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# Single-electron tunnelling in two vertically coupled quantum dots 

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#### Abstract

Electron states in two vertically coupled quantum dots are analysed using an exactdiagonalization method. In the two-electron system, the ground state at zero field is a spin-singlet state, and this state is eventually replaced by spin-triplet states by applying a vertical magnetic field. One of the triplet states is stable under the conditions of very weak coupling and larger asymmetry between the two dots. In the transition from the three- to the four-electron state, we find a parameter region where the tunnelling current is strongly suppressed because of the orthogonality of the quantum states. An isospin selection rule is effective under strong-coupling conditions.


## 1. Introduction

The atom-like properties of a single quantum dot confined in a double-barrier heterostructure have been studied by measuring Coulomb oscillations (COs) in the tunnelling current as a function of the Schottky gate voltage [1]. The separation between the CO peaks reflects a 'shell structure' and 'Hund's rule' originating from the degenerate set of single-electron levels of the system with a cylindrical symmetry. Moreover, CO peaks shift in a magnetic field and clearly show transitions in the many-electron ground states (GSs) because of the competition of kinetic energy and intra-dot Coulomb energy evolving with the magnetic field. A system of two such quantum dots coupled face to face is especially interesting since we can control two other energies, namely, an inter-dot quantum mechanical coupling energy and an inter-dot Coulomb energy, while maintaining the cylindrical symmetry. The two vertically coupled quantum dots (TVCQDs) can be considered as an artificial molecule [2] if the coupling to the contacts is much smaller than the inter-dot coupling energy. Such coupled-dot systems are also interesting in that they can represent the few-electron analogue of a system of coupled, parallel two-dimensional electrons.

The system of coupled dots was first studied in a lateral configuration (by partly depleting a two-dimensional electron gas with surface gates or by ion implantation) [3-5], and resonant current peaks, electrostatic couplings of the two dots, and photon-assisted tunnelling have been demonstrated. Detailed analysis of the CO peaks shows splitting depending on the centralbarrier conductance $[6,7]$. This has been done for relatively large coupled-dot systems as in reference [3], where the single-particle level structure can be neglected. Recently, several experiments had been conducted on TVCQDs using a triple-barrier heterostructure [8, 9]. In reference [8], single-particle energy levels of only one of the dots were observed since the confined levels of the two dots were almost out of resonance, whereas the system of
reference [9] is ideal for studying an artificial molecule, since current was observed near zero bias when using InGaAs as a well material, and the relative energy offset of the dots with respect to the contact was controlled by a gate contact. The following discussion assumes the system of reference [9].

There are four important energy scales in this system, namely, the intra-dot Coulomb energy

$$
E_{\text {intra }} \sim e^{2} /\left(4 \pi \epsilon^{*} l_{0}\right)
$$

where $l_{0}$ is the typical lateral size of the dot and $\epsilon^{*}$ is a dielectric constant of the material, the lateral confinement energy $\hbar \omega_{0}$ (which is assumed for simplicity to be the same for the two dots), the energy difference between the symmetric and antisymmetric states, $\Delta_{\mathrm{SAS}}$, due to the inter-dot quantum mechanical coupling of the otherwise nearly degenerate energy levels in the two dots, and finally the inter-dot Coulomb energy given by

$$
E_{\text {inter }} \sim e^{2} /\left(4 \pi \epsilon^{*} \sqrt{l_{0}^{2}+d^{2}}\right)
$$

where $d$ is the separation of the two dots. The level width $\Gamma$ given by the tunnelling to the contacts is much smaller than the other energies. The energy misalignment of the two dots, $\delta$, may also be included by assuming realistic experimental conditions, namely, a small difference in the well thickness or a fluctuation of the In mole fraction in the InGaAs wells [10]. The cylindrical symmetry-breaking potential induced by the in-plane fluctuation of $5 \%$ of the In atoms is negligible since the envelope function spreads over a much longer scale.

Experimentally, $\Delta_{\mathrm{SAS}}$ and $E_{\text {inter }}$ are controlled by appropriately designing the centralbarrier thickness $d$ and its height. If $\Delta_{\text {SAS }}$ is the largest among these energies, TVCQDs are nothing more than a thick single dot in the few-electron regime, which has been demonstrated using CO peak characteristics for $d=2.5 \mathrm{~nm}$ TVCQDs in reference [9]. If $d$ becomes small, the two energies $E_{\text {intra }}$ and $E_{\text {inter }}$ become comparable and there emerges an interesting situation where isospin becomes a good quantum number and $\Delta_{\text {SAS }}$ is an effective magnetic field for an isospin [11]. In this case, the occupation of an electron in one of the dots corresponds to an isospin-down state, while the occupation in the other dot corresponds to an isospin-up state (equivalently, the occupation of an electron in a symmetric state corresponds to a rotated isospin-down state, while the occupation in an antisymmetric state corresponds to a rotated isospin-up state). On the other hand, if $d$ becomes large and $E_{\text {intra }} \gg E_{\text {inter }}, E_{\text {inter }}$ can be treated as a small perturbation to the two separated dots [12, 13]. In reference [9] with $d=7.5 \mathrm{~nm}$, the experimental results strongly suggest that the CO peaks originated from the process of tunnelling into a state localized in one of the two dots. The case where $\Delta_{\mathrm{SAS}}$ is comparable to or smaller than $\hbar \omega_{0}$ is quite interesting, since correlation effects become important in the complicated level degeneracy as in a single dot under a large magnetic field. This electron correlation also strongly affects the tunnelling current [14-16]. Therefore, a full understanding of all of the regimes determined by these four energy scales is quite important.

There have been several theoretical studies on such a system [11, 17-22], although no systematic study seems to have been conducted yet. This work generalizes the Hamiltonian, treats the interaction effect by an exact-diagonalization method, and explores the states in different regimes. Special emphasis is put on the tunnelling characteristics at low temperatures, but not below the Kondo temperature. Extension of our work to higher temperature is straightforward.

This paper is organized as follows. Section 2 describes our model of the system, and the $N$-electron Hamiltonian is defined; then in section 3 the results for TVCQDs with $N=2$ are presented. Then the results are discussed with isospin representations. Section 4 discusses the phase diagrams and several mechanisms controlling the tunnelling currents of TVCQDs with $N=3$ and 4 , and conclusions follow in section 5 .

## 2. The model of the system

The model of the TVCQDs is shown schematically in figure 1. The lateral confining potential is parabolic with a frequency $\omega_{0}$, and the vertical ( $z$-direction) confining potential is formed by a triple-barrier heterostructure [9]. The rectangular wells with thickness $W$ are separated by a central barrier with thickness $d$. The well thickness $W$ is assumed to be much smaller than any other length scales, i.e. an effective Bohr radius and the wave function spreading in the lateral direction

$$
l_{0}=\sqrt{\hbar /\left(m^{*} \omega_{0}\right)}
$$

where $m^{*}$ is an effective mass; hence, only the lowest state in the $z$-direction is taken into account, and the effects of the excited states are neglected. If the quantum mechanical tunnelling through the central barrier is negligible, we have two independent sets of states, $\Psi_{n m \mathrm{U}}(\rho, \phi, z)$ and $\Psi_{n m \mathrm{~L}}(\rho, \phi, z)$ where $n, m$ are the radial and the angular quantum numbers of the parabolically confined states in the $x-y$ plane ( $n=0,1,2, \ldots$ and $m=0, \pm 1, \pm 2, \ldots$ ) and $U$ and $L$ mean upper and lower dots, respectively. The confinement energy and the wave function in the $z$-direction are $E_{z \mathrm{U}}, E_{z \mathrm{~L}}$ and

$$
\zeta_{\mathrm{U} / \mathrm{L}}(z)=\sqrt{\frac{2}{W}} \sin \frac{\pi}{W}\left(z \pm\left(W+\frac{d}{2}\right)\right) \quad \text { for } \frac{d}{2}<|z|<W+\frac{d}{2}
$$

A magnetic field $B$ is applied in the $z$-direction, and the lateral confinement energy of the [ $n, m$ ] Darwin-Fock state is

$$
\begin{equation*}
E_{n m}=(2 n+|m|+1) \hbar \Omega-\frac{m \hbar \omega_{c}}{2} \tag{1}
\end{equation*}
$$

where $\omega_{c}$ is the cyclotron frequency given by $e B / m^{*}$, and $\Omega=\sqrt{\omega_{0}^{2}+\omega_{c}^{2} / 4}$.


Figure 1. A schematic diagram of the two vertically coupled quantum dots and the corresponding energy diagram.

Coupled single-electron states of TVCQDs split into symmetric (S) states and antisymmetric (AS) states with an energy difference

$$
\Delta_{\mathrm{SAS}}=\sqrt{\Delta_{0}^{2}+\delta^{2}}
$$

which consists of the energy difference between the isolated levels, $\delta=E_{z \mathrm{U}}-E_{z \mathrm{~L}}$, and the quantum mechanical coupling energy, $\Delta_{0}$. We introduce an angle, $\theta=\arccos \left(\Delta_{0} / \Delta_{\mathrm{SAS}}\right)$, characterizing the amount of asymmetry between the dots $(\theta=0$ is a symmetric case). The wave functions are given by

$$
\begin{align*}
& \zeta_{\mathrm{S}}(z)=\zeta_{\mathrm{L}} \cos \Theta+\zeta_{\mathrm{U}} \sin \Theta  \tag{2}\\
& \zeta_{\mathrm{A}}(z)=\zeta_{\mathrm{L}} \sin \Theta-\zeta_{\mathrm{U}} \cos \Theta \tag{3}
\end{align*}
$$

where $\theta=\pi / 2-2 \Theta$ and the electron probability in the barrier $(|z|<d / 2)$ is neglected in evaluating the Coulomb matrix elements in the following, by assuming that the tunnelling barrier is sufficiently high (that is the case of reference [9]). Since the lateral confinement potentials of these dots are assumed to be the same, no level mixing occurs by quantum mechanical coupling; therefore, the single-particle energy spectrum is determined by $(q, \sigma)=$ $(n, m, p, \sigma)$ where $p$ is the electron-rotated isospin with $p_{z}=\mp \frac{1}{2}$ depending on an S/AS state and $\sigma$ is the electron spin.

The Coulomb matrix element $\left\langle q_{1} q_{2}\right| V\left|q_{3} q_{4}\right\rangle$ is calculated as follows:
$V^{\mathrm{DA}}=\langle\mathrm{SS}| V|\mathrm{SS}\rangle=\langle\mathrm{AA}| V|\mathrm{AA}\rangle=V_{\text {intra }}\left(\cos ^{4} \Theta+\sin ^{4} \Theta\right)+2 V_{\text {inter }} \sin ^{2} \Theta \cos ^{2} \Theta$
$V^{\mathrm{DB}}=\langle\mathrm{SA}| V|\mathrm{AS}\rangle=\langle\mathrm{AS}| V|\mathrm{SA}\rangle=2 V_{\text {intra }} \sin ^{2} \Theta \cos ^{2} \Theta+V_{\text {inter }}\left(\cos ^{4} \Theta+\sin ^{4} \Theta\right)$
$V^{\mathrm{XA}}=\langle\mathrm{AA}| V|\mathrm{AS}\rangle=-\langle\mathrm{SS}| V|\mathrm{SA}\rangle=\frac{1}{4}\left(V_{\text {inter }}-V_{\text {intra }}\right) \sin 4 \Theta$
$V^{\mathrm{XB}}=\langle\mathrm{SS}| V|\mathrm{AA}\rangle=\langle\mathrm{SA}| V|\mathrm{SA}\rangle=\frac{1}{2}\left(V_{\text {intra }}-V_{\text {inter }}\right) \sin ^{2} 2 \Theta$
where in the definitions of $V^{\mathrm{XA}}$ and $V^{\mathrm{XB}}$ there are six and two other equivalent combinations of $S$ and $A(=A S)$ states, respectively. In the equations, a set of quantum numbers [ $n_{1}, m_{1}, n_{2}, m_{2}, n_{3}, m_{3}, n_{4}, m_{4}$ ] is implicit, with the constraint $m_{1}+m_{2}=m_{3}+m_{4}$ from the cylindrical symmetry of the system. The intra- and inter-Coulomb integrals are given by

$$
\begin{align*}
& V_{\text {intra }}=\langle\mathrm{LL}| V|\mathrm{LL}\rangle=\langle\mathrm{UU}| V|\mathrm{UU}\rangle  \tag{8}\\
& V_{\text {inter }}=\langle\mathrm{LU}| V|\mathrm{UL}\rangle=\langle\mathrm{UL}| V|\mathrm{LU}\rangle \tag{9}
\end{align*}
$$

respectively, with the definition

$$
\begin{equation*}
\langle s 1 s 2| V|s 3 s 4\rangle=\int \mathrm{d} r_{1} \mathrm{~d} r_{2} \Psi_{s 1}^{*}\left(r_{1}\right) \Psi_{s 2}^{*}\left(r_{2}\right) \frac{e^{2}}{4 \pi \epsilon^{*}\left|r_{1}-r_{2}\right|} \Psi_{s 3}\left(r_{2}\right) \Psi_{s 4}\left(r_{1}\right) \tag{10}
\end{equation*}
$$

The indices $s$ stand for $n m \mathrm{U}$ or $n m \mathrm{~L}$. Other integrals such as $\langle\mathrm{LL}| V|\mathrm{LU}\rangle$ vanish because of the negligible electron probability in the barrier region.

Now the Hamiltonian for the TVCQDs is

$$
\begin{align*}
H=\sum_{q, \sigma}\left(E_{n m}\right. & \left.+p_{z} \Delta_{\mathrm{SAS}}+\sigma_{z} g \mu_{B} B\right) a_{q, \sigma}^{\dagger} a_{q, \sigma} \\
& +\frac{1}{2} \sum_{q_{1}, q_{2}, q_{3}, q_{4}, \sigma, \sigma^{\prime}}\left\langle q_{1} q_{2}\right| V\left|q_{3} q_{4}\right\rangle a_{q_{1}, \sigma}^{\dagger} a_{q_{2}, \sigma^{\prime}}^{\dagger} a_{q_{3}, \sigma^{\prime}} a_{q_{4}, \sigma} \tag{11}
\end{align*}
$$

where $g$ is an effective $g$-factor, $\mu_{B}$ is the Bohr magneton, and $a_{q, \sigma}$ and $a_{q, \sigma}^{\dagger}$ are annihilation and creation operators of a state $q$ and spin $\sigma$, respectively. We employ an exact-diagonalization technique with single-particle basis sets as far as the fourth shell (ten levels for each S/AS state) to find the $N$-electron eigen-energies $E_{N, j}$, and the eigen-states of the total spin $S$ and the total angular momentum $\boldsymbol{M}$, which are represented by a pair $(\boldsymbol{M}, \boldsymbol{S})[16,23]$. The probability of occupation of the highest energy level is quite small for the ground and excited states discussed in the rest of the text. The Coulomb integrals $V_{\text {intra }}$ and $V_{\text {inter }}$ for possible sets
of quantum numbers $\left[n_{1}, m_{1}, n_{2}, m_{2}, n_{3}, m_{3}, n_{4}, m_{4}\right.$ ] are evaluated numerically, which reduce to single integrals, including the finite spreading of the wave functions in the $z$-direction. We restricted the values of $\left(\Delta_{0}, d\right)$ to experimentally accessible pairs corresponding to TVCQDs with $\hbar \omega_{0} \sim 4 \mathrm{meV}$, and InGaAs wells 12 nm thick. All of the energies are scaled with respect to $\hbar \omega_{0}$ in the following.

The CO current for tunnelling through this triple-barrier structure is estimated using a standard formula, assuming the probability of tunnelling to the collector to be much smaller than that of tunnelling to the emitter (the charging condition). At low temperatures, the tunnelling current is composed of all possible paths that the electron can tunnel along into the $N$-electron GS, which then becomes the $(N+1)$-electron $j$ th state if the condition $\mu_{e}>\mu_{N, j, G}>\mu_{c}$ is fulfilled, where

$$
\mu_{N, j, i}=E_{N+1, j}-E_{N, i}-E_{\text {gate }} .
$$

$E_{\text {gate }}$ is the energy offset controlled by a gate contact, and $E_{N, G}$ is the $N$-electron GS energy [24]. $\mu_{e}$ and $\mu_{c}$ are the electrochemical potentials of the emitter and the collector, respectively. (For the $N+1$ state empty, an additional condition $\mu_{e}>\mu_{N, G, G}>\mu_{c}$ is required.) Such a process has a spectral weight

$$
\left.S_{N, j, G} \equiv\left|\left\langle\Psi_{N+1, j}\right| \sum_{q, \sigma} a_{q, \sigma}^{\dagger}\right| \Psi_{N, G}\right\rangle\left.\right|^{2} .
$$

More explicitly, the current is obtained from

$$
-e \Gamma S_{N, j, G}\left[f\left(\mu_{e}-\mu_{N, j, G}\right)-f\left(\mu_{c}-\mu_{N, j, G}\right)\right]
$$

summed for all possible $j$-states, where $f$ is a Fermi distribution function in the contacts [25]. $\Gamma=2 \pi D t_{c}^{2} / \hbar$, where $D$ and $t_{c}$ are the collector density of states and the energy of tunnelling to the collector, respectively. We assume that the tunnelling probability is independent of the single-particle levels.

If $\Delta_{0}<\Gamma$ (weakly coupled dots), we cannot treat the coupled dot as a whole, and the tunnelling current formula should be modified. The $d=75 \mathrm{~nm}$ dot in reference [9] has $\Delta_{0} \sim 0.1 \mathrm{meV}$ which is comparable to $\Gamma$. Moreover, in such a situation the electron is apt to occupy a localized state in one of the dots because of intrinsic asymmetry (finite $\delta$ ) or extrinsic asymmetry (an applied electric field), and the probability of tunnelling to the contacts varies substantially for different $N$-electron states. In the following, we assess the relative amplitude of the current with the spectral weight $S_{N, j, i}$ assuming $\Delta_{0} \gg \Gamma$.

## 3. A two-electron system

First, we discuss the smallest non-trivial system, two electrons in TVCQDs. Figure 2 shows the two-electron energy spectrum as a function of $\Delta_{\text {SAS }}$ with zero magnetic field and $\delta=0$. The GS is a spin singlet, (0,0), occupying symmetric states like $|S \uparrow S \downarrow\rangle$ for strong-coupling conditions. If $d \rightarrow \infty, V_{\text {intra }} \gg V_{\text {inter }} \gg \Delta_{\mathrm{SAS}}$, where the Coulomb energy dominates, this state approaches the Mott-insulator phase in which singlet electrons occupy symmetric and antisymmetric states coherently:

$$
(|\mathrm{S} \uparrow \mathrm{~S} \downarrow\rangle-|\mathrm{AS} \uparrow \mathrm{AS} \downarrow\rangle) / \sqrt{2}=(|\mathrm{U} \uparrow \mathrm{~L} \downarrow\rangle-|\mathrm{U} \downarrow \mathrm{~L} \uparrow\rangle) / \sqrt{2}
$$

This coherence makes the GSs more stable for smaller $\Delta_{\text {SAS }}$. The ( $\mathbf{0}, \mathbf{0}$ ) state is asymptotically degenerate with the spin-triplet state (0, 1), $|\mathrm{S} \uparrow \mathrm{AS} \uparrow\rangle=|\mathrm{U} \uparrow \mathrm{L} \uparrow\rangle$, in the limit where $\Delta_{\mathrm{SAS}}=0$. The other low-energy triplet excited state is made up of one $[n, m]=[0,0]$ electron and one $[0, \pm 1]$ electron, $( \pm \mathbf{1}, \mathbf{1})$. If a magnetic field is applied in the $z$-direction, one of the degenerate
states ( $[0,1]$ ) becomes stable. As shown in the $\omega_{c}-\Delta_{\text {SAS }}$ phase diagram, figure 3 , the ground state eventually evolves into spin-triplet states, (0,1), favoured by Zeeman energy, or into $(\mathbf{1}, \mathbf{1})$, favoured by exchange energy with reduced kinetic energy, depending on the value of $\Delta_{\mathrm{SAS}}$ (singlet-triplet transition) [19]. Then how should we understand the transition between $(\mathbf{0}, \mathbf{1})$ and $(\mathbf{1}, \mathbf{1})$ ?


Figure 2. The two-electron energy diagram as a function of $\Delta_{\mathrm{SAS}}$ for symmetric dots and zero field. ( $\mathbf{0}, \mathbf{0}$ ): thick solid curves; $(\mathbf{1}, \mathbf{0})$ : thin solid curves; $(\mathbf{0}, \mathbf{1})$ : thick dotted curves; $(\mathbf{1}, \mathbf{1})$ : thin dotted curves. See the text for the notation ( $\boldsymbol{M}, \boldsymbol{S}$ ). The aligned three boxes and two arrows show the most probable configurations of two electrons with spin. The lower box shows the $n=0, m=0$ state and the two upper boxes show the $n=0, m= \pm 1$ states. The area to the left of each curve is for symmetric states and that to the right is for antisymmetric states. Note that the actually realized configuration is a linear combination of the states having the same ( $\boldsymbol{M}, \boldsymbol{S}$ ) quantum number including the one shown.

An isospin representation makes the physics of this system clearer, where the isospin $p_{z}=\mp \frac{1}{2}$ corresponds to an S/AS state (the rotated isospin representation) [11]. In the following we simply refer to the rotated isospin as the 'isospin' for simplicity. The isospin operators are defined as

$$
\begin{align*}
& \rho_{l_{1}, l_{2}}=\xi_{l_{1}}^{\dagger} \mathbf{1} \xi_{l_{2}}  \tag{12}\\
& \zeta_{l_{1}, l_{2}}=\xi_{l_{1}}^{\dagger} \boldsymbol{\sigma} \xi_{l_{2}} \tag{13}
\end{align*}
$$



Figure 3. The phase diagram of the symmetric two-electron system as a function of $\Delta_{\text {SAS }}$ and magnetic field $\omega_{c}$. The inset shows the phase diagram as a function of the asymmetry parameter $\theta$ and $\omega_{c}$ for $\Delta_{\mathrm{SAS}}=0.1$.
where $\mathbf{1}$ is a $2 \times 2$ unit matrix, $\sigma$ is the Pauli's spin matrix, and $\xi_{l}=\left(a_{l, \mathrm{~A}}, a_{l, \mathrm{~S}}\right)^{\mathrm{t}}, \xi_{l}^{\dagger}=\left(a_{l, \mathrm{~A}}^{\dagger}, a_{l, \mathrm{~S}}^{\dagger}\right)$ with $l=(n, m, \sigma)$. The Hamiltonian for the TVCQDs is therefore

$$
\begin{align*}
H=\sum_{l}\left(E_{l} \rho_{l, l}\right. & \left.+\frac{\Delta_{\mathrm{SAS}}}{2} \zeta_{l, l}^{z}\right)+\frac{1}{2} \sum_{l_{1}, \ldots, l_{4}} V_{D}^{l_{1}, \ldots, l_{4}} \rho_{l_{1}, l_{4}} \rho_{l_{2}, l_{3}} \\
& +\frac{1}{2} \sum_{l_{1}, \ldots, l_{4}} V_{E}^{l_{1}, \ldots, l_{4}}\left[\zeta_{l_{1}, l_{4}}^{x} \zeta_{l_{2}, l_{3}}^{x} \cos ^{2} \theta+\zeta_{l_{1}, l_{4}}^{z} \zeta_{l_{2}, l_{3}}^{z} \sin ^{2} \theta\right] \tag{14}
\end{align*}
$$

omitting linear terms in $\rho_{l, l^{\prime}}, \zeta_{l, l^{\prime}}$ and $E_{l}=E_{n m}+\sigma_{z} g \mu_{B} B$. The Coulomb energy consists of $V_{D}=\frac{1}{2}\left(V_{\text {intra }}+V_{\text {inter }}\right)$ and $V_{E}=\frac{1}{2}\left(V_{\text {intra }}-V_{\text {inter }}\right)$. The terms proportional to $V_{E}$ and $\Delta_{\mathrm{SAS}}$ break the $\mathrm{SU}(2)$ isospin symmetry. If we can neglect the contribution of $V_{E}, P=\sum_{k=1}^{N} p_{k}$ will be a good quantum number. The intra-dot Coulomb energy, $V_{\text {intra }}$, is apparently independent of the separation, $d$, between the two dots; however, the inter-dot Coulomb energy, $V_{i n t e r}$, is approximately inversely proportional to $d$, and $V_{\text {intra }}=V_{\text {inter }}$ for $d=0$. Therefore, $V_{E}(d)$ is
a positive monotonically increasing function of $d$ (or a monotonically decreasing function of $\Delta_{\mathrm{SAS}}$ in our case) with $V_{E}(0)=0$ and

$$
\lim _{d \rightarrow \infty} V_{E}(d)=V_{\text {intra }} / 2
$$

The spin triplet-triplet transition found in figure 3 could be understood as an isospin singlet-triplet transition since $P$ changes from 0 to 1 , which may seem surprising since this transition occurs for rather small $\Delta_{\mathrm{SAS}}$ (or large $d$ ) when the $V_{E}$-term is not small. This is because the isospin is a good quantum number irrespective of the coupling constant in a spin-polarized two-electron system, which can be shown by rewriting the Hamiltonian for the two-electron relative-motion wave function [11].

The inset of figure 3 shows the phase diagram as a function of $\theta$ for $\Delta_{\mathrm{SAS}}=0.1$. The $(\mathbf{0}, \mathbf{1})$ state, corresponding to the situation where two electrons of parallel spin occupy the two dots, $|\mathrm{U} \uparrow \mathrm{L} \downarrow\rangle-|\mathrm{U} \downarrow \mathrm{L} \uparrow\rangle$, is stable if there is an asymmetry between the two dots. Because of the Pauli exclusion principle, the electrons cannot hop to the other dot to gain energy of the order of $\Delta_{0}^{2} / E_{\text {intra }}$ without losing kinetic energy $\hbar\left(\Omega-\omega_{c} / 2\right)$. This is not the case for the $(\mathbf{0}, \mathbf{0})$ and $(\mathbf{1}, \mathbf{1})$ states. However, if $\theta \rightarrow \pi / 2$ (or $\Delta_{0} \rightarrow 0$ ), the other states cannot gain by quantum mechanical coupling any longer, and the ( $\mathbf{0}, \mathbf{1}$ ) state becomes stable by the gain of the Zeeman energy.

## 4. Three- and four-electron systems

The GS phase diagrams of the system of three and four electrons are more complicated. Figure 4 shows the phase diagrams in a parameter area of $\omega_{c}$ and $\Delta_{\mathrm{SAS}}$ for symmetric dots with $\theta=0$. Phases for $\Delta_{\mathrm{SAS}}>0.7$ show GS transitions quite similar to those of a single dot. This is consistent with the experiments [9] with $d=2.5 \mathrm{~nm}\left(\Delta_{\mathrm{SAS}} \sim 1\right)$. For $N=4$ near zero magnetic field, a spin-polarized phase obeying Hund's rule is seen. For $\omega_{c}>1.5$, the angular momentum $M$ of the GS shows a one-by-one increase, and finally the system drops into a quite stable maximum-density droplet (MDD) phase (for $N=3,(\mathbf{3}, \mathbf{3} / \mathbf{2})$, and for $N=4,(\mathbf{6}, \mathbf{2})$ ). The phases for smaller $\Delta_{\mathrm{SAS}}$ are very different from those of a single dot.

The CO peak corresponding to the transition from an $N$-electron system to an $(N+1)$ electron system is suppressed at low temperatures if the change of spin $|\Delta \boldsymbol{S}| \neq \frac{1}{2}$ (spin blockade) [26]. Spin blockade has also been predicted for TVCQDs for the transition from $N=2$ to $N=3$ [20] and for $N>12$ in a non-parabolic potential [22]. We find it here for a transition from $N=3$ to $N=4$ for the area of $\Delta_{\mathrm{SAS}}<0.1$ and $\omega_{c} \sim 1.5$ as shown in figure 4 , since the transition corresponds to $|\Delta \boldsymbol{S}|=\frac{3}{2}$.

In the limit of $d=0, V_{E}$ vanishes, so the total isospin quantum number $\boldsymbol{P}$ is exactly conserved; then isospin blockade is also expected. It might be interesting to see some evidence of isospin blockade in the situation where $V_{E}$ is not zero. We evaluated the spectral weight of possible $N$ - and $(N+1)$-electron eigen-functions for zero field. Since $\boldsymbol{P}$ is approximately a good quantum number for strong coupling, we expect that several CO excitation peaks with $|\Delta \boldsymbol{P}| \neq \frac{1}{2}$ will be suppressed. Figure $5(a)$ shows the spectral weight as a function of $\Delta_{\mathrm{SAS}}$ for transitions from $N=2$ to $N=3\left(\omega_{c}=0\right)$. The solid thick curves correspond to GS-to-GS transition. The small spectral weight of the GS-GS transition for very small $\Delta_{\text {SAS }}((\mathbf{0}, \mathbf{0})$ to $(\mathbf{0}, \mathbf{1} / \mathbf{2})$ ) could be understood from the stiffness of the $N=2$ Mott insulating phase. The curve indicated by an arrow corresponds to the transition from ( $\mathbf{0}, \mathbf{1}$ ) to $(\mathbf{1}, \mathbf{1} / \mathbf{2})$, so no spin selection rule applies. However, the weight decreases to almost zero with increasing $\Delta_{\text {SAS }}$, since this transition is approximately from $P_{z}=0$ to $3 / 2$. The weight is restored to a finite value for $\Delta_{\mathrm{SAS}}>1.7$ where the transition is now from $P_{z}=1$ to $3 / 2$. More dramatically, we predict that the CO peak for the transition between $(\mathbf{0}, \mathbf{1} / \mathbf{2})$ for $N=3$ and $(\mathbf{0}, \mathbf{1})$ for $N=4$ is almost


Figure 4. Phase diagrams of symmetric three-electron (a) and four-electron (b) systems in $\Delta_{\mathrm{SAS}}-\omega_{c}$ space.
completely suppressed (figure 5(b)). This suppression is more peculiar than the previous one since it is almost independent of $\Delta_{\text {SAS }}$. The origin of this suppression is twofold. Among the configurations making up the $N=3,(\mathbf{0}, \mathbf{1} / \mathbf{2})$ and $N=4,(\mathbf{0}, \mathbf{1})$ states, transitions with $\left|\Delta P_{z}\right| \neq \frac{1}{2}$ are prohibited by a normal isospin selection rule. And most of the weights of the other processes vanish because of the wave-function orthogonality. The exception is for the processes such that all of the electrons occupy $m=0$ states-for example $[0,0],[1,0],[2,0]$
(a)


(b)

Figure 5. (a) The spectral weight for two-to-three-electron transition as a function of $\Delta_{\text {SAS }}$ for zero field. The thick solid curve shows the GS-GS transition. The dotted curve shows the process with the spectral weight suppressed with $\Delta_{\text {SAS }}$. The three numbers in the brackets show $(\boldsymbol{M}, \boldsymbol{S}, \boldsymbol{P})$. (b) The spectral weight for three-to-four-electron transition as a function of $\Delta_{\text {SAS }}$ for zero field.
to $[0,0],[1,0],[2,0],[3,0]$. Therefore this suppression is not complete; however, the weight is of the order of $10^{-30}$ in the range of $\Delta_{\mathrm{SAS}}$ indicated. A similar effect of the cancelling out of the matrix elements, although not so strong, had been reported for a single dot in a quasi-onedimensional square well [27]. The excited state is about 0.03 (of the order of 1 K ) above the $N=4$ GS energy, which suggests that this current blocking could be observed experimentally. This strong cancellation of the spectral weight originates from the transition processes to the spin-triplet pair of $N=4,(\mathbf{0}, \mathbf{1})$ (parallel spins occupying $m= \pm 1$, for example, obeying Hund's rule). Similar strong cancellation is also found in the transitions from $N=2,(\mathbf{0}, \mathbf{1})$ with isospin $P=1$ to $N=3,(\mathbf{0}, \mathbf{3} / \mathbf{2})$. This indicates that the TVCQD system offers several new and interesting mechanisms controlling the tunnelling current.

## 5. Conclusions

Electron states and tunnelling characteristics for two vertically coupled quantum dots are analysed. The GS phase diagrams are obtained for two-, three-, and four-electron systems. In the two-electron system, a spin-singlet state is the GS at zero field, and this state is eventually replaced by spin-triplet states on applying a vertical magnetic field. One of the triplet states is stable under conditions of very weak quantum mechanical coupling and larger asymmetry between the two dots. An isospin selection rule is demonstrated in the two- to three-electron transitions, which is effective under strong-coupling conditions. In the transitions from the three-electron to the four-electron state, we find parameter regions where the tunnelling current is strongly suppressed because of the spin selection rule or the orthogonality of the quantum states.

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