Spin hot spots in vertically coupled few-electron isolated quantum dots

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The effects of spin-orbit (SO) coupling arising from the confinement potential in single and two vertically coupled quantum dots have been investigated. Our work indicates that a dot containing a single electron shows the lifting of the degeneracy of dipole-allowed transitions at \( B = 0 \) due to the SO coupling which disappears for a dot containing two electrons. For coupled dots with one electron in each dot, the optical spectra is not affected by the coupling and is the same as the dot containing one electron. However, for the case of two coupled dots where one partner dot has two interacting electrons while the other dot has only one electron, a remarkable effect is observed where the oscillator strength of two out of four dipole-allowed transition lines disappear as the distance between the dots is decreased.

Interest in spin properties of semiconductor nanostructures has increased significantly in recent years due to the exciting possibility to manipulate it in solid state devices. The role of spin-orbit (SO) coupling in nanostructured systems is important in this context because this coupling would provide a means to influence the spin states via the orbital degrees of freedom. Quantum dots (QDs) are particularly promising systems for these studies as the electron spin states are very stable in these zero-dimensional systems and are measurable.

In quantum dots, spin hot spots are composed of two or more states that are degenerate in the absence of the SO coupling but the degeneracy is lifted due to the SO coupling. The importance of these hot spots lies in the fact that this lifting of degeneracy allows mixing of the spin-up and spin-down states and opens up the possibility for spin-flip transitions in the presence of the SO coupling. Recent studies have indicated that for laterally coupled quantum dots, there is no contribution of the Bychkov-Rashba SO potential to the spin hot spots at zero magnetic field.

We have explored the spin hot spots in vertically coupled quantum dots where they are readily identifiable and reflect interesting physical properties in the presence of SO coupling through the low-lying energy levels as well as in the dipole-allowed optical absorption spectra. To be specific, we have studied the effect of Bychkov-Rashba SO coupling in the optical transition spectra and the energy levels of two parabolic dots placed vertically and interacting only through the Coulomb interaction. We assume the dots to be isolated in the sense that there is no tunneling between the dots. Interestingly, the zero-field spin hot spots in our vertically coupled QDs manifests in the dipole transition energies. For coupled QDs with one dot containing two electrons while the other with a single electron, the SO effect strongly depends on the interdot separation. It should be pointed out that a vast literature exists on the electronic properties of vertically coupled quantum dots, but without any spin-orbit interaction included. The interest on the role of SO coupling in coupled quantum dots has reached its peak recently due to its importance in quantum information processing.

We begin with the low-lying energy levels and the transition energies of a single electron in a vertically coupled parabolic quantum dot in the presence of a SO coupling. From the Dirac equation we know that whenever a spin-half particle with charge \( q \) moves under the four-potential \( (\vec{A}, \phi) \) the lowest-order relativistic correction leads to the SO potential \( V_{\text{SO}} \) of the form

\[
V_{\text{SO}} = \frac{q \hbar}{4 m^* c^2} \mathbf{\nabla} \phi(\vec{r}) \cdot \mathbf{\sigma} \left( \frac{\vec{p}}{c} - \frac{q}{c} \vec{A}(\vec{r}) \right)
\]

\[
= -\frac{q \hbar}{4 m^* c^2} \vec{E}(\vec{r}) \cdot \mathbf{\sigma} \left( \vec{p} - \frac{q}{c} \vec{A}(\vec{r}) \right).
\]

In quantum dots the electric field can arise, for example, from the inversion asymmetry of the potential restricting the motion of the electrons (charge \( e < 0 \) and effective mass \( m^* \)) to a two-dimensional plane. Then the electric field would be perpendicular to the plane of the motion. Furthermore, since we may well assume the field to be nearly homogenous within the range of the electron wave functions it can be replaced to a good approximation with its average value. It is also customary to collect all the parameters including the average of the electric field into a single coupling constant \( \beta \) leading to the familiar Bychkov-Rashba potential

\[
V_{\text{SOI}} = \beta \left[ \mathbf{\sigma} \left( \vec{p} - \frac{e}{c} \vec{A}(\vec{r}) \right) \right]_z.
\]

for the SO coupling due to the inversion asymmetry.

Another source for the electric field in the quantum dot is of course the potential \( V_c \) that confines the electrons into the dot in the two-dimensional plane. The field \( \vec{E} \) now lies in the plane of motion and, if the confinement is rotationally symmetric it will be parallel to the radius vector \( \vec{r} = (x, y) \). It is easy to see that the SO coupling can now be written as

\[
V_{\text{SOC}} = \frac{\alpha}{\hbar} \frac{d V_c(\vec{r})}{d \theta} \left( p_\theta - \frac{e}{c} A_\phi(\vec{r}) \right),
\]

where \( p_\theta \) and \( A_\phi \) stand for the angular components of the momentum and the vector potential, and where most of the parameters are combined to the Bychkov-Rashba spin-orbit coupling parameter, \( \alpha = -q \hbar^2/4 m^* c^2 \). As compared to the
V_{SO} we see two essential differences in V_{SOC}. First, the coupling depends on the position, in particular in the case of the parabolic confinement \( V_c = \frac{1}{2} m^* \omega_c^2 r^2 \) it will be proportional to \( \omega_c^2 r \). Second, it is diagonal in spin space and, consequently \( S_z \) is a good quantum number, a fact that will be utilized throughout this work. From our point of view this latter property makes it very attractive because it allows us to find analytic solutions for the single-particle problem. It should be noted, however that in order to see the effects arising from the confinement-induced SO coupling \( V_{SOC} \), the confinement itself must be rather large. Typically, \( \hbar \omega_0 \) must be of the order of \( 10-20 \) meV. \(^{11}\)

The Hamiltonian describing our coupled-dot system is given by

\[
\mathcal{H} = \sum_i \mathcal{H}^o_i + \sum_{i<j} \frac{\epsilon^2}{i^2 + j^2 + d^2},
\]

where \( d \) is interdot separation (in units of magnetic length \( \ell_B \)), \( \mathcal{H}_i^o \) is the Hamiltonian governing a single electron confined in a parabolic quantum dot\(^{9,9}\) and is given by

\[
\mathcal{H}_i^o = \mathcal{H}^o + \mathcal{H}_{so},
\]

\[
\mathcal{H}^o = \frac{1}{2m} \left( \hat{p}^2 + \frac{e}{c} \mathbf{A} \right)^2 + \frac{1}{2} \sigma \mu_B g_B B + \frac{1}{2} m^* \omega_c^2 r^2,
\]

\[
\mathcal{H}_{so} = \sigma_z \alpha \frac{dV_c(r)}{dr} \left( k^2 + \frac{e}{2\hbar} Br \right) = \sigma_z \alpha \left( m \omega_c^2 r \right) \left( k^2 + \frac{e}{2\hbar} Br \right),
\]

where \( \sigma \) is the Pauli \( z \) matrix. It is to be noted that the first term of \( \mathcal{H}_{so} \) is independent of the external magnetic field \( B \). At \( B=0 \) it lifts the spin degeneracy because of the magnetic field originating from the orbital motion of the electron in the presence of electric field coming from the confinement potential. \(^{11}\)

The energy eigenfunctions are then given by

\[
\psi_{n, \ell, \sigma} = \frac{1}{\sqrt{2}} \exp(i \ell \phi) R_{n, \ell, \sigma}(r),
\]

where

\[
R_{n, \ell, \sigma}(r) = \sqrt{\frac{2}{\ell + 1}} \frac{1}{(n + |\ell|)!} \exp\left(-\frac{\ell^2}{2 \sigma^2} \right) \times \left( \frac{\ell^2}{\sigma^2} \right)^{|\ell|/2} L_n^{|\ell|} \left( \frac{\ell^2}{\sigma^2} \right),
\]

where \( r_s = (\hbar / m^* \Omega_\sigma)^{1/2} \) and \( L_n^{|\ell|} \) is the generalized Laguerre polynomial.

The corresponding electron energy levels are

\[
E_{n, \ell, \sigma} = \hbar \Omega_\sigma (2n + |\ell| + 1) + \ell \frac{\hbar \omega_c}{2} + \sigma \left( \frac{\mu_B}{2} g_B + \ell \alpha m^* \omega_c^2 \right),
\]

where

\[
\Omega_\sigma^2 = \omega_c^2 + \frac{\omega_c^2(B)}{4} + \sigma \alpha m^* \omega_c^2 / \hbar \omega_c.
\]

Fig. 1. The (a) dipole transition energies and (b) a few low-lying energy levels of the single-electron energy spectrum of a single quantum dot in the presence of the SO coupling. The states are labeled as \( (\ell, \sigma) \) where \( \ell \) and \( \sigma \) denote the orbital and spin quantum numbers, respectively. The spin-up and spin-down projections are denoted by 1 and \( -1 \), respectively. At \( B=0 \), the degeneracy (without the SO coupling) is lifted making the states involved as spin hot spots. The states with antiparallel \( \ell \) and spin are lower in energy.

and \( \omega_c \) is the cyclotron frequency. Clearly, the SO coupling influences \( \Omega_\sigma \) [Eqs. (3) and (2)] which results in an increase of the energy of the up-spin and a decrease in energy of the down-spin. Another effect due to the SO coupling is from the last term of Eq. (2) which is independent of an external magnetic field. As mentioned earlier, at \( B=0 \) it lifts the spin degeneracy of the states with the same orbital momentum. The energy of the states with antiparallel spin and \( \ell \) is lowered while the states with the parallel \( \ell \) and spin show an increase in energy at \( B=0 \). The Coulomb energy is evaluated by the exact diagonalization method, that is well established in the literature,\(^{5,8,10}\) in particular, for the case of parabolic quantum dots.

The dipole-allowed transition energies of a single parabolic dot in the presence of the SO coupling are presented in Fig. 1(a) while the energy eigenvalues are presented in Fig. 1(b). In all our calculations, the material parameters are for the InAs dots as listed in Ref. 11. Transitions take place from the \( |\ell=0, \uparrow\rangle \) state to \( |\ell=1, \uparrow\rangle \) and \( |\ell=-1, \downarrow\rangle \) states. These two transitions are not degenerate at \( B=0 \) because of the SO coupling: \( |\ell=1, \uparrow\rangle \) has lower energy than that of \( |\ell=-1, \downarrow\rangle \) [Fig. 1(b)]. It is interesting to note that this splitting between the \( L=+1 \) and \( L=-1 \) branches at \( B=0 \) disappears if the dot contains two electrons [Fig. 2(a)]. In the energy spectrum of a two-electron dot [Fig. 2(b)], the lowest line represents a two-electron state where the electrons occupy \( |0, \uparrow\rangle \) and \( |0, \downarrow\rangle \) states. In order to understand the degeneracy of the \( L=+1 \) and \( L=-1 \) branches at \( B=0 \), let us look at the states involved in the transition to (say) the \( L=+1 \) branch. In this case, any
of the two electrons occupying \( |0 \uparrow \rangle \) and \( |0 \downarrow \rangle \) states can be excited: the electron is excited either from \( |0 \uparrow \rangle \) to \( |1 \uparrow \rangle \) or from \( |0 \downarrow \rangle \) to the \( |1 \downarrow \rangle \) state. Due to the SO interaction, the excitation energies are not degenerate at \( B=0 \). Since there are now two electrons, the Coulomb interaction between them mixes the \( |1 \uparrow \rangle \) and \( |1 \downarrow \rangle \) states. The eigenstate is a combination of \( |1 \uparrow \rangle \) and \( |1 \downarrow \rangle \) states due to the Coulomb interaction. Similarly, the \( L=-1 \) transition can occur in two ways: the electron can either jump from \( |0 \uparrow \rangle \) to the \( |1 \downarrow \rangle \) state or from \( |0 \downarrow \rangle \) to the \( |1 \uparrow \rangle \) state. Again, these two possibilities for \( L=-1 \) are not degenerate at \( B=0 \) but due to the Coulomb interaction the eigenstate is a combination of these two alternatives. However, the state \( |−1 \uparrow \rangle \) is degenerate at \( B=0 \) with \( |1 \downarrow \rangle \) and so are the states \( |−1 \downarrow \rangle \) and \( |1 \uparrow \rangle \) [Fig. 2(b)]. Therefore, we do not observe a splitting at \( B=0 \) between the \( L=+1 \) and \( L=−1 \) branches in the optical spectra of a dot containing two interacting electrons.

The results for two quantum dots each containing one electron and are vertically coupled (via only the Coulomb interaction) are displayed in Fig. 3. For a large separation of the dots (e.g., \( d=9.5 \ell_B \)), the transition energies, quite expect-edly, resemble those of a single dot with one electron [Fig. 1(a)]. As the dots are brought closer, the interdot interaction becomes stronger but that modifies only the energy spectrum, leaving the optical spectra unchanged [Fig. 3(a)]. Figure 3(b) shows the low-lying energy levels for two dots at a separation of \( d=0.5 \ell_B \). An electron in the ground state \( |0 \uparrow \rangle \) in any of the two dots can make a transition to \( |1 \downarrow \rangle \) state. There are now two states corresponding to \( L=\ell_{D1}+\ell_{D2}=1, S=s_{D1}+s_{D2} \) where \( \ell_{D1}, s_{D1} \) and \( \ell_{D2}, s_{D2} \) represent the quantum numbers for the first and second dot, respectively. When the interdot interaction is very weak, the two states \( (\ell_{D1}=1, \ell_{D2}=0) \) and \( (\ell_{D1}=0, \ell_{D2}=1) \) are degenerate. However, as the separation between the dots is decreased, the Coulomb interaction lifts the degeneracy between the two eigenstates (which are a linear combination of the above two states). For \( L=−1 \), we similarly have two levels. However, the oscillator strength of the lower state is nearly zero and the transition takes place only to the higher state. Therefore, there are only two lines (for \( L=±1 \)) in the optical spectra for all distances between the two dots [Fig. 3(a)].

The most interesting situation is found to occur when one dot has a single electron while the other dot contains two electrons. Figure 4 shows the transition energies of the two dots for two different values of the interdot separation: (a) \( d=0.5 \ell_B \) and (b) \( d=9.5 \ell_B \). For a large separation of the dots \( (d=9.5 \ell_B) \), there are four lines as a function of the magnetic field [Fig. 4(b)], whereas there are only two lines for a much smaller separation \( (d=0.5 \ell_B) \) [Fig. 4(a)]. This is because when the dots are far apart the uncoupled two-electron dot does not show the SO splitting between the \( L=1 \) and \( L=−1 \) branches at \( B=0 \) and as a result, there are two middle lines that are degenerate at \( B=0 \). The one-electron dot, on the other hand, shows a splitting and results in the lowest line corresponding to the \( L=−1 \) branch while the uppermost line corresponds to the \( L=1 \) branch. Hence we have two \( L=1 \) branches and two \( L=−1 \) branches for the two dots. As

![FIG. 2.](image)

FIG. 2. The (a) dipole-transition energy spectrum and (b) the few low-lying energy levels of a two-electron dot in the presence of the SO coupling. In (b) the lowest line represents the eigenvalues of the state \( L=\ell_1+\ell_2=0, S=s_1+s_2=0 \). The eigenvalues for the \( L=1 \), \( S=1,0,−1 \) states are drawn as dashed lines.

![FIG. 3.](image)

FIG. 3. The (a) transition energy spectrum and (b) the few low-lying energy levels of two vertically coupled dots separated by \( d=0.5 \ell_B \) in the presence of the SO coupling. Each dot contains a single electron. In (b), the three lowest lines correspond to the eigenvalues for the states \( L=\ell_{D1}+\ell_{D2}=0, S=s_{D1}+s_{D2}=0, ±1 \). The eigenvalues for the \( L=1 \) states are drawn as dashed lines.

![FIG. 4.](image)

FIG. 4. The transition energy spectrum of two vertically coupled dots separated by (a) \( d=0.5 \ell_B \) and (b) \( d=9.5 \ell_B \), in the presence of the SO coupling. In this case, one dot confines a single electron while the other dot contains two interacting electrons.
the distance between the dots decreases, the excited \( L=1 \) state of the two dots are coupled by the Coulomb interaction. The transition probability for the lower state decreases while it increases for the higher state. At \( d=0.5 \ell_B \) the transition to the lower state is zero and hence we have only one line corresponding to the \( L=1 \) branch and similarly one line for the \( L=-1 \) branch [Fig. 4(a)]. The result we observe here is that, unlike in the case of two coupled dots with one electron in each dot, in the present system, for a large separation, the \( L=1 \) branch coming from the two-electron dot is not degenerate with the \( L=1 \) branch coming from the one-electron dot. Therefore, one could observe the disappearance of one of the two \( L=1 \) branches (same for the two \( L=-1 \) branches) as the distance between the two dots is decreased. It should be pointed out that the \( L=1 \) branch of the dot containing two electrons is not degenerate with the \( L=1 \) branch of the dot containing a single electron because the two-electron dot does not show the SO splitting between the \( L=\pm 1 \) branches while the one-electron dot does show the splitting.

In summary, we have investigated a single parabolic QD and two vertically coupled QDs, containing one or two (interacting) electrons, in the presence of the SO coupling. For single dots, the SO interaction that we considered to be arising from the confinement potential, lifts the degeneracy of the dipole-transition energies at \( B=0 \) for a dot containing one electron. The splitting disappears for a dot containing two electrons. The lifting of the degeneracy at \( B=0 \) is also observed for two coupled QDs, each containing a single electron. In case of two coupled dots where one partner dot has two interacting electrons while the other has only one electron, the dipole transition energies show a remarkable dependence on the interdot separation. For a large separation, the spectra consist of four lines corresponding to a combination of one and two electron spectra. However, as the separation between the dots is decreased, the oscillator strength for the lower eigenstates of \( L=+1 \) and \( L=-1 \) decreases and the optical spectra contains only two lines instead of four.

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