x,y) = V_b \exp \left( -\frac{x^2}{l_{hx}^2} - \frac{y^2}{l_{hy}^2} \right) - V_0 \left[ \exp \left( -\frac{(x-x_0)^2}{l_x^2} - \frac{y^2}{l_y^2} \right) + \exp \left( -\frac{(x+x_0)^2}{l_x^2} - \frac{y^2}{l_y^2} \right) \right].
\]

The second and the third Gaussians (with strength of \( V_0 \)) are for the individual wells which will form a double dot structure, and the first Gaussian (with strength of \( V_b \)) will control the height of the central barrier which separates the QDs.

The eigenfunctions are of the form of two-component spinors

\[
\psi = \sum_\kappa c_{\kappa} \phi_{\kappa} \chi^\dagger,
\]

where \( \chi^\dagger \) and \( \chi \) are eigenvectors of the \( s_z \) operator with their respective eigenvalues being \( \pm \hbar/2 \) and \( \kappa \) is a set of quantum numbers. For the spatial portion of the spinors, we choose the complete set of orthonormal eigenvectors which are the solution of the two-dimensional harmonic oscillator, i.e.,

\[
\phi_{\kappa; n_1 n_2} = \left( \frac{1}{a_x a_y} \right)^{1/4} \frac{1}{\sqrt{\pi}} \left( \frac{1}{2^{n_1} n_1! 2^{n_2} n_2!} \right)^{1/2} e^{-a_x^2/2} H_{n_1}(x/a_x) e^{-a_y^2/2} H_{n_2}(y/a_y),
\]

where \( a_x \) and \( a_y \) are the characteristic lengths in \( x \) - and \( y \) - directions, and \( H_n(x) \) are the Hermite polynomials. Using the single-particle basis \( \phi_{\kappa; n_1 n_2} \), we are able to obtain the exact analytic form for the Coulomb interaction matrix elements

\[
\langle n_1' n_2' | V | n_1 n_2 \rangle = \int \psi_{n_1 n_2}^{*}(x_1, y_1) \psi_{n_1' n_2'}^{*}(x_2, y_2) \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|} \psi_{n_1 n_2}(x_1, y_1) \psi_{n_1' n_2'}(x_2, y_2) dx_1 dy_1 dx_2 dy_2
\]

\[
= \frac{1}{a_x a_y \sqrt{2\pi}} (-1)^{s_1 + s_2 + n_1' + n_2'} e^2 \left( \frac{n_1'^4}{n_{1x}^4} + \frac{n_1'^4}{n_{1y}^4} + \frac{n_2'^4}{n_{2x}^4} + \frac{n_2'^4}{n_{2y}^4} \right)^{1/2}
\]

\[
\times \sum_{k_x, 0} \left( \frac{n_1'^4}{n_{1x}^4} - k_x \right) \sum_{k_y, 0} \left( \frac{n_1'^4}{n_{1y}^4} - k_y \right) \sum_{k_x', 0} \left( \frac{n_1'^4}{n_{1x}^4} - k_x' \right) \sum_{k_y', 0} \left( \frac{n_1'^4}{n_{1y}^4} - k_y' \right)
\]

\[
\times \left[ s_x + k_x + k_x' + 1 \right] \left[ s_x + k_x + k_x' + \frac{1}{2} \right]
\]

\[
\times \left[ s_y + k_y + k_y' + 1 \right] \left[ s_y + k_y + k_y' + \frac{1}{2} \right]
\]

\[
\times \left[ 2 s_x + s_y + k_x + k_y + k_x' + k_y' + 1 \right] \left[ 2 s_x + s_y + k_x + k_y + k_x' + k_y' + \frac{1}{2} \right]
\]

\[
\times \text{F}_1(1, 2; s_x + s_y + k_x + k_y + k_x' + k_y' + 1 + 1, 1 - \gamma^2),
\]

where \( n_{1x}^d = \max(n_1, n_1') \), \( n_{1y}^d = \min(n_1, n_1') \), \( 2 s_x = n_{1x}^d - n_{1x}^{d-1} + n_{1x}^{d+1} - n_{1x}^c \) with \( s_x \in \mathbb{N} \) and \( \gamma = a_x/a_y \). The method used for extracting a set of low-lying eigenvalues and eigenvectors from the Hamiltonian matrix (that could be up to the order of \( 10^5 \) in the worst case treated) was the Davidson–Liu diagonalization algorithm \cite{9}.

The material parameters used in the numerical calculation were those appropriate for a GaAs QD, i.e., \( m^* = 0.067 m_e \), and \( \varepsilon = 13.1 \). To characterize a double dot system, we also need to determine the radius \( R \) and the interdot distance \( d \). In this work, we choose \( R = 100 \text{nm} (l_x = l_y = 100) \). In the absence of the magnetic field the orbital parts of the eigenstates of the Hamiltonian \( \mathcal{H}_0 \) transform according to the irreducible representations of the point group consisting of the two-fold rotational symmetry and a mirror symmetry (group \( C_{2v} \)) \cite{10}. At the vanishing interdot distances \( d \to 0 \), i.e., in the case of a single rotationally symmetric dot the energy states can be labelled by the radial and angular momentum quantum numbers \( (n, l) \). At increasing interdot distances the orbital nondegenerate ground state \( (0,0) \) transforms to a corresponding, still nondegenerate parity eigenstate. The degenerate single-dot eigenstates \( (0,1) \) and \( (0,-1) \) are split into two nondegenerate double dot states, of which the lower one merges with the ground state when the interdot
distance is further increased. The chosen parameter \( d = 96 \text{ nm} \) \((x_0 = 64, l_hx = 50, l_hy = 55)\) is the region where the transformed ground state and the first excited state are close.

The far-infrared (FIR) spectroscopy can be of great help in determining the underlying structure of the QD. According to the Fermi golden rule, the intensity of absorption of the dipole transition is proportional to \([1,9]\)

\[
I = |\langle f|\chi(0)|0\rangle|^2 + |\langle f|\psi(0)|0\rangle|^2,
\]

when the transition goes from the ground state \(|0\rangle\) to a final \(|f\rangle\) state. In Fig. 1, we show the energy levels and dipole-allowed transition of a single electron in a Gaussian double QD. With the spherical symmetry broken, the first excited state approaches the ground state. The level separation between the first excited state and the ground state is small. Optical transitions are dominated by the jump to the first excited state. In the absorption spectra, it shows a thick branch at \(E \rightarrow 0\), which is present because of the broken rotational symmetry. As \(d \rightarrow 0(\infty)\) \((or \ V_h \gg 1)\), it becomes two individual QDs, and the thick branch in transition spectra will disappear.

Fig. 2 shows the low-lying energy levels for few-interacting electrons in a GDQD. A striking feature visible in Fig. 2(a) for two electrons is the absence of the singlet–triplet crossing \((the\ triplet\ state\ becomes\ the\ ground\ state\ in\ the\ high\ magnetic\ field\ limit)\). This result is remarkably different from all the earlier works reported in the literature. The physical reason behind this noncrossing configuration is rather subtle. Let us first consider the exchange energy \(J\) which is the energy difference between the energy level ‘1’ \((E_1)\) and energy level ‘0’ \((E_0)\). It can be expressed as

\[
J = \langle E_1|\mathcal{H}|E_1\rangle - \langle E_0|\mathcal{H}|E_0\rangle = J_{\text{dir}}(B) + J_{\text{exch}}(B) + J_{\text{conf}},
\]

where \(J_{\text{dir}}(B)\) is from the direct Coulomb interaction, \(J_{\text{exch}}(B)\) is from the exchange Coulomb interaction which gives the negative value, and \(J_{\text{conf}}\) is from the confinement. As proposed by Loss and DiVincenzo [3], two electrons in a parabolic confined double QD show a singlet–triplet crossing, i.e., \(J\) changes sign at the finite strength of a magnetic field. Within the Heitler–London approximation in molecular physics, and with increasing magnetic field the magnitude of \(J_{\text{dir}}\) and \(J_{\text{conf}}\) cannot compensate the contribution from \(J_{\text{exch}}\). Eventually, it leads to a sign change from the antiferromagnetic \(J > 0\) to a ferromagnetic \(J < 0\). Other authors [4] using the exact diagonalization method in the same model found the singlet–triplet crossing at \(B \neq 0\). For a GDQD, and in this approximation a larger \(J_{\text{conf}}\) is possible [5]. But, it does not dominate over the \(J_{\text{exch}}\) and one still finds the singlet–triplet crossing. The exact diagonalization method but with only the lowest Landau level wavefunction as the basis has been used in the Gaussian potential model [7], and the crossing associated with a very small exchange energy has been found. In addition to the GDQD, several authors employed a self-consistent 3D Poisson equation to have a better fit of the confinement potential [8]. However, in their numerical calculation, they also found the crossing.

We find that for the two electron case \(J\) is zero, i.e., there is no singlet–triplet crossing (the dashed line in Fig. 3). The main difference in our approach, as opposed to the earlier investigations is that we deal with the Gaussian confinement, but use the exact diagonalization method [9] with the complete set of single-particle eigenfunction as the basis. In our results, the energy level ‘0’ (spin-singlet) keeps its status as the ground state for all values of the magnetic field. It results from a large enough \(J_{\text{conf}}\) and \(J_{\text{dir}}\) to compensate the negative value of \(J_{\text{exch}}\). As a result, we observe the
unique noncrossing behavior. The corresponding feature in the absorption spectra associated with the absence of level crossing is the disappearance of discontinuities in the absorption spectra. Interestingly, we do recover the singlet–triplet crossing if we reduce the number of basis states.

We now consider cases of GDQD with more electrons. In Fig. 2(b) and (c), we show the energy spectrum for three and four electrons, respectively. Obviously, in these cases the contribution from the Coulomb interaction is larger than that in the two-electron case. With increasing magnetic field, the higher energy state will become, due to the Coulomb interaction, energetically favorable to be the ground state. The crossing (but not the singlet–triplet crossing) which is also found by other groups [11] occurs and results in a change of sign of $B \approx 2T$ (the solid and dotted lines in Fig. 3). The crossing behavior also causes the appearance of discontinuities of the absorption spectra (the thick branch at $B \approx 2T$). From Fig. 3 it is also clear that the magnitude of $J$ for the two-electron case is larger than that for the three- and four-electron cases.

To further illustrate the unique behavior of the two-electron case, we take a closer look at $B = 0$. As shown in Fig. 4, the exchange energy depends on $V_b$. At $V_b = 0$, the system is a single QD. The first excited states are three-fold degenerate with finite energy level separation from the ground state, i.e., the exchange energy is $\sim 0.27$ meV. With increasing $V_b$ the energy level separation becomes smaller. The system forms a double QD. At large values of $V_b (> 10$ meV), the system is a double QD and has a vanishing exchange energy. The first excited states eventually merge with the ground state at a rate that is hyper-exponentially dependent on $V_b$. The ground state is now four-fold degenerate which is uniquely present at $B = 0$. In addition, at large values of $V_b$ the system is now in a very favorable state to accommodate two electrons. Each electron is in one of the two nearly isolated dots and experiences a seemingly circular symmetry.

Unlike for the parabolic confinement and the self-consistent numerical confinement [8], an exponential dependence of the exchange energy, as seen in the experiments [12], is clearly exhibited in our GDQD. The hyper-exponential behavior of the exchange energy allows a fast control of the degeneracy of the ground state, i.e., control the separation between the ground state (singlet) and the first excited states (triplet). The gate voltage controlled singlet–triplet separation is also called the singlet–triplet splitting. This splitting can be used to switch the spin states. The way it has been demonstrated in the experiments [12]. The computer terminology for the operation which converts $|\uparrow\downarrow\rangle$ to $|\uparrow\uparrow\rangle$, is a SWAP. In Ref. [12], a proposal to measure the coherent control of two-electron spin states in a double QD has been put forward. The technique is based on the electrical control of the exchange interaction. In our model, such a control of the singlet–triplet splitting can be achieved by controlling the barrier height. The SWAP can then be performed in three steps: first, we consider the $V_b$ to be small or zero. The system is then in the spin-singlet ground state (2)$S$ (we follow the convention of Ref. [12], where $(m)$ and $(m,n)$ indicate the number of electrons in a single dot or a double dot, respectively). The corresponding triplet states (2)$T$ are energetically inaccessible, being $\sim 2$ meV above (2)$S$ are ignored in the following discussion. The inset in Fig. 4 shows the energy level separation of the first two excited states as a function of $V_b$. Second, we tune $V_b$ to be large such that a double-well potential is formed with a weak interdot tunnelling and (1,1) is the new ground state. Here, one singlet (1,1)$S$ is degenerate with the three triplet (1,1)$T$ states. The separated electrons would then hop about the degenerate states and as a result there will be a fast mixing of the (1,1)$S$ and (1,1)$T$ states. Third, the central barrier is depressed to make (2)$S$ again the ground state. Then (1,1)$S$ states evolve into the (2)$S$ state. However, due to spin selection rules, only (1,1)$S$ can tunnel to (2)$S$ while the (1,1)$T$ to (2)$S$ transitions are blocked. These steps complete the SWAP process. Most importantly, the exponential behavior of the exchange energy, as found in our model, would allow this operation, as proposed in the experiments [12].

In conclusion, we have evaluated very accurately the energy levels of a Gaussian double QD by using the exact diagonalization method. Contrary to all the earlier reported results, we observe that for the two-electron case

![Fig. 3. Exchange energy $J = E_1 - E_0$ as a function of a magnetic field with the values taken from Fig. 2.](image1)

![Fig. 4. The hyper-exponential dependence of the exchange energy versus the Gaussian parameter $V_b$, in the absence of a magnetic field for the two-electron system.](image2)
the singlet–triplet crossing (due to electron correlations only) is absent. Without the antiferromagnetic/ferromagnetic transition, only the electrical control of a quantum gate and the coherent manipulation of two electron spins are applicable. In our model, the barrier potential can be used to tune a double QD. An exponential dependence of the exchange energy facilitates the changes of the degeneracy of the ground state, i.e., the singlet–triplet splitting. In addition to be of fundamental interest, such a tunable double QD can be used as a quantum gate device with the novel properties of the exchange energy found here. For example, a computer operation, the spin SWAP, is achievable using the voltage-controlled exchange as demonstrated in recent experiments [12]. A gate voltage controlled double QD can also efficiently generate entanglement, which makes the quantum computing more faster or secure [13].

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