Electronic properties of single and coupled anisotropic quantum dots in a magnetic field, spin interactions and switching.

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We determined the eigenstates of a single electron in a parabolic anisotropic 2D quantum dot in a magnetic field. Using obtained expressions for these eigenstates, we study the spin coupling $J$ between two electrons located in two laterally coupled anisotropic quantum dots (QD). The exchange coupling $J$ is calculated using the Heitler-London and Hund-Mulliken approaches. We found that the exchange $J$ changes sign at certain values of parameters of the system, in particular at certain anisotropy of the QD. Therefore, we present a new method to switch on and off the spin coupling between QDs: switching by means of changing shape of the QD. Switching the spin coupling is essential for quantum computation using electronic spins as qubits. We note that our calculations can be applied to the system of vertically coupled QD as well.

I. INTRODUCTION.

The last decade has seen a great interest in quantum dots, i.e. little islands of electron gas confined by an artificial potential (see Ref. [1]). One of the most challenging proposals concerning QD is the idea of using the electron spin in quantum dots as the basic information carrier (the qubit) in a quantum computer (see, for example, Ref. [2]). Quantum logic gates between these qubits are effected by allowing the electrons to tunnel between two coupled quantum dots. For the application of coupled quantum dots as a quantum gate, it is important that the coupling between the spins can be switched on and off via externally controlled parameters such as magnetic field and interdot distance. In the recent paper of G.Burcard et al. [2] the spin interaction for two laterally coupled isotropic QD defined in a two-dimensional electron system (2DES) was calculated as a function of these external parameters and it was shown that the interaction $J$ can be switched on and off with exponential sensitivity to that parameters. In the present paper, we consider a different setup consisting of two laterally coupled anisotropic quantum dots with a magnetic field applied perpendicular to that 2DES (see Fig.1). We especially interested in calculation of interaction $J$ as a function of anisotropy of the QD since our proposal is to switch on and off the interaction $J$ by changing shape of the QD, e.g. by applying gate voltage to each quantum dot. We note that in the setup being proposed in Ref. [2] it was assumed that the interdot distance is controlled by varying the barrier height between the QD. In real experimental setup varying the barrier height might lead to changing shape of the QD from circular to elliptic. Also, probably in future quantum computers based on large integrated circuits of QD it will be simpler to change shape of the QD (and, in case of necessity, interdot distance), than change interdot distance alone, preserving circular shape of the QD. This is one of the reasons which motivated our study.

In order to study coupled anisotropic quantum dots, one needs to find firstly the eigenstates of a single electron in a single anisotropic quantum dot in a magnetic field. The latter problem is of fundamental interest in mesoscopic physics. Surprisingly, it seems that this important problem was not solved so far.

The eigenstates of a single two-dimensional electron confined by a radial potential of the form $\frac{1}{2} m_e \omega^2 r^2$ with a magnetic field perpendicular to the plane of the system are called Fock-Darwin states. That system was investigated by Fock [3] and Darwin [4] a long time ago. The system where an electron is confined by an anisotropic potential of the form $\frac{1}{2} m_e (\omega_x^2 x^2 + \omega_y^2 y^2)$ was studied only recently by A.V. Madhav and Tapash Chakraborty. [5] Their studies were motivated, in particular, by the experiments on anisotropic quantum dots (see Ref. [6]). They obtained energy eigenvalues of the system, but not the eigenfunctions of it. In their paper, the transformation of coordinates and momenta of the system was performed. In the new Hamiltonian, variables are separated and one can easily obtain both the energy eigenvalues and the eigenstates of the system. However, in order to obtain the eigenstates of the system in old (initial) coordinates, one needs to transform the eigenfunctions of the new Hamiltonian. It was not done in Ref. [6]. In the section II of the present paper, we performed such a transformation and obtained exact analytical expressions for the eigenstates of that system. Note that the system of an anisotropic quantum dot in a magnetic field was considered also in Ref. [7], where only approximate solution for the ground state of the system was obtained (see Appendix D in that paper). In the section III we study coupled anisotropic QD using expressions obtained in section II. Following Ref. [3], we employ Heitler-London approximation and Hund-Mulliken approach. In section IV we give brief conclusion.

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II. SINGLE ANISOTROPIC QUANTUM DOT.

Let us consider a single electron in a lateral anisotropic parabolic confinement potential in the presence of a perpendicular magnetic field. The Hamiltonian is

$$\mathcal{H} = \frac{1}{2m_e} \left[ p - \frac{e}{c} A \right]^2 + V_{\text{conf}}(x, y),$$

where $m_e$ is the effective mass of the electron and the confinement potential is

$$V_{\text{conf}}(x, y) = \frac{1}{2} m_e (\omega_x^2 x^2 + \omega_y^2 y^2).$$

Choosing the symmetric gauge vector potential $A = \frac{1}{2} B (y, -x, 0)$, we get

$$\mathcal{H} = \frac{1}{2m_e} \left[ p_x^2 + \Omega_1^2 x^2 + p_y^2 + \Omega_2^2 y^2 + m_e \omega_c (y p_x - x p_y) \right],$$

$$\Omega_{1,2}^2 = m_e (\omega_x^2 + \frac{1}{4} \omega_c^2),$$

$$\omega_c = e B / m_e c.$$

Following Ref. [3], we make the following transformations:

$$x = \mu q_1 + \eta p_2,$$
$$y = \mu q_2 + \eta p_1,$$
$$p_x = \mu p_1 - \zeta q_2,$$
$$p_y = \mu p_2 - \zeta q_1,$$

where

$$\mu = \sqrt{\Omega_2^2 + \Omega_2^2 - \Omega_2^2}, \eta = \sqrt{\Omega_2^2 + \Omega_2^2 - \Omega_2^2},$$

$$\zeta = \sqrt{(\Omega_1^2 + \Omega_2^2 - \Omega_2^2)(\Omega_1^2 + \Omega_2^2)},$$

$$\Omega_2^2 = [(\Omega_1^2 - \Omega_2^2)^2 + 2 m_e \omega_c^2 (\Omega_1^2 + \Omega_2^2)]^{1/2}.$$

The transformations [3] are consistent with the commutation relations $[p_i, q_j] = -i \hbar \delta_{ij}$, $[q_i, q_j] = 0$ and the resulting Hamiltonian is diagonal (see also Ref. [3]):

$$H = \frac{1}{2m} \left( \alpha_1^2 p_1^2 + \alpha_2^2 p_2^2 + \beta_1^2 q_1^2 + \beta_2^2 q_2^2 \right),$$

where

$$\alpha_1^2 = \frac{2 \Omega_1^2 + \Omega_2^2 + \Omega_2^2}{2(\Omega_1^2 + \Omega_2^2)}, \quad \beta_1^2 = \frac{1}{4} (3 \Omega_1^2 + \Omega_2^2 + \Omega_2^2),$$

$$\alpha_2^2 = \frac{3 \Omega_1^2 + \Omega_2^2 - \Omega_2^2}{2(\Omega_1^2 + \Omega_2^2)}, \quad \beta_2^2 = \frac{1}{4} (3 \Omega_1^2 + 3 \Omega_2^2 - \Omega_3^2).$$

One can easily obtain eigenvalues and eigenstates of the Hamiltonian:

$$E_{m,n} = (m + \frac{1}{2}) \hbar \omega_1 + (n + \frac{1}{2}) \hbar \omega_2,$$

$$\psi_{m,n}(q_1, q_2) = c_{m,n} e^{-\frac{\gamma_2^2 q_2^2}{2}} e^{-\frac{\gamma_1^2 q_1^2}{2}} H_m(\gamma_1 q_1) H_n(\gamma_2 q_2),$$

where $c_{m,n} = \left( \frac{(\gamma_1^2 \gamma_2^2)^{1/2}}{2} \right)^{1/2}$, $\omega_i = \alpha_i \beta_i / m_e$, $\gamma_i^2 = \beta_i / (\alpha_i \hbar)$, $H_k$ is the Hermite polynomial. The question is how one can return back to coordinates $(x, y)$, i.e. how to obtain eigenstates $\Psi_{m,n}(x, y)$ of the Hamiltonian [3].

Since $\psi(q_1, q_2) = \langle q_1, q_2 | \Psi \rangle$, $\Psi(x, y) = \langle x, y | \Psi \rangle$, and $| \Psi \rangle = \int_{-\infty}^{\infty} dq_1 dq_2 | q_1, q_2 \rangle \psi(q_1, q_2)$, we have the following formula for the eigenstates $\Psi_{m,n}(x, y)$:

$$\Psi_{m,n}(x, y) = \int_{-\infty}^{\infty} dq_1 dq_2 \langle x, y | q_1, q_2 \rangle \psi(q_1, q_2)$$

Let us denote $\Phi(x, y, q_1, q_2) = \langle x, y | q_1, q_2 \rangle$. Function $\Phi(x, y, q_1, q_2)$ is the eigenstate of operators $\hat{q}_1, \hat{q}_2$ in the $(x, y)$ representation and should obey the following relations:

$$\hat{q}_1 \Phi = [\mu \hat{x} - \eta \hat{p}_y] \Phi = q_1 \Phi,$$
$$\hat{q}_2 \Phi = [\mu \hat{y} - \eta \hat{p}_x] \Phi = q_2 \Phi.$$

On the other hand, $\Phi^*(x, y, q_1, q_2) = \langle q_1, q_2 | x, y \rangle$ ($^*$ denotes complex conjugating) and therefore it should obey the following relations:

$$\hat{x} \Phi^* = [\mu \hat{q}_1 + \eta \hat{p}_y] \Phi^* = x \Phi^*,$$
$$\hat{y} \Phi^* = [\mu \hat{q}_2 + \eta \hat{p}_x] \Phi^* = y \Phi^*.$$

Therefore, finally we have the following system of differential equations defining $\Phi(x, y, q_1, q_2)$:

$$\left\{ \begin{array}{ll}
(i \hbar \frac{\partial}{\partial y} + \mu x) \Phi(x, y, q_1, q_2) &= q_1 \Phi(x, y, q_1, q_2), \\
(i \hbar \frac{\partial}{\partial x} + \mu y) \Phi(x, y, q_1, q_2) &= q_2 \Phi(x, y, q_1, q_2),
\end{array} \right.$$
where \( \sigma = \mu / (\eta \hbar \gamma_1 \gamma_2) \), \( d = \sqrt{1 + \sigma^2} \). Let us firstly find the ground state of our system \( \Psi_{00}(x, y) \). Differentiating expression for \( I_{00}(z_1, z_2) \) over \( z_1 \) and \( z_2 \) and solving obtained differential equations, one can find that
\[
I_{00}(z_1, z_2) = \dot{C}_{00} e^{-\frac{z_1^2}{2} - \frac{z_2^2}{2}} e^{-i\sigma z_1 z_2},
\]
where \( \dot{C}_{00} \) is a constant. Therefore, the ground state of the system is
\[
\Psi_{00}(x, y) = C_{00} e^{i\nu_2(1-\nu_2) - \frac{z_1^2}{2} - \frac{z_2^2}{2}},
\]
where normalization constant is \( C_{00} = \sqrt{\frac{n(n+1)}{2}} \). \( \nu_1 = \nu \gamma_1 \), \( \nu_2 = \nu \gamma_2 \). One can see that \( C_{00} = \nu \gamma_1 \), \( \nu_2 = \nu \gamma_2 \). Let us now note that \( H_{\nu_1} = \frac{\nu_1}{\bar{z}} x \), \( \nu_2 = \frac{\nu_2}{\bar{z}} y \). Let \( \nu_1 = \nu \gamma_1 \), \( \nu_2 = \nu \gamma_2 \), \( \nu \gamma_1 = \nu \gamma_2 \).

A similar procedure for the coordinate \( z_2 \) can be executed. Now one can easily find the following expression for \( I_{m,n}(z_1, z_2) \):
\[
I_{m,n}(z_1, z_2) = D_m^{z_2} D_n^{z_1} I_{00}(z_1, z_2),
\]
where operators \( \hat{D}_a \) are defined as
\[
\hat{D}_a = H_k \left( \frac{i}{d} \frac{\partial}{\partial z_2} \right) = \frac{\partial}{\partial z_2} (k) \cdot \frac{(\partial)_{k-2}}{\partial z_2} + ... \]

So, we finally have the following expression for the eigenstates of the Hamiltonian [8]:
\[
\Psi_{m,n}(x, y) = \sqrt{\frac{\kappa x \kappa y}{\pi^{m+n} n!}} D_{m}^{z_2} D_{n}^{z_1} I(x, y),
\]
where \( I(x, y) = \exp \left\{ -\frac{x^2}{2} - \frac{y^2}{2} - i\sigma \kappa x \kappa y xy \right\} \). The lowest excited states of the system are
\[
\Psi_{01}(x, y) = \frac{1}{d} \sqrt{\frac{2\kappa x \kappa y}{\pi}} (\kappa x - i\kappa y) F_{00}(x, y),
\]
\[
\Psi_{10}(x, y) = \frac{1}{d} \sqrt{\frac{2\kappa x \kappa y}{\pi}} (\kappa x - i\kappa y) F_{00}(x, y),
\]
\[
\Psi_{11}(x, y) = \frac{2}{d^2} \sqrt{\frac{\kappa x \kappa y}{\pi}} (\kappa x - i\kappa y) (1 - \sigma^2) + i\sigma (\kappa x^2 - \kappa y^2) - i\sigma F_{00}(x, y),
\]
where
\[
F_{00}(x, y) = e^{i\nu_2(1-\nu_2) - \frac{z_1^2}{2} - \frac{z_2^2}{2}} = C_{00}^{-1} \Psi_{00}(x, y).
\]

Note that in degenerate case of isotropic dot we have \( \Omega_1 = \Omega_2, \nu = \sigma = 1 \), and the eigenstates \( \Psi_{00}(x, y) \) coincide with the corresponding Fock-Darwin states.

### III. COUPLED ANISOTROPIC QUANTUM DOTS.

#### A. Model.

The Hamiltonian which we use for the description of two laterally coupled quantum dots is
\[
H = \sum_{i=1,2} h(r_i, p_i) + C,
\]
\[
h(r, p) = \frac{1}{2m_e} \left( p - \frac{e}{c} A(r) \right)^2 + V(r),
\]
\[
C = \frac{e^2}{\kappa |r_1 - r_2|},
\]
where \( C \) is the Coulomb interaction and \( h \) is the single-particle Hamiltonian. The dielectric constant \( \kappa \) and the effective mass \( m_e \) are material parameters. For the lateral confinement \( V \) we choose the quartic potential
\[
V(x, y) = \frac{m_e \omega_x^2}{8a_0^2} (x^2 - a^2)^2 + \frac{m_e \omega_y^2}{2} y^4,
\]
which separates (for \( x \) around \( \pm a \)) into two anisotropic harmonic wells in the limit of large inter-dot distance, i.e. for \( 2a > 2a_B x, y \), where \( a \) is half the distance between the centers of the dots, and the lateral effective Bohr radii \( a_B x, y = \sqrt{\hbar / m_e \omega_x, y} \) are a measure for the lateral extension of the electron wave function in the dots (see Fig. 1). In Ref. [2] the potential similar to (24) was considered, but there \( \omega_x = \omega_y = \omega_0 \). It was also shown in Ref. [3] that spin-orbit contribution and Zeeman splitting can be neglected in relevant cases. For material parameters, we choose that of GaAs (\( \kappa = 13.1, m_e = 0.067 m \), where \( m \) is the mass of the electron).

#### B. Heitler-London approach.

Here we consider firstly the Heitler-London approximated, and then refine this approach by including (see subsection C) double occupancy in a Hund-Mulliken approach. In the Heitler-London approach, one starts from single-dot ground-state coordinate wavefunctions \( \varphi(\mathbf{r}) \) and combines them into the (anti-)symmetric two-particle state vector
\[
|\Psi_\pm\rangle = \frac{|12\rangle \pm |21\rangle}{\sqrt{2(1 \pm S^2)}},
\]
the positive (negative) sign corresponding to the spin singlet (triplet) state, and \( S = \int d^2r \varphi_+^\ast \varphi_- \) denoting the overlap of the right and left orbitals. A non-vanishing overlap implies that the electrons tunnel between the dots (see also Ref. [2]). Here, \( \varphi_-^\ast(\mathbf{r}) = (\mathbf{r}|1\rangle \) and \( \varphi_+^\ast(\mathbf{r}) = (\mathbf{r}|2\rangle \) denote the one-particle orbitals centered at \( \mathbf{r} = (\mp \mathbf{a}, 0) \), and \( \langle ij \rangle = \langle i|j \rangle \) are two-particle
product states. The exchange energy is then obtained as
\[ J = \epsilon_t - \epsilon_0 = \langle \Psi_{-\sigma} | H | \Psi_{+\sigma} \rangle - \langle \Psi_{+\sigma} | H | \Psi_{-\sigma} \rangle. \]
The single-dot orbital for anisotropic harmonic confinement in two dimensions in a perpendicular magnetic field is the ground state being obtained in section II. The ground state centered at the origin is
\[ \varphi(x,y) = \frac{k_x k_y}{\pi} e^{\gamma x y} e^{-k_x^2 x^2/2} e^{-k_y^2 y^2/2}, \]
where \( \gamma = \mu(1 - \nu^2) / \hbar \), and \( \kappa_x \) and \( \kappa_y \) were introduced in section II.

Shifting the single particle orbitals to \((\pm a, 0)\) in the presence of a magnetic field we obtain \( \varphi_{\pm a}(x,y) = \exp(\pm i a / 2l_2) \varphi(x \mp a, y) \). The phase factor involving the magnetic length \( l_B = \sqrt{\hbar C / eB} \) is due to the gauge transformation \( A_{\pm a} = B(-y, x \mp a, 0) / 2 \to A = B(-y, x, 0) / 2 \). We rewrite the Hamiltonian, adding and subtracting the potential of the single left (right) dot for electron 1(2) in \( H \). The Hamiltonian then takes the form
\[ H = h^0_{\pm a}(r_1) + h^0_{\pm a}(r_2) + \mp e_a(1/2m_a + m_a \omega_x^2 / 2 + m_a \omega_y^2 / 2), \]
and \( W(r_1, r_2) = \sum_{i=1,2} V(x_i, y_i) - m_a \omega_x^2 ((x_1 + a)^2 + (x_2 - a)^2) / 2 - m_a \omega_y^2 (y_1^2 + y_2^2) / 2 \). The formal expression for \( J \) is now
\[ J = \frac{252}{1 - S^2} \left( (12C + W|12) - \text{Re}(12C + W|21) \right), \]
where the overlap becomes \( S = \exp(-\kappa_x^2 a^2 - \kappa_y^2 l_-^2) \).

Here we denoted \( l_0 = (a \gamma - a / 2l_2)^{-1} \). Evaluation of the matrix elements of \( C \) and \( W \) provides us with the result,
\[ J = \left[ c \kappa x e^{-k^2 x^2} K \left( 1 - \kappa_x^2 \kappa_y^2 \right) I_0(\kappa_x^2 a^2) - c \kappa y e^{-k^2 y^2} K \left( 1 - \kappa_y^2 \kappa_x^2 \right) I_0(\kappa_y^2 l_-^2) + 3 m_a \omega_x^2 (\kappa_x^2 a^2 + 1) / \kappa_x^2 \right] e^{\gamma x y} e^{-k_x^2 x^2/2} e^{-k_y^2 y^2/2}, \]
which \( e = \sqrt{2/\pi e^2 / \kappa} \), is the complete elliptic integral of the first kind, and \( I_0 \) is the zeroth order Bessel function. The first and second term in Eq. (28) are due to Coulomb interaction \( C \), where the exchange term enters with a minus sign. The last term comes from the confinement potential \( W \). Note that in the degenerate case of isotropic QD our result coincide with that being obtained in Ref. 3.

We plotted \( J \) as a function of \( \omega_y \) and \( \omega_z \) at different values of magnetic field \( B \). Note singlet-triplet crossing \(( J = 0 \)\) at certain parameters of the system.

C. Hund-Mulliken approach.

Following Ref. 3, we now apply the Hund-Mulliken approach to calculate the exchange energy of the double-dot system. We introduce the orthornormalized one-particle wave functions \( \Phi_{\pm a} = (\varphi_{\pm a} - g \varphi_{\mp a}) / \sqrt{1 - 2Sg + g^2} \), where \( S \) again denotes the overlap of \( \varphi_{-a} \) with \( \varphi_{+a} \) and \( g = (1 - \sqrt{1 - S^2}) / S \). Using \( \Phi_{\pm a}, \) we generate four basis functions to which we diagonalize the two-particle Hamiltonian \( H \) : the states with double occupation, \( \Psi_{\pm a}^d(r_1, r_2) = \Phi_{\pm a}(r_1) \Phi_{\pm a}(r_2) \) and the states with single occupation, \( \Psi_{\pm a}^s(r_1, r_2) = \left[ \Phi_{+a}(r_1) \Phi_{-a}(r_2) \pm \Phi_{-a}(r_1) \Phi_{+a}(r_2) \right] / \sqrt{2} \). Diagonalization of
\[ H = 2 \epsilon_t + \begin{pmatrix} U & X & -\sqrt{2t_H} & 0 \\ X & U & -\sqrt{2t_H} & 0 \\ -\sqrt{2t_H} & -\sqrt{2t_H} & V_+ & 0 \\ 0 & 0 & 0 & V_- \end{pmatrix} \]
yields the eigenvalues \( \epsilon_{s \pm} = 2 \epsilon_t + U_H / 2 + V_+ \pm \sqrt{U_H^2 / 4 + 4t_H^2} \), \( \epsilon_{0} = 2 \epsilon_t + U_H - 2X + V_+ \) (singlet), and \( \epsilon_1 = 2 \epsilon_t + V_- \) (triplet), where the following quantities were introduced:
\[ \epsilon = \langle \Phi_{\pm a} | h | \Phi_{\pm a} \rangle, \]
\[ t_H = t - w = -\langle \Phi_{\pm a} | h | \Phi_{\mp a} \rangle - \langle \Psi_{\pm a}^d | C \Psi_{\mp a}^d \rangle / \sqrt{2}, \]
\[ V = V_+ - V_- = \langle \Phi_{\mp a}^d | C \Psi_{\mp a}^d \rangle - \langle \Psi_{\pm a}^d | C \Psi_{\pm a}^d \rangle, \]
\[ X = \langle \Psi_{\pm a}^d | C \Psi_{\mp a}^d \rangle, \]
\[ U_H = U - V_+ + X = \langle \Phi_{\pm a}^d | C \Phi_{\mp a}^d \rangle - \langle \Psi_{\pm a}^d | C \Psi_{\mp a}^d \rangle + \langle \Psi_{\pm a}^d | C \Phi_{\mp a}^d \rangle, \]
The exchange energy is the gap between the lowest singlet and the triplet state
\[ J = \epsilon_t - \epsilon_{s-} = V - \frac{U_H}{2} + \frac{1}{2} \sqrt{U_H^2 + 16t_H^2}. \]

The results of evaluation of matrix elements are given in Appendix. We plotted resulting \( J \) as a function of \( \omega_y \) and \( \omega_z \) at different values of magnetic field \( B \) in Fig. 2.

IV. CONCLUDING REMARKS.

In summary, we obtained the eigenstates of two-dimensional anisotropic oscillator in a magnetic field (Eq. (21)) which in degenerate isotropic case become the well-known Fock-Darwin states. We used obtained analytical expressions to study a system of two coupled elliptic QD in a magnetic field. We have calculated the exchange energy \( J(B, a, \omega_x, \omega_y) \) between spins of coupled QD as a function of magnetic field, interdot distance and parameters \( \omega_x, \omega_y \) defining shape of a single quantum dot. We have shown that by varying \( \omega_x \) or \( \omega_y \) the exchange coupling \( J \) can be switched on and off. This opens up the alternative way (compared to that being investigated in Ref. 3) of performing quantum computing operations using coupled QD as quantum gates. In the present paper, we didn’t consider spin-orbit contribution, Zeeman
splitting and interplay between nonadiabaticity of varying the system parameters and excitation of higher energy levels. We consider these questions in a separate paper (see Ref. [3]). We emphasize that our results can easily be applied to the system of two vertically coupled three-dimensional QD with in-plane magnetic field \( B \) being studied in Ref. [3], since the Hamiltonian of that problem separates on \( B \)-independent part, which is merely a harmonic oscillator, and \( B \)-dependent part which actually coincides with the Hamiltonian of two laterally coupled anisotropic QD being studied in the present paper.

To conclude, we believe that our results bring closer the day the first quantum computer\(^9\) to work.

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**APPENDIX A: HUND-MULLIKEN MATRIX ELEMENTS**

Here, we give the explicit expressions for the matrix elements defined in Eqs. (29) and (30). The single-particle matrix elements are given by

\[
\epsilon = \frac{3}{8} \frac{m_e \omega_\perp^2}{\kappa_\perp^2 a^2} + \frac{3}{8} \frac{S^2}{1 - S^2} \frac{m_e \omega_\perp^2}{\kappa_\perp^2} (1 + \kappa_\perp^2 a^2) + \frac{\hbar \omega_\perp \beta_1}{2m_e} + \frac{\hbar \omega_\perp \beta_2}{2m_e},
\]

\[
t = \frac{3}{8} \frac{S}{1 - S^2} \frac{m_e \omega_\perp^2}{\kappa_\perp^2} (1 + \kappa_\perp^2 a^2),
\]

where \( S = \exp(-\kappa_\perp^2 a^2 - \kappa_\perp^2 a^2) \).

The (two-particle) Coulomb matrix elements are formally equal to that given in Ref. [3], where only \( F_1 \) have to be changed. We give here the complete set of expressions for convenience:

\[
V_+ = c N^4 \left( 4g^2 (1 + S^2) F_1 + (1 + g^2)^2 F_2 + 4g^2 F_3 - 16 g^2 F_4 \right),
\]

\[
V_- = c N^4 (1 - g^2)^2 (F_2 - S^2 F_3),
\]

\[
U = c N^4 \left( (1 + g^4 + 2g^2 S^2) F_1 + 2g^2 F_2 + 2g^2 S^2 F_3 - 8g^2 F_4 \right),
\]

\[
X = c N^4 \left( (1 + g^4) S^2 + 2g^2 \right) F_1 + 2g^2 F_2 + 2g^2 S^2 F_3 - 8g^2 F_4,
\]

\[
w = c N^4 \left( -g(1 + g^2)(1 + S^2) F_1 - g(1 + g^2)^2 F_2 - g(1 + g^2) S^2 F_3 + (1 + 6g^2 + g^4) S^2 F_4 \right),
\]

with \( N = 1/\sqrt{1 - 2Sg + g^2} \), \( c = \frac{\omega_\perp}{\sqrt{\pi}} \), and \( g = (1 - \sqrt{1 - S^2})/S \). Here, we make use of the functions

\[
F_1 = \kappa_\perp K \left( 1 - \kappa_\perp^2 \kappa_\perp^2 \right),
\]

\[
F_2 = \kappa_\perp K \left( 1 - \kappa_\perp^2 \kappa_\perp^2 \right) e^{-\kappa_\perp^2 a^2} I_0 \left( \kappa_\perp^2 a^2 \right),
\]

\[
F_3 = \kappa_\perp K \left( 1 - \kappa_\perp^2 \kappa_\perp^2 \right) e^{\kappa_\perp^2 a^2} I_0 \left( \kappa_\perp^2 a^2 \right),
\]

\[
F_4 = \kappa_\perp K \left( 1 - \kappa_\perp^2 \kappa_\perp^2 \right) e^{\kappa_\perp^2 a^2 - \kappa_\perp^2 a^2} \times \sum_{k=\infty} \left( -1 \right)^k I_{2k} \left( \frac{\kappa_\perp^2 a^2 + \kappa_\perp^2 a^2}{4} \right) I_{2k} \left( \frac{\kappa_\perp^2 a^2}{2\kappa_\perp^2 a^2} \right),
\]

where \( I_n \) denotes the Bessel function of \( n \)-th order.

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Figure captions.

Figure 1. Two coupled anisotropic QD with one valence electron per dot. Each electron is confined to the xy plane. The magnetic field $B$ is perpendicular to the plane, i.e. along the z axis. The quartic potential $V(x, y)$ is given in Eq. (24) and is used to model the coupling of two anisotropic harmonic wells centered at $(\pm a, 0, 0)$.

Figure 2. Exchange energy $J$ in units of meV plotted against anisotropy $\omega_y/\omega_x$, as obtained from Heitler-London approximation. Upper graph: $\omega_x$ was fixed ($\hbar \omega_x = 3$ meV), $\omega_y$ was varied; interdot distance $a=0.7 a_{Bx}$. Bottom graph: $\omega_y$ was fixed ($\hbar \omega_y = 3$ meV), $\omega_x$ was varied; interdot distance $a$ is the same as in the upper graph. For both graphs, solid line: magnetic field $B=0.8T$; dashed-dot line: $B=1.2T$; dotted line: $B=4T$.

Figure 3. Exchange energy $J$ in units of meV plotted against anisotropy $\omega_y/\omega_x$, as obtained from Hund-Mulliken approach. Upper graph: $\omega_x$ was fixed ($\hbar \omega_x = 3$ meV), $\omega_y$ was varied; interdot distance $a=0.7 a_{Bx}$. Bottom graph: $\omega_y$ was fixed ($\hbar \omega_y = 3$ meV), $\omega_x$ was varied; interdot distance $a$ is the same as in the upper graph. Solid line: $B=0.8 T$; dashed-dot line: $B=1.2 T$; dotted line: $B=4$ T.
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