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Charge localization and isospin blockade in vertical double quantum dots

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Charge localization seems unlikely to occur in two vertically coupled symmetric quantum dots even if a small bias voltage breaks the exact isospin-symmetry of the system. However, we find a strong localization of charges in one of the dots at certain vertically applied magnetic fields. The charge localization is directly connected to ground state transitions between eigenstates differing only in parity. The transitions are driven by magnetic-field-dependent Coulomb correlations between the electrons and give rise to strong isospin blockade signatures in transport through the double-dot system.

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Quantum dot structures are excellent systems to investigate few and many particle physics[1] due to the high experimental control over the system parameters. In this context double quantum dots are particularly interesting in two different ways: as an implementation of quantum bits (qubit)[2] and as a model system for molecular binding under controlled conditions.[3–5]

In this paper we describe a correlation effect in a vertically coupled double quantum dot (DQD) in a perpendicular magnetic field, which strongly changes the molecular binding and at the same time defines a two-level system that can be manipulated in a controlled way and could serve as a qubit. This effect is manifest in the energy spectrum and the transport properties of the DQD. Sweeping the magnetic field we find ground state (GS) crossings in a perfectly symmetric DQD which occur between states with same spin and angular momentum. In contrast to the well known crossings between states that differ in angular momentum and/or spin[6] and that affect the lateral motion and occur in single dots already, the crossing discussed here involves a transition in the parity of the GS that characterizes the vertical degree of freedom. Therefore, by slightly breaking the symmetry between the two dots, e.g., by applying an infinitesimally small voltage, the crossing turns into an anticrossing, which for an odd number of electrons results in charge localization. Due to the charge localization of the GS, transport through the DQD is strongly suppressed at the anticrossing. In analogy to the well known spin blockade[7] this strong suppression can be seen as an isospin blockade at the anticrossing with the isospin describing the vertical degree of motion.

We describe the DQD within the layer model,[6,8] which is applicable if the external potentials separate in a strong vertical and a considerably weaker lateral component. We assume the in-plane confinement for the electrons to be parabolic and circular symmetric. Additionally a magnetic field B can be applied in the vertical direction. The in-plane motion of the electrons is then described in the effective mass approximation by the Fock-Darwin-Hamiltonian[9] $\hat{H}_{\mathrm{FD}}$ and the Zeeman term $\hat{H}_Z$,

$$\hat{H}_{\mathrm{FD}} + \hat{H}_Z = \frac{1}{2m^*}(\vec{p} + e\vec{A})^2 + \frac{m^*\omega_0^2}{2}r^2 + g^*\frac{\mu_B}{\hbar}B\hat{S}_z, \qquad (1)$$

where ω_0 is the strength of the parabolic confinement, m^* is the effective mass, μ_B the Bohr magneton, and g^* the effective Landé factor.[10] The eigenstates of the in-plane motion are the Fock-Darwin states $|n,m\rangle$ with the principal quantum number $n \in \mathbb{N}$ and the angular momentum quantum number (z component) $m \in \mathbb{Z}$. The Hamiltonian (1) conserves the angular momentum $\hat{L}_z$ as well as the z component of the spin $\hat{S}_z$ and the square of the spin $\hat{S}^2$, described by m, s_z, and s, respectively.

The vertical motion is reduced to tunneling between two δ sheets, labeled by the quantum number $\alpha \in \{+,-\}$. $\alpha = \pm$ corresponds to the upper dot (+) or lower dot (−), respectively. In analogy with the real electron spin one can define a spin operator algebra, where the z component of the isospin $\hat{I}_z$ is given by α.[8]

The interdot tunneling $\hat{H}_T|\pm\rangle = t|\mp\rangle$ which transfers electrons between the two dots can be expressed by isospin operators:

$$\hat{H}_T = t\left(\hat{I}_+ + \hat{I}_-\right) = 2t\,\hat{I}_x \qquad (2)$$

with the real hopping parameter $t<0$.[6] $\hat{I}_\pm$ are the raising and lowering operators for the z component of the isospin, and $\hat{I}_x$ is its x component. The eigenstates of $\hat{I}_x$ and thus of $\hat{H}_T$ are the symmetric and antisymmetric linear combinations of the isospin eigenstates $|\pm\rangle$. Due to tunneling the electrons are delocalized and the eigenstates of the Hamiltonian $\hat{H}_{\mathrm{FD}} + \hat{H}_T + \hat{H}_Z$ are no longer eigenstates of I_z. However, in the case of symmetric dots the two layers are identical, so that the isospin-parity $\hat{P}$ is conserved. In the case of more than one electron inside the DQD, the Coulomb interaction $\hat{\mathcal{V}}_c$ between the electrons has to be included such that the few-electron Hamiltonian reads

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_{\mathrm{FD}} + \hat{\mathcal{H}}_T + \hat{\mathcal{H}}_Z + \hat{\mathcal{V}}_c = \sum_{i=1}^{N_e}\left(\hat{\mathrm{H}}_{\mathrm{FD}}^{(i)} + \hat{\mathrm{H}}_{\mathrm{T}}^{(i)} + \hat{\mathrm{H}}_{\mathrm{Z}}^{(i)}\right) + \frac{e^2}{4\pi\epsilon\epsilon_0}\sum_{i<j}\hat{V}_c^{(i,j)}. \qquad (3)$$

Since Coulomb interaction is invariant under spatial and spin rotations, total angular momentum $\hat{\mathcal{L}}_z$ and total spin $\hat{\mathcal{S}}^2, \hat{\mathcal{S}}_z$ are still conserved and are described by the quantum numbers M and S, S_z, respectively. For a symmetric DQD also the total isospin parity $\hat{P}=2^{N_e}\cdot\hat{I}_x^{(1)}\otimes\cdots\otimes\hat{I}_x^{(N_e)}$, which flips the isospins of all electrons (i.e., it moves all electron orbitals from the upper dot to the lower dot and vice versa), is conserved, described by the quantum number $P\in\{+1,-1\}$. Due to the Coulomb interaction the electrons are correlated. In a vertical double quantum dot the Coulomb interaction can be divided into two parts: $\hat{V}_c^{(i,j)}=\hat{V}_{\mathrm{intra}}^{(i,j)}+\hat{V}_{\mathrm{inter}}^{(i,j)}$. The *intradot* Coulomb interaction $\hat{V}_{\mathrm{intra}}^{(i,j)}=1/r_{ij}$ describes the interaction between electrons localized in the same dot, whereas the *interdot* Coulomb interaction $\hat{V}_{\mathrm{inter}}^{(i,j)}=1/(r_{ij}^2+d^2)^{1/2}$ describes the interaction between electrons localized in different dots. Here $r_{ij}=|\vec{r}_i-\vec{r}_j|$ is the lateral separation of two electrons i and j and d is the vertical separation between the dots. The Coulomb operator commutes with the z component of the total isospin $\hat{\mathcal{I}}_z$ but does not commute with $\hat{\mathcal{I}}_x$ and accordingly $\hat{\mathcal{H}}_{\mathrm{T}}$. The commutator between the Coulomb interaction and tunneling depends on the difference between *intradot* and *interdot* Coulomb interaction[8] and vanishes only in the limit $d\to 0$.

Increasing the vertical magnetic field effectively leads to a stronger lateral confinement of the electrons and hence to an increase of the Coulomb energy. Additionally intradot interaction increases faster with increasing magnetic field than the interdot interaction, which is limited to $1/d$.[6] This different scaling causes magnetic-field-dependent correlations in the eigenstates. We show that this can lead to a GS crossing to fixed M,S,S_z for symmetric DQDs and charge polarization in slightly asymmetric dots.

To take correlations into account we compute the eigenstates and the corresponding eigenenergies by numerically diagonalizing the many-body Hamiltonian (3), i.e., we expand the eigenstates in a finite basis of Slater determinants.[11]

In the following we discuss calculations of the eigenspectrum in a three-electron DQD for a particular set of external parameters, where a slight asymmetry causes charge localization in a small magnetic field window whereas the GS is nearly unpolarized for different magnetic fields. However, we want to point out that this effect is general and that it exists for different parameters and subsets of quantum numbers as well as for different electron numbers in the DQD.

Calculating the magnetic-field dependence of the energy spectrum for three electrons inside a symmetric DQD to angular momentum $M=-5$ and spin $S=S_z=3/2$, we find a crossing between the two energetically lowest states as illustrated in Fig. 1. Since the crossing states only differ in parity, the accidental crossing converts into an anticrossing if the parity conservation is broken by a slight asymmetry between the dots leading to two strongly charge-polarized states. For specific parameters the parity crossing and hence the charge polarization found for this subspace of quantum numbers becomes visible in the GS as illustrated in Fig. 2. The asymmetry between the dots can be either intrinsic or caused by a small bias voltage, as it is applied in transport experiments.[12] We model the asymmetry between the dots by adding the term $\hat{\mathcal{V}}_z=V_z\cdot\hat{\mathcal{I}}_z$ to the Hamiltonian (3), where V_z is the energy difference between upper and lower dot for a single electron. While the GS is nearly unpolarized for general magnetic field strengths, Fig. 2 shows a strongly polarized GS at the magnetic field where the anticrossing occurs. The minimal value of $\langle\mathcal{I}_z\rangle=-0.5$ corresponds to two electron charges in the lower dot and one in the upper. Thus we find the astonishing effect that electrons become localized in one of the dots by simply changing the vertical magnetic field. It is important to note that the strength of the asymmetry (i.e., V_z) only determines the width of the localization dip in Fig. 2 but even for arbitrarily small asymmetries the GS is strongly polarized at the anticrossing with $\langle\mathcal{I}_z\rangle=-0.5$. Since $[\hat{\mathcal{L}}_z,\hat{\mathcal{V}}_z]=[\hat{\mathcal{S}}^2,\hat{\mathcal{V}}_z]=[\hat{\mathcal{S}}_z,\hat{\mathcal{V}}_z]=0$, $\hat{\mathcal{V}}_z$ couples only states with same total angular momentum and total spin. Therefore a similar effect does not occur in the well known GS crossing between states that differ in M and/or S[6].

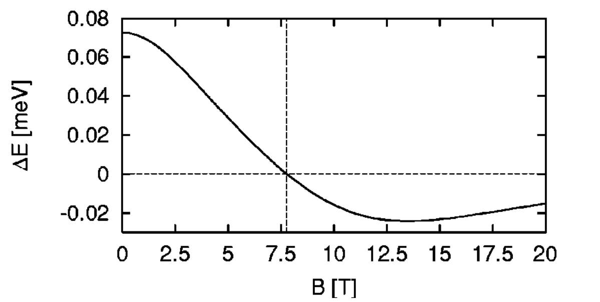

FIG. 1. Energy difference of the lowest two eigenstates to $\hat{\mathcal{H}}(M=-5$ and $S=S_z=3/2)$ as a function of the magnetic field B. $t=-0.059$ meV, $\hbar\omega_0=2.96$ meV, and $d=19.6$ nm. The crossing takes place at $B=7.77$ T (dashed vertical line).

In the following we study the reported parity crossing in the GS of a symmetric DQD in more detail. Without tunneling I_z is conserved and since both dots are identical the GS will be twofold degenerate with $I_z=\pm 0.5$. Switching on tunneling their degeneracy is lifted and the GS splits in two nondegenerate parity eigenstates $|P=\pm 1\rangle$ because of their different occupations of symmetric and antisymmetric orbitals. In particular Fig. 1 illustrates that for magnetic fields $B<7.8$ T the state $|P=-1\rangle$ is favored by tunneling, i.e., it has a higher occupation of symmetric orbitals than $|P=+1\rangle$. However, due to magnetic-field-dependent correlations the occupation of symmetric orbitals decreases for $|P=-1\rangle$ but

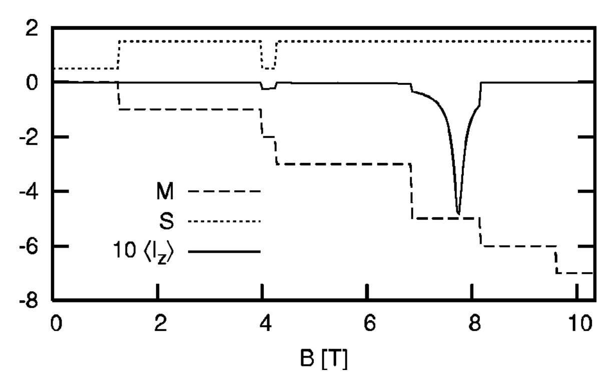

FIG. 2. Angular momentum M, total spin S, and expectation value of the z component of isospin $\langle\mathcal{I}_z\rangle$ for three electron GS to $\hat{\mathcal{H}}+\hat{\mathcal{V}}_z$. $\hat{\mathcal{V}}_z=5.9\times 10^{-4}\hat{\mathcal{I}}_z$ meV. The peak in $\langle\hat{\mathcal{I}}_z\rangle$ illustrates the charge localization that corresponds to the parity crossing (see text). Other parameters are as in Fig. 1.

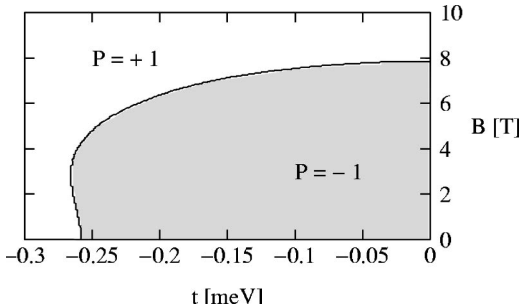

FIG. 3. Dependence of parity P for $M=-5$ and $S=3/2$ on magnetic field B and tunneling t. The solid line indicates where the crossing between the parity eigenstates takes place. Other parameters are as in Fig. 1.

increases for $|P=+1\rangle$, so that by increasing the magnetic field finally $|P=+1\rangle$ becomes the GS. Figure 3 shows the parity as a function of tunneling and external magnetic field for the subspace $M=-5$ and spin $S=S_z=3/2$. The crossing exists from zero tunneling up to $t\approx 0.27$ meV, which suggests to treat the tunneling t as a small perturbation. For small tunneling (tunneling much smaller than the energy spacing between degenerate GS and first excited state at $t=0$) the parity eigenstates are to first-order perturbation theory given by $|P=\pm 1\rangle \approx (|I_z=\frac{1}{2}\rangle \pm |I_z=-\frac{1}{2}\rangle)/\sqrt{2}$ and their energy splitting is $2\langle I_z=\frac{1}{2}|\hat{\mathcal{H}}_{\mathrm{T}}|I_z=-\frac{1}{2}\rangle(B)$. As indicated this matrix element depends on the magnetic field due to the magnetic-field-dependent correlations present in the states $|I_z=\pm\frac{1}{2}\rangle$. To first order the crossing occurs at $B=7.85$ T where the matrix element vanishes, and is independent of t in good agreement with the exact results for small tunneling (see Fig. 3). For strong tunneling, however, higher-order effects (coupling to higher states) come into play causing the crossing to disappear for $t>0.27$ meV. Breaking the vertical symmetry of the DQD the two parity eigenstates are coupled and the parity crossing converts into an anticrossing, thereby lifting their accidental degeneracy by an amount V_z. At the anticrossing the eigenstates are approximately given by $I_z=\pm\frac{1}{2}$ and are thus strongly charge polarized. We want to note that the parity crossing and the related strong charge polarization is not restricted to the total angular momentum and total spin chosen here but also occurs for other sets of quantum numbers. Furthermore, a symmetric DQD containing any odd number of electrons has a degenerate GS at $t=0$ and similar parity crossings occur for higher odd numbers of electrons in the DQD. The GS of an even number of electrons at $t=0$ has $I_z=0$ and is nondegenerate, so that the parity crossings also found for an even number of electrons do not lead to strong charge localization in the presence of arbitrarily small asymmetry.

The polarization of the three-electron GS can be detected in a transport experiment through the DQD.[4,5,12,13] If a small transport voltage, V_{SD}, across the DQD is applied[14] at constant magnetic field, the conductance G has a peak structure as a function of the gate voltage. The height of the conductance peaks G^{peak} corresponding to the transitions between two and three electrons or three and four electrons inside the DQD are shown as a function of the magnetic field and for two different constant temperatures in Fig. 4. A comparison with Fig. 2 shows that the current through the DQD is suppressed at the magnetic field, where the three-electron GS becomes polarized. We want to point out that since the asymmetry between the dots is weak only the two lowest three-electron states are polarized (in opposite direction) whereas the other states and in particular the two and four electron GS are unpolarized (in contrast to Ref. 5). In our calculations we assume that transport is described by sequential tunneling processes in and out of the many-particle eigenstates of the isolated DQD.[15] This is a good approximation for weak tunnel contacts between the reservoirs and the DQD, i.e., the tunneling strength to the external reservoirs is smaller than the interdot tunneling and the finite lifetime broadening of the DQD states is smaller than temperature.[16] For the tunneling events a transition rate can be calculated, which we call $T^{+}(T^{-})$ for a transition caused by a tunneling event through the upper (lower) barrier. In the following we discuss the transition between two and three electrons in the dot, but the arguments are equally valid also for the next conductance peak.

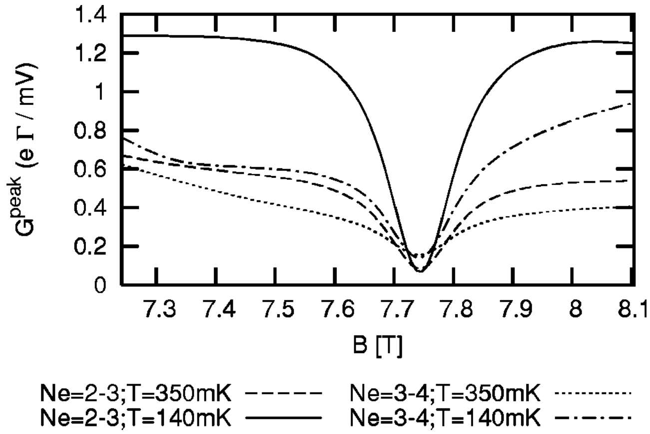

FIG. 4. Height of the third and fourth conductance peaks (transition from $N_e=2$ to $N_e=3$ or from $N_e=3$ to $N_e=4$) as a function of B for two temperatures and $V_{sd}=12\ \mu$V. $\Gamma=\mathrm{DOS}|T|^2(2\pi/\hbar)$ determines the coupling to the external reservoirs, where DOS is the density of states in the reservoirs and T denotes the tunnel matrix elements to the reservoirs. Other parameters are as in Figs. 1 and 2. In particular the asymmetry between the lower and upper dot $V_z=10^{-2}|t|\approx 0.6\ \mu$eV.

Assuming that an electron in the upper (lower) reservoir can only tunnel into the upper (lower) dot (in contrast to Ref. 15), the transition rate T^{+} between a two-particle state and a three-particle state is proportional to the spectral weight $T^{+}_{N_e=3\rightarrow N_e=2}\propto\sum_{n,m,\sigma}|\langle N_e=2|d_{nm+\sigma}|N_e=3\rangle|^2$,[17] where $d_{nm+\sigma}$ denotes the annihilation operator for the orbital $|nm+\sigma\rangle$ in the upper dot,[11] similarly $T^{-}_{N_e=3\rightarrow N_e=2}\propto\sum_{n,m,\sigma}|\langle N_e=2|d_{nm-\sigma}|N_e=3\rangle|^2$. Due to the small transport voltage only the two transport channels that include the unpolarized two-electron GS and one of the polarized three-electron states (GS and first excited state) lie within the transport window. Higher channels only contribute due to the finite temperature and can be further suppressed by lowering the temperature. For both transport channels that include polarized three-electron states one of the transition rates either for the tunneling in or tunneling out process is isospin blocked. $T^{-}(T^{+})$ is suppressed if the three-electron state has two electrons localized in the upper (lower) dot. For a current to flow through the DQD both tunneling processes are necessary, which is expressed by the effective tunneling rate proportional to $(T^{-}T^{+})/(T^{-}+T^{+})$.[18] Therefore, the current is strongly reduced due to an isospin blockade of both channels. Away from the crossing the three-electron states are no longer polarized so that the transition through both barriers is possible.

We conclude as follows. Magnetic-field-dependent Coulomb correlations affect the eigenstates' tunneling energies differently, depending on their parity leading to additional magnetic-field-induced level crossings between states with different parity but same angular momentum and spin in a perfectly symmetric DQD. In symmetry-broken DQDs with an odd number of electrons the anticrossing of two eigenstates with different parity leads to a magnetic-field-dependent charge polarization. The charge polarization also takes place in the GS (as presented in this paper for $N_e=3$ electrons) and is detectable in a transport experiment through the DQD as it leads to an isospin blockade at the magnetic field where the polarization occurs. The resulting polarized eigenstates $|\frac{1}{2}\rangle$ and $|-\frac{1}{2}\rangle$ can be seen as a qubit that can be switched by the applied bias voltage. A controlled superposition of the two states can then be achieved by adjusting the magnetic field.

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