Spin properties of single electron states in coupled quantum dots

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Spin properties of single electron states in laterally coupled quantum dots in the presence of a perpendicular magnetic field are studied by exact numerical diagonalization. Dresselhaus (linear and cubic) and Bychkov-Rashba spin-orbit couplings are included in a realistic model of confined dots based on GaAs. Group theoretical classification of quantum states with and without spin orbit coupling is provided. Spin-orbit effects on the g-factor are rather weak. It is shown that the frequency of coherent oscillations (tunneling amplitude) in coupled dots is largely unaffected by spin-orbit effects due to symmetry requirements. The leading contributions to the frequency involves the cubic term of the Dresselhaus coupling. Spin-orbit coupling in the presence of magnetic field leads to a spin-dependent tunneling amplitude, and thus to the possibility of spin to charge conversion, namely spatial separation of spin by coherent oscillations in a uniform magnetic field. It is also shown that spin hot spots exist in coupled GaAs dots already at moderate magnetic fields, and that spin hot spots at zero magnetic field are due to the cubic Dresselhaus term only.

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I. INTRODUCTION

The possibility of tuning spin-orbit coupling in low-dimensional semiconductor electronic structures has stirred great interest in spin properties of lateral semiconductor electronic systems in the presence of Dresselhaus and Bychkov-Rashba spin-orbit couplings. The former appears in low-dimensional systems lacking inversion symmetry in the bulk (such as zinc-blende semiconductors), the latter in low-dimensional structures with asymmetric confining potentials. The principal question is what spin and charge properties and to what degree can be affected and manipulated by this tuning. Such questions are of fundamental importance for spintronics.

Electron spins in coupled quantum dot systems have been proposed to perform universal gating of quantum computers. The spin acts as a qubit and exchange coupling provides the physical realization of two-qubit gates. Another application of a controlled coupling between dots is spin entanglement distillation in which singlet and triplet states get spatially separated during adiabatic passage through trapped states. Understanding of spin-orbit properties of coupled dots is thus of great interest to quantum information processing.

Spin-orbit coupling provides a way for orbital degrees of freedom to influence spin states. As a result the spin dynamics is affected, making spin qubit operations more complex (it was shown, though, that two qubit operations can be performed reliably even in the presence of spin-orbit interaction which leads to anisotropic exchanges). Furthermore, spin-orbit coupling leads to spin decoherence and relaxation due to phonons, limiting the operation time. The impressive experimental progress in coherent oscillations in coupled dot systems, as well in spin dephasing and spin manipulation in single and double dots, provides additional strong impetus for investigating spin states in double dots. Spin-orbit properties of single dots have been already extensively investigated.

In this paper we investigate the role of spin-orbit coupling, represented by the Dresselhaus (both linear and cubic) and Bychkov-Rashba terms, in spin and charge properties of two laterally coupled quantum dots based on GaAs materials parameters. We perform numerically exact calculations of the energy spectrum using the method of finite differences. We first study the general structure of the energy spectrum and the spin character of the states of the double dot system. We construct the group theoretical correlation diagram for the single and double dot states and indicate the possible transitions due to spin-orbit coupling. This group theoretical classification is used in combination with Löwdin perturbation theory to explain analytically our numerical results. In particular, we show that while allowed by symmetry, the specific forms of the linear spin-orbit interactions do not lead to spin hot spots in the absence of magnetic field (spin hot spots are nominally degenerate states lifted by spin-orbit coupling). Only the cubic Dresselhaus term gives spin hot spots. If identified experimentally, the strength of the cubic term can be detected.

We next focus on two important measurable parameters: electronic g-factor and tunneling amplitude. In single dots the variation of the effective g-factor with the strength of the spin-orbit interaction has been investigated earlier. The effect is not large, amounting to a fraction of a percent. Similar behavior is found for double dots. In our case of GaAs the contribution of the g-factor from spin-orbit coupling is typically about 1%, due to the linear Dresselhaus term.

More exciting is the prospect of influencing coherent tunneling oscillations between the dots by modulating the spin-orbit coupling strength. Two effects can appear: (i) the tunneling amplitude or frequency can be modulated by spin-orbit coupling and, (ii) the tunneling amplitude can be spin dependent. We show how a
naive application of perturbation theory leads to a misleading result that (i) is present in the second order in linear spin-orbit coupling strengths, giving rise to an effective tunneling Hamiltonian involving spin-flip tunneling at zero magnetic field. Both numerical calculations and an analytical argument, presented here, show that this is incorrect and that there is no correction to the tunneling Hamiltonian in the second order of linear spin-orbit terms. The dominant correction in the second order comes from the interference of linear and cubic Dresselhaus terms. We propose to use this criterion, that the corrections to linear terms vanish in the second order, to distinguish between single and double dots as far as spin properties of the states are concerned. Indeed, at very small and very large intradot couplings the states have a single dot character and the correction to energy due to linear spin orbit terms depends on the interdot distance (except for the two lowest states which provide tunneling). We find that dots are “coupled” up to the interdot distance of about five single-dot confinement lengths.

In the presence of magnetic field the time reversal symmetry is broken. The presence of spin-orbit coupling then in general leads to a spin dependent tunneling amplitude. Spin up and spin down states will oscillate between the corresponding spin state, realizing effectively the interference of linear and cubic Dresselhaus terms. We propose to use this criterion, that the corrections to linear terms vanish in the second order, to introduce dimensionless strengths of the individual terms.

The paper is organized as follows. In Sec. II we introduce the model, the numerical technique, and materials and system parameters. In Sec. III we review the benchmark case of single dots with spin-orbit coupling and magnetic field. Coupled double dots are studied in Sec. IV, separately in zero and finite magnetic fields. We conclude with the discussion of our results in Sec. V.

II. MODEL

We consider conduction electrons confined in a [001] plane of a zinc-blende semiconductor heterostructure, with additional confinement into lateral dots given by appropriately shaped top gates. A magnetic field $B$ is applied perpendicular to the plane. In the effective mass approximation the single-electron Hamiltonian of such a system, taking into account spin-orbit coupling, can be decomposed into several terms:

$$H = T + V_C + H_Z + H_{BR} + H_D + H_{D3}. \quad (1)$$

Here $T = \hbar^2 K^2/2m$ is the kinetic energy with the effective electron mass $m$ and kinetic momentum $\hbar \mathbf{k} = \hbar \mathbf{p} + e \mathbf{A} = -i \hbar \nabla + e \mathbf{A}$; $e$ is the proton charge and $\mathbf{A} = B(-y/2, x/2, 0)$ is the vector potential of $\mathbf{B} = (0, 0, B)$. Operators of angular momentum with mechanical and canonical momenta are denoted as $L = r \times (\hbar \mathbf{K})$ and $I = r \times (\hbar \mathbf{k})$. The quantum dot geometry is described by the confining potential $V_C(r)$. Single dots will be described here by a parabolic potential $V_C = (1/2)m_0 \omega_0^2 r^2$, characterized by confinement energy $E_0 = \hbar \omega_0/2$ and confinement length $l_0 = (\hbar/m_0 \omega_0)^{1/2}$, setting the energy and length scales, respectively. Coupled double dots will be described by two displaced (along $x$) parabolas:

$$V_C^{dd} = \frac{1}{2}m_0 \omega_0^2 (|x| - l_0 d)^2 + y^2; \quad (2)$$

the distance between the minima is $2d$ measured in the units of $l_0$. The Zeeman energy is given by $H_Z = (g^* / 2) \mu_B \sigma_z B$, where $g^*$ is the conduction band g-factor, $\mu_B$ is the Bohr magneton, and $\sigma_z$ is the Pauli matrix. In order to relate the magnetic moment of electrons to their orbital moment, we will use dimensionless parameter $\alpha_Z = g^* m / 2m_e$, where $m_e$ is the free electron mass.

Spin-orbit coupling gives additional terms in confined systems. The Bychkov-Rashba Hamiltonian, appears if the confinement is not symmetric in the growth direction (here $z$). The strength $\tilde{\alpha}_{BR}$ of the interaction can be tuned by modulating the asymmetry by top gates. Due to the lack of spatial inversion symmetry in zinc-blende semiconductors, the spin-orbit interaction of conduction electrons takes the form of the Dresselhaus Hamiltonian, which, when quantized in the growth direction $z$ of our heterostructure gives two terms, one linear and one cubic in momentum:

$$H_{BR} = \tilde{\alpha}_{BR} (\sigma_x K_y - \sigma_y K_x), \quad (3)$$

appears if the confinement is not symmetric in the growth direction (here $z$). The strength $\tilde{\alpha}_{BR}$ of the interaction can be tuned by modulating the asymmetry by top gates. Due to the lack of spatial inversion symmetry in zinc-blende semiconductors, the spin-orbit interaction of conduction electrons takes the form of the Dresselhaus Hamiltonian, which, when quantized in the growth direction $z$ of our heterostructure gives two terms, one linear and one cubic in momentum:

$$H_D = \frac{\gamma_c}{2} \langle K_z^2 \rangle (-\sigma_z K_x + \sigma_y K_y), \quad (4)$$
$$H_{D3} = \langle \gamma_c / 2 \rangle (\sigma_x K_x K_y^2 - \sigma_y K_y K_x^2) + H.c., \quad (5)$$

where $\gamma_c$ is a material parameter. The angular brackets in $H_D$ denote quantum averaging in the $z$ direction—the magnitude of $H_D$ depends on the confinement strength. We will denote the sum of the two linear spin-orbit terms by $H_{lin} = H_D + H_{BR}$. The complete spin-orbit coupling is then $H_{SO} = H_{lin} + H_{D3}$. We find it useful to introduce dimensionless strengths of the individual terms of the spin-orbit interaction by relating them to the confinement energy of a single dot $E_0$. We denote $\alpha_{BR} = \tilde{\alpha}_{BR} / E_0 l_0$ and $\alpha_D = \gamma_c / 2 E_0 l_0$ for linear terms, and $\alpha_{D3} = \gamma_c / 2 E_0 l_0^3$ for the cubic Dresselhaus term.
In our numerical examples we use $E_0 = \hbar \omega_0/2 = 1.43$ meV for the confinement energy, which corresponds to the confinement length of $l_0 = 20$ nm. We further use bulk GaAs materials parameters: $m = 0.067 m_e$, $g^* = -0.44$, and $\gamma_c = 27.5$ eVÅ. For $\langle k_z^2 \rangle$ we choose $5.3 \times 10^{-4}$ Å$^2$, which corresponds to $\gamma_c(k_z^2) = 14.6$ meV Å. This value of $\langle k_z^2 \rangle$ corresponds to the ground state of a 6 nm thick triangular potential well. For $\alpha$ we choose a generic value of 4.4 meV Å, which is in line of experimental observations. The dimensionless parameter of the Zeeman splitting then is $\alpha_Z = -0.015$, while the strengths of the spin-orbit interactions are $\alpha_{BR} \approx 0.015$, $\alpha_D \approx 0.05$, and $\alpha_{D3} \approx 0.001$. Except for anti-crossings, the spin-orbit interaction is a small perturbation to the electronic structure; it is, however, essential for investigating spin properties.

Our analytical calculations will often refer to the Fock-Darwin spectrum, which is the spectrum of Hamiltonian $H_{SO} = 0$. The corresponding wave functions $\Psi$ (expressed in polar coordinates $r$ and $\phi$), and energies $\epsilon$ are

$$\Psi_{n,l,\sigma}(r,\phi) = C \rho |l| e^{-\gamma^2/2} L_n(\rho^2) e^{i l \phi} \xi(\sigma),$$  \hspace{1cm} (6)

$$\epsilon_{n,l,\sigma} = 2E_0 \frac{l_B^2}{l_B^2}(2n + |l| + 1) + B \frac{\hbar c}{2m} (l + \alpha_Z \sigma), (7)$$

where $\rho = r/l_B$ is the radius in the units of the effective confinement length $l_B$, defined by $l_B^2 = \left| \frac{l_B^2}{l_B^2} \right| \sqrt{1 + B^2 e^2 l_B^2 / \hbar^2}$; $n$ and $l$ are the principal and orbital quantum numbers, respectively, $C$ is the state dependent normalization constant, and $L_n^{\alpha l}$ are associated Laguerre polynomials. Spinors $\xi(\sigma)$ describe the spin $\sigma$ state of the electrons. Since the parabolic dot has rotational symmetry in the plane, the states have well defined orbital momentum $l$ and spin $\sigma$ in the $z$ direction. We also introduce a useful dimensionless measure $\theta$ of the strength of the magnetic field induced confinement compared to the potential confinement: $\theta = B e l_B^2 / 2 h$, $0 < \theta < 1$. The parameter $\theta$ gives the number of magnetic flux quanta through a circle with radius $l_B$. For large magnetic fields, $\theta \approx 1 - (Be l_B^2 / 2h)^2 / 2$. The confining length can be expressed as $l_B = l_0(1 - \theta^2)^{1/4}$.

As it is not possible to solve for the spectrum of Hamiltonian $H_{SO}$ analytically, we treat it numerically with the finite differences method using Dirichlet boundary conditions (vanishing of the wave function at boundaries). The magnetic field is included via the Peierls phase: if $H(r_i, r_j)$ is the discretized Hamiltonian connecting grid points $r_i$ and $r_j$ at $B = 0$, the effects of the field are obtained by adding a gauge phase: $H(r_i, r_j) \exp[\mu(\hbar / e) \int_{r_i}^{r_j} A \cdot dl]$. In our simulations we typically use $50 \times 50$ grid points. The resulting matrix eigenvalue problem is solved by Lanczos diagonalization. The achieved accuracy is about $10^{-5}$.

### III. SINGLE DOTS

As a starting point we review the effects of spin-orbit coupling in single dots. We are interested in the changes to the spectrum and, in particular, to the magnetic moment of the lowest states, that is, to the effective $g$-factor. The calculated spectrum of a single dot is shown in Fig. 4.

There are three ways in which spin-orbit coupling influences the spectrum: (i) First, the levels are uniformly shifted down, in proportion to $\alpha^2$ (by $\alpha$ here we mean any of $\alpha_{BR}$, $\alpha_D$, or $\alpha_{D3}$). (ii) Second, the degeneracy at $B = 0$ is lifted, again in proportion to $\alpha^2$. (iii) Finally, at some magnetic field the level crossing of the Fock-Darwin levels is lifted by spin-orbit coupling. The resulting level repulsion is linear in $\alpha$.

The states here are the spin hot spots, that is states in which both Pauli spin up and down species contribute significantly.

The above picture can be understood from general symmetry considerations within the framework of perturbation theory. All spin-orbit terms commute, at $B = 0$, with the time inversion operator $T = i \sigma_y C$, where $C$ is the operator of complex conjugation. Therefore Kramer’s degeneracy is preserved so that the states are always doubly degenerate. The linear terms can be transformed into each other by a unitary transformation $(\sigma_z + \sigma_y)/\sqrt{2}$ (spin rotation around $[110]$ by $\pi$), which commutes with $H_0$. Therefore the effects on the energy spectrum induced individually by the linear Dresselhaus and the Bychkov-Rashba terms are identical at $B = 0$. At finite magnetic fields the two interactions give qualitatively different effects in the spectrum, especially for spin hot spots, as discussed below.

For any $B$ the following commutation relations hold for the linear terms:

$$[H_{BR}, l_z + s_z] = 0, \quad [H_D, l_z - s_z] = 0. \quad (8)$$

This means that $H_{BR}$ commutes with the angular momentum, while $H_D$ does not. This will influence the interference between the two terms in the energy spectrum.

We can use the Fock-Darwin states as a basis for perturbation theory. Up to the second order the energy of state $|i\rangle = \Psi_{n,l,\sigma}$ is

$$E_i = \epsilon_i + |\langle i | H_{SO} | i \rangle| + \sum_{j \neq i} \frac{\langle i | H_{SO} | j \rangle \langle j | H_{SO} | i \rangle}{\epsilon_i - \epsilon_j}. \quad (9)$$

The first order correction is zero for all spin-orbit terms since $H_{SO}$ contain only odd powers of $K$ whose expectation values in the Fock-Darwin states vanish. If the perturbation expansion is appropriate, the spin-orbit interactions have a second order (in $\alpha$) effect on energy.

Both linear spin-orbit terms couple states with orbital momenta $l$ differing by one. It then follows from the commutation relations that $H_{BR}$ preserves the total angular momentum $l + s$, while $H_D$ preserves the quantity $l - s$. As a result, there is no correction to
and from the data. For clarity, a linear trend was subtracted to grow as \( \alpha \). The Fock-Darwin spectrum, Eq. (7). b) Lowest orbital excited states with \( \alpha \) about 13 T. For clarity, a linear trend was subtracted from the data.

The Bychkov-Rashba and Dresselhaus Hamiltonians act independently on the Fock-Darwin spectrum (up to the second order). To gain more insight into the perturbed structure of the spectrum at \( B = 0 \), we rewrite Eq. (9) using an auxiliary anti-hermitian operator \( H_{SO}^{op} \) defined by the commutation relation \( [H_0, H_{SO}^{op}] = H_{SO} \). If such an operator exists, the second order correction in \( \alpha \) is then

\[
\sum_{j \in \mathcal{N}} \langle \alpha | H_{SO} | j \rangle \langle j | H_{SO} | \alpha \rangle = \langle \alpha | \frac{1}{2} [H_{SO}^{op}, H_{SO}] | \alpha \rangle + \text{Re} \langle \alpha | H_{SO} P_N H_{SO}^{op} | \alpha \rangle,
\]

where \( P_N \) is the projector on the subspace \( \mathcal{N} \) of the states included from the summation. In our case here it is just one state, \( \mathcal{N} = \{ | \alpha \rangle \} \). The last term in (10) then vanishes. The auxiliary operator for \( H_{D3} \) is not known and if found, it must depend on the confining potential. Operators for the linear terms are:

\[
H_{D3}^{op} = -i(\alpha_D/2l_0)(x\sigma_y - y\sigma_x),
\]

(11)

\[
H_{BR}^{op} = i(\alpha BR/2l_0)(y\sigma_x - x\sigma_y).
\]

(12)

The corresponding commutators are (in the zero magnetic field \( K = k \), \( L_z = l_z \), \( \theta = 0 \); the last expression will be useful later)

\[
[H_{D3}^{op}, H_D] = -E_0\alpha_D^2(1 - \sigma_z L_z),
\]

(13)

\[
[H_{BR}^{op}, H_{BR}] = -E_0\alpha_{BR}^2(1 + \sigma_z L_z),
\]

(14)

\[
[H_{D3}^{op}, H_{D3}] = E_0\alpha_D^2\alpha_D\alpha_{D3} \left( K_z^2 + K_y^2 - 2\sigma_z [x K_y K_z^2 - y K_x K_y^2 - 2i(x K_x + y K_y)] \right)
\]

(15)

Because \( [H_{D3}^{op}, H_{BR}] = [H_{D3}^{op}, H_D] = 0 \), the corrections to the second order perturbation add independently for \( H_{BR} \) and \( H_D \) (as also noted above from the selection rules), we can introduce \( H_{lin}^{op} = H_{D3}^{op} + H_{BR}^{op} \). An alternative route to Eq. (10) is to transform the Hamiltonian with \( \exp (-H_{SO}^{op}) \) to \( \hat{H} = H_0 - (1/2)[H_{SO}, H_{SO}] \) in the second order of \( \alpha \). The final result can be also obtained in a straightforward way by using the Thomas-Reiche-Kuhn sum rule in the second order of perturbation theory with the original spin-orbit terms. The resulting effective Hamiltonian is (terms depending on \( \alpha_{D3} \) are omitted here)

\[
\hat{H} = H_0 - E_0(\alpha_D^2 + \alpha_{BR}^2)/2 + E_0\sigma_z L_z(\alpha_D^2 - \alpha_{BR}^2)/2.
\]

(16)

This Hamiltonian, in which the spin-orbit coupling appears in its standard form, neatly explains point (ii) about the lifting of the degeneracy at \( B = 0 \). The levels in Fig. (1b), for example, are four fold degenerate (\(| l | = 1 \), \(| | = 1 \) without spin-orbit coupling. Turning on, say, \( H_D \), will split the levels into two groups: energy of the states with \( \sigma > 0 \) would not change in the second order, while the states with \( \sigma < 0 \) will go down in energy by \( E_0\alpha_D^2/2 \), as seen in Fig. (1b).

A. Spin hot spots

Spin hot spots are states formed by two or more states whose energies in the absence of spin-orbit coupling are degenerate or close to being degenerate, while turning on
The coupling removes the degeneracy. Such states are of great importance for spin relaxation, which is strongly enhanced by their presence. The reason is that the degeneracy lifting mixes spin up and spin down states and so transitions between states of opposite magnetic moment will involve spin flips with a much enhanced probability compared to normal states.

Figure II shows an interesting situation where two degenerate levels are lifted by spin-orbit coupling. The lifting is of the first order in $\alpha$, unlike the lifting of degeneracy at $B = 0$ in which case the degenerate states are not directly coupled by $H_{SO}$. In a finite magnetic field, at a certain value $B_{acr}$, the states of opposite spins and orbital momenta differing by one cross each other, as follows from the equation (16). The crossing field is $B_{acr} \approx |\alpha Z|^{-1/2} \hbar/(e\ell_0^2)$, which is about 13.4 T for our parameters (making the confinement length larger the magnitude of the field would decrease). Spin-orbit interaction couples the two states thereby lifting the degeneracy. For GaAs, where $g^* < 0$, only the Bychkov-Rashba term couples the two states. The Dresselhaus terms are not effective ($H_{D3}$ would introduce such a splitting at $3B_{acr}$). The energy splitting due to $H_{BR}$ is

$$\Delta = cE_0\alpha_{BR}(1 - \theta_{acr})(1 - \theta^2_{acr})^{1/4},$$

(17)

where $c$, which is a number of order 1, depends on the quantum numbers of the two states. Since spin hot spots at $B_{acr}$ are due only $H_{BR}$, the splittings could help to sort out the Bychkov-Rashba versus Dresselhaus contributions. Figure II shows the calculated level repulsion for states $n = 0, l = 0, \sigma = \downarrow$ and $n = 0, l = -1, \sigma = \uparrow$. The magnitude of $\Delta$, though being linear in $\alpha_{BR}$, is on the order of $10^{-3}$ meV and thus comparable to the energy scales associated with quadratic spin-orbit perturbations.

### B. Effective g-factor

When probing spin states in quantum dots with magnetic field, important information comes from the measured Zeeman splitting. We will focus here on the two lowest spin states and calculate the effective g-factor as $g = (E_{0,0,\downarrow} - E_{0,0,\uparrow})/(\mu_B B)$. If $H_{SO} = 0$, then the effective g-factor equals to the conduction band value $g^*$. The actual value in the presence of spin-orbit coupling is important for understanding single spin precession in magnetic field, which seems necessary to perform single qubit operations in quantum dots. We have obtained the following contributions to the g-factor from non-degenerate states (is, excluding spin hot spots) second-order perturbation theory [Eq. (16)] (for linear spin-orbit terms these are derived also in the text):

$$\delta g_{D-D} = -\frac{\alpha_{\downarrow}^2}{2m/m_e} \frac{\sqrt{1 - \theta^2} [1 - \theta^2 - 2(1 + \theta^2)\alpha Z]}{1 - \theta^2(1 + 4\alpha Z + 4\alpha^2 Z)} ,$$

$$\delta g_{BR-BR} = \frac{\alpha_{BR}^2}{2m/m_e} \frac{\sqrt{1 - \theta^2} [1 - \theta^2 + 2(1 + \theta^2)\alpha Z]}{1 - \theta^2(1 + 4\alpha Z + 4\alpha^2 Z)} ,$$

$$\delta g_{D-D3} = \frac{\alpha_{D\alpha D3}}{m/m_e} \frac{[1 - \theta^2 - 2(1 + \theta^2)\alpha Z]}{1 - \theta^2(1 + 4\alpha Z + 4\alpha^2 Z)} ,$$

$$\delta g_{D3-D3} = \frac{\alpha_{\downarrow}^2}{8m/m_e \theta(1 - \theta^2)} \frac{2(1 - \theta^2)^2}{1 - \theta(1 + 2\alpha Z)} + \frac{(1 - \theta)^2(1 + \theta^2)}{3 - \theta^2(1 + 2\alpha Z)} - \frac{3(1 + \theta)^6}{3 + \theta(3 - 2\alpha Z)} - \frac{2(1 + \theta)^2(1 + \theta^2)^2}{1 - \theta(1 + 2\alpha Z)} - \frac{(1 - \theta)^2(1 + \theta^4)}{3 + \theta(3 + 2\alpha Z)} \right) .$$

(18)

Here $\delta g_{A-B}$ stands for a correction that is proportional to $\alpha_{\downarrow}^2 / \alpha_{\uparrow}$. The functions $\delta g_{A-B}$ are plotted in Fig. II. We can understand the limits of $\delta g$ at $B \to \infty (\theta \to 1)$ if we notice that in the natural length unit $l_B$ the momentum $K_x = -i\partial_x - yBc/2\hbar = l_B^{-1}[-i\partial_x/l_B - \theta\partial_y/l_B]$. In the limit $B \to \infty$ the matrix elements of $H_D$, which is linear in $K$, scale as $l_B^{-1}$, while the Fock-Darwin energies scale as $l_B^{-2}$. The second order D-D correction to $E_{0,0,\downarrow} - E_{0,0,\uparrow}$ is thus independent of $l_B$; it converges to $-E_0\alpha_{\downarrow}^2/(1 + \alpha Z)$. The BR-BR correction is analogous, with the limit $E_0\alpha_{\downarrow}^2/\alpha_{\downarrow}$, to get the g-factor we divide the energy differences by $\mu_B B$ and get $\delta g_{D-D} (\theta \to 1) \propto B^{-1}$; similarly for $H_{D3}$. Since $H_{D3}$ scales as $l_B^{-3}$ one gets $\delta g_{D3-D3} (\theta \to 1) \propto 2\alpha_{D\alpha D3}m/(1 + \alpha Z)m_e$ and $\delta g_{D3-D3} (\theta \to 1) \propto B$. It seems that for increasing $B$
| magnetic field | SO terms | symmetries of $H$ |
|---------------|----------|------------------|
| $B = 0$       | none     | $I_x, I_y, I, T, R_B$ |
|               | $BR$     | $-i\sigma_x I_x, -i\sigma_y I_y, -i\sigma_z I, T$ |
|               | $D, D_3$ | $-i\sigma_y I_x, -i\sigma_z I_y, -i\sigma_z I, T$ |
| $B > 0$       | none     | $-i\sigma_z I, T$ |
|               | any      | $-i\sigma_z I$ |

There inevitably comes a point where the influence of $H_{D3}$ on the g-factor dominates. But at $B = B_{ac}$ there is an anti-crossing of the states ($0, 0, \downarrow$) and ($0, -1, \uparrow$) so for larger $B$ the g-factor does not describe the energy difference between the two lowest states, but between the second excited state and the ground state. The value of $B$ where $\delta_{BD3-D3} = \delta_{BD-0}$ is given by $B \approx (\hbar/eB_0) \alpha_{D3}/\sqrt{2}$. For GaAs parameters it is $\approx 25$ T. After anti-crossing the first exited state is $\Psi_{\uparrow} \rightarrow \Psi_{\downarrow}$, and its energy difference to the ground state is divided by $\mu B$ is $\approx 1/B^2$ for $H_0$. The corrections from spin-orbit terms are $D-D, BR-BR \propto 1/B^5$, $D-D_3 \propto 1/B^4$, and $D_3-D_3 \propto 1/B^3$.

## IV. DOUBLE DOTS

A double dot structure comprises two single dots close enough for their mutual interaction to play an important role. Here we consider symmetric dots modeled by $V_C^d$ of Eq. (2). Such a potential has an advantage that in the limits of small $d \rightarrow 0$ and large $d \rightarrow \infty$, the solutions converge to the single dot solutions centered at $x = 0$ and $\pm l_0d$, respectively. We denote the displaced Fock-Darwin states as $\Psi^{\pm d}_{n,l,\sigma}(x, y) \equiv \Psi_{n,l,\sigma}(x \pm l_0d, y)$.

The symmetries of the double dot Hamiltonian with spin-orbit couplings are listed in Tab. I. The time symmetry is always present at $B = 0$, giving Kramer’s double degeneracy. The rotational space symmetry from the single dot case is lost; instead there are two discrete symmetries – reflections $I_x$ about $y$ and $I_y$ about $x$. In zero magnetic field and without spin-orbit terms, the Hamiltonian has both $I_x$ and $I_y$ symmetries. If only Rashba or Dresselhaus terms are present, we can still preserve symmetries $I_x$ and $I_y$ by properly defining the symmetry operators to act also on the spinors (forming the double group). The Bychkov-Rashba term, $H_0 + H_{BR}$, is invariant to operations defined by the spatial invariance. This is not the case of $H_D$, since here the operators $-i\sigma_y I_x$ and $-i\sigma_z I_y$ do not describe a spatial reflection of both the orbital and spinor parts. The symmetry operations for $H_{BR}$ and $H_D$ are connected by the unitary transformation $\sigma_x \rightarrow \sigma_y/\sqrt{2}$, which connects the two Hamiltonians themselves. Finally, if both spin-orbit terms are present, or at $B > 0$, the only space symmetry left is $I = I_x I_y$.

In the following we consider separately the cases of zero and finite magnetic fields.

### A. Energy spectrum in zero magnetic field, without spin-orbit terms.

If no spin-orbit terms are present the group of our double dot Hamiltonian is $C_{2v} \otimes SU(2)$. The $SU(2)$ part accounts for the (double) spin degeneracy. The orbital parts of the eigenstates of the Hamiltonian therefore transform according to the irreducible representations of $C_{2v}$. The representations $\Gamma_i, i = 1..4$, along with their transformation properties under the symmetries of $C_{2v}$, are listed in Tab. II. The symmetry properties will be used in discussing the perturbed spectrum.

We denote the exact eigenfunctions of the double dot Hamiltonian with $H_{SO} = 0$ as $\Gamma_i a^\dagger b$, where $a(b)$ is the single dot level to which this eigenfunction converges as $d \rightarrow 0(\infty)$; $i$ labels the irreducible representation, $\sigma$ denotes spin. We have chosen the confining potential to be such, that at $d \rightarrow 0(\infty)$ the solutions of the double dot $H_0$ converge to the (shifted) Fock-Darwin functions, if properly symmetrized according to the representations of $C_{2v}$. These symmetrized functions will be denoted as $g_i^{n,l,\sigma}$, where (up to normalization)

$$g_i^{n,l,\sigma} = (\Psi_{n,l,\sigma}^d + D_i \Psi_{n,-l,\sigma}^d)/2 = \Gamma_i (\Psi_{n,l,\sigma} + D_i \Psi_{n,-l,\sigma}).$$

The numbers $D_i(L_i)$ for different irreducible representations are in the Tab. III.

Generally, up to normalization, the exact solution can be written as a linear combination of any complete set of functions (we omit the spin index which is the same for all terms in the equation)

$$\Gamma_i = \sum_{n,l} c(n, l) g_i^{n,l} = g_i^{n_0, l_0} + \sum_{n,l} c(n, l) g_i^{n,l}.\quad (20)$$

The last equation indicates the fact, that for a function $\tilde{\Gamma}_i \equiv \Gamma_i^{ab}$ in the limit $d \rightarrow 0(\infty)$, there will be a dominant $g$-
function in the sum with the numbers \( n_0, l_0 \) given by the level \( a(b) \) and the coefficients \( c \) for the other functions will converge to zero. We term the approximation \( c(n, l) = 0 \) as a linear combination of single dot orbitals (LCSDO).

Knowing the representations of the double dot Hamiltonian and the fact that Fock-Darwin functions form \( SO(2) \) representations (reflecting the symmetry of single dot \( H_0 \)) we can decompose all single dot levels into the double dot representations and thus formally construct the energy spectrum of a double dot using the symmetry considerations only.

Following the standard technique for constructing such correlation diagrams (connecting states of the same representation and avoiding crossing of lines of the same representation) we arrive at the spectrum shown in Fig. 3. The ground state transforms by the symmetry operations according to \( \Gamma_1 \) (identity), while the first excited state according to \( \Gamma_2 \) (\( x \)). This is expected for the symmetric and antisymmetric states formed by single dot ground states. The symmetry structure of the higher excited states is important to understand spin-orbit coupling effects. Indeed, the spin-orbit terms couple two opposite spins according to certain selection rules. Since \( H_D \), for example, transforms similarly to \( x \oplus y \), it couples the ground state \( \Gamma_1 \) with \( \Gamma_2 \) and \( \Gamma_4 \). In general, odd numbered representations can couple to even numbered representations. The same holds for \( H_{BR} \) and \( H_{D3} \). If we include either \( H_{BR} \) or \( H_D \) into the Hamiltonian, and consider spinors as the basis for a representation, the states would transform according to \( \Gamma_5 \), the only irreducible representation of the double group of \( C_{2v} \).

The calculated numerical spectrum for our model structure is shown in Fig. 3. There is a nice qualitative correspondence with Fig. 3. In Fig. 4 by vertical bars we denote coupling through \( H_D \) or \( H_{BR} \) \((\langle i|H_D|j\rangle = \langle i|H_{BR}|j\rangle \)). The couplings follow the selection rule described above. Since there are several level crossings in the lowest part of the spectrum, a question arises if spin hot spots are formed in the presence of spin-orbit coupling. It turns out, that there is no first-order level repulsion at the crossings due to the linear spin-orbit terms because the levels are not coupled by the linear terms, even though such couplings are allowed by symmetry. There are no spin hot spots due to the linear spin-orbit terms at zero magnetic field. For example \( \Gamma_1^{11} \) and \( \Gamma_1^{21} \) are not coupled by spin-orbit terms, and therefore their degeneracy (at \( 2d_0 \approx 50 \text{ nm} \)) is not lifted by linear spin-orbit terms as we would expect from symmetry (actually, there is an anti-crossing which is of the order \( \alpha_B^2 \), instead of the expected \( \alpha_B^2 \)). The cubic Dresselhaus term gives here (and also in other crossings that conform with the selection rules) a linear anti-crossing, as one expects. The absence of anti-crossings from the linear spin-orbit terms will be explained in the next section.

Since our main goal here is to study the effects of spin-orbit coupling on the tunneling between the two dots, we first look at the tunneling for \( H_{SO} = 0 \). The tunneling energy, \( \delta E_t / 2 \), is given by the difference between the energies of the symmetric ground state and the asymmetric first excited orbital state: \( \delta E_t = E_A - E_S \). We compare the LCSDO approximation with our numerically exact calculations. The functions Eq. (10) are not orthogonal. If we introduce the overlap integrals between these functions (all the indices of a \( g \)-function are denoted by one letter here) by \( S_{ij} = \langle i|j \rangle \), and the Hamiltonian matrix elements \( H_{ij} = \langle i|H|j \rangle \), variational theory gives for the expansion coefficients \( c_i \) of a double dot state \( \Gamma = \sum_i c_i|i\rangle \) the generalized eigenvalue equation,

\[
\sum_j H_{ij} c_j = E \sum_j S_{ij} c_j. \tag{21}
\]

We will compute the energy of the two lowest orbital double dot states, \( \Gamma_1^{00} \equiv \Gamma_S^0 \), \( \Gamma_1^{20} \equiv \Gamma_A^{20} \), which are a symmetric and an antisymmetric double dot state with respect to \( x \).

The energies are denoted as \( E_S^{(0)}, E_A^{(0)} \), where index zero indicates the absence of spin-orbit coupling.

FIG. 3: Single electron spectrum of a symmetric \((C_{2v})\) lateral double dot structure as a function of the interdot separation, at \( B = 0 \), derived by applying group theoretical considerations. Single dot states at \( d = 0 \) and \( d = \infty \) are labeled by the principal \((n)\) and orbital \((l)\) quantum numbers, while the double dot states are labeled according to the four irreducible representations \( \Gamma_i \) of \( C_{2v} \). The lowest double dot states have explicitly written indices showing the excitation level of the \( d = 0 \) and \( d = \infty \) states they connect. Every state is doubly (spin) degenerate, and spin index is not given.

We first use the LCSDO approximation suitable for the limit \( d \rightarrow \infty \), that is we approximate \( \Gamma_1 \) by \( \Gamma_{10} \). This means the basis in Eq. (21) consists of one function and the solution for the energy is \( E_i = H_{ii}/S_{ii} \). For the considered states we obtain:

\[
E_S^{(0)} = 2E_0 \frac{1 - |1 - 2d_0|/\sqrt{\pi} d^2 e^{-d^2} + d^2 \text{Erf}(d) \bigg|}{1 + e^{-d^2}},
\]

\[
E_A^{(0)} = 2E_0 \frac{1 - e^{-d^2} + d^2 \text{Erf}(d) \bigg|}{1 - e^{-d^2}}. \tag{22}
\]
The off-diagonal element in the matrix \( \langle 22 \rangle \), the other for the limiting case of large \( d \) forms of \( \delta E_0 \) and get the basis for Eq. (21) to be
take the next excited function of the same symmetry ample, for the ground state to go beyond LCSDO, we
of \( (\Psi_{0,0,\sigma}) \) is plotted in Fig 5. The complete expression is in excel-
H 
H
\[
\delta E_0 \approx E_0 \frac{4}{\sqrt{\pi}} d e^{-d^2}.
\]
(23)
To understand this result, we get it once again by taking a two dimensional basis in Eq. (21) consisting of functions \( \Psi_{0,0,\sigma} \) and \( \Psi_{0,0,\sigma} \). In the limit \( d \rightarrow \infty \) both diagonal elements of the matrix \( H \) converge to the energy of the Fock-Darwin ground state (2\( E_0 \)). Then the difference of the eigenvalues of \( H \) is given by the off-diagonal matrix element, which is
\[
H_{12} = \langle \Psi_{0,0,\sigma} | H | \Psi_{0,0,\sigma} \rangle \sim (\Psi_{0,0,\sigma}^d \Psi_{0,0,\sigma}^d) (r = 0) \sim e^{-d^2}.
\]
Any further refinement beyond LCSDO would not contribute significantly to the calculated \( \delta E_0 \). For example, for the ground state to go beyond LCSDO, we take the next excited function of the same symmetry and get the basis for Eq. (21) to be \( \{ g_{0,0,\sigma}, g_{1,1,\sigma} \} \). The off-diagonal element in the matrix \( H \) is
\[
H_{12} = \langle \Psi_{0,0,\sigma} | H | \Psi_{0,0,\sigma} \rangle \approx E_0 P(d) e^{-d^2},
\]
where \( P(d) \) is a polynomial in \( d \). Since now \( H_{11} - H_{22} \) is of the order of \( E_0 \), the correction from non-diagonal terms will be of the order of \( (e^{-d^2})^2 \) and will not change the leading order result.

The numerical result, together with the analytical forms of \( \delta E_0 \) [one using the complete expressions Eq. (22), the other for the limiting case of large \( d \), Eq. (23)], is plotted in Fig 5. The complete expression is in excellent agreement with the numerics, over the whole range of \( d \), including the limit \( d \rightarrow 0 \). As for the leading order expression, it becomes an excellent description for the tunneling energy at distances roughly twice the dot confinement length (40 nm in our case), as seen from the inset to Fig. 5.

Using a LCSDO approximation \( g_{0,0,\sigma} \) for the ground state is correct for both limits \( d \rightarrow 0 \) and \( d \rightarrow \infty \), because \( H_{10} \) converges to the single dot level 0 in both limits. Therefore it is reasonable to expect that the approximation will be equally good for the whole range of \( d \). However, for the first excited state \( H_{10} \) the two limits go into different single dot levels and the proper LCSDO approximations for this state are \( g_{0,0,\sigma} \) and \( g_{0,1,\sigma} \) in the limit \( d \rightarrow \infty \) and \( d \rightarrow 0 \) respectively. However \( g_{0,0,\sigma} \sim g_{2,1,\sigma} \sim g_{4,1,\sigma} \) as \( d \rightarrow 0 \) and thus for both ground and first excited states using a LCSDO approximation suitable for \( d \rightarrow \infty \) gives good results in the whole range of \( d \). We will see, that this will not be true for a non-zero magnetic field and describing \( H_{10} \) by \( g_{0,0,\sigma} \) will give a much higher error. A remedy is to go beyond LCSDO for \( H_{10} \), for example by taking the base for Eq. (21) to include two \( g \)-functions, each correct in one of the limits \( d \rightarrow 0 \), \( d \rightarrow \infty \). We will not present the results of such computations since formulas become more complicated without giving better understanding.

Higher orbital states can be treated similarly. Starting from level 2 there are more functions of the same representation in one single dot level, therefore the basis for the Hamiltonian Eq. (21) giving the leading order must contain more that one function.
the linear Dresselhaus term. Spin-dependent tunneling term contributes, either by itself or in combination with correction is the mixed spin-orbit couplings are shown in Fig 6. The dominant spin-orbit contributions to tunneling fail to explain the above results. We use the example of the linear Dresselhaus term. The simplest way to include this term is to begin with the two lowest orbital states (that are four states including spin), $g_1^{0,0,\sigma}$ and $g_2^{0,0,\sigma}$. Because of the time reversal symmetry the resulting 4 × 4 matrices $H$ and $S$ from Eq. [21] block diagonalize into two equal 2 × 2 matrices with elements $H_{11} = E_1^{(0)}$, $H_{22} = E_2^{(0)}$, and $H_{12} = (g_1^{0,0,\sigma})|H_D|g_2^{0,0,\sigma}| = -iE_D\alpha de^{-d^2}$; $S$ is the unit matrix now, since the two states are orthogonal due to symmetry. Using the large $d$ limit for $\delta E_t$, Eq. [25] we obtain the perturbed energies $E_{S(A)} = 2E_0 \pm E_0\sqrt{4/\pi + \alpha^2_D de^{-d^2}}$ with the minus (plus) sign for $S$ ($A$). In the second order of $\alpha_D$ the symmetric and antisymmetric level energies have opposite contributions, giving $\delta E_t \approx (4E_0/\sqrt{\pi}) + (E_0\sqrt{\pi}/2)|\alpha^2_D|d\exp(-d^2)$, in contrast to the numerical results where there is no dependence on $\alpha^2_D$ in the second order. Enlarging the basis by the first excited orbital states (all together 12 states including spin), that is, include $g_3^{0,1,\sigma}$, the symmetric and antisymmetric level energies will have the correct limit for the spin-orbit contributions, $-E_0\alpha^2_D/2$, at $d \rightarrow \infty$. At finite values of $d$ the difference from this limit value is less than 2%. That means there are still terms of order $\alpha^2_D$ in $\delta E_t$. Could using a renormalized basis help? We could, for example, use symmetrized states of the separated dots that include spin-orbit terms. It is not difficult to see that this would not work either: the perturbed single dot ground state, for example, contains the spin admixture from the first excited orbital states. This is then similar to using the 12 state basis in the variational approach.

From the previous example one can see that to get a correct spin-orbit contribution to the energy of a state, it is not enough to include just a few terms in the sum in Eq. [9]. Instead we employ the operators $H^{op}$ given in Eqs. [11] and [12]. To get a contribution for a particular state, say $|i\rangle$, we apply the Löwdin perturbation theory. For this one has to identify states $|j\rangle$ which are degenerate with $|i\rangle$ with respect to the perturbation $H_{SO}$ and which have to be treated exactly. The rest of the states can be treated perturbatively. The condition for a degeneracy of two states can be taken as $|E_i^{(0)}| - |E_j^{(0)}| \leq \alpha_{SO,\alpha_{in}}$, when one considers linear and cubic terms respectively. The finite set of the degenerate states will be denoted by $N$. The effective Hamiltonian $H^{eff}$ acting in $N$ is

$$H^{eff}_{ij} = (H_0 + H_{SO})_{ij} + \frac{1}{2\alpha_{SO,\alpha_{in}}^2 \sqrt{N}} \sum_{k \neq N} \left( (H_{SO})_{ik} (H_{SO})_{kj} - (H_{SO})_{ik} (H_{SO})_{kj} \right).$$

For the example of the linear Dresselhaus term, we can now use Eq. [10] and [13] to obtain

$$H^{eff}_{ij} = (H_0 + H_D)_{ij} - \frac{1}{2} \alpha_D^2 E_0 (1 - \sigma_z l_z)_{ij} + R_{ij},$$

where

$$R_{ij} = \frac{1}{2} (i |H_D P_N H^{op}_D - H^{op}_D P_N H_D |j).$$

FIG. 6: Calculated corrections to the tunneling energy $\delta E_t$ from spin-orbit terms at $B = 0$. The labels indicate which spin-orbit terms are involved. Only D-D3 and D3-D3 are of second order. The remaining contributions are of fourth order.

### B. Corrections to energy from spin-orbit coupling in zero magnetic field.

When we add $H_{SO}$ to $H_0$, the structure of the corrections to the energies of the two lowest states up to the second order in spin-orbit couplings can be expressed as

$$E_t^{(2)} = -A_i (\alpha_D^2 + \alpha_{BR}^2) - B_i \alpha^2_D + C_i \alpha_D \alpha_{BR},$$

where $i$ is either $S$ or $A$. The coefficients $A, B, C$ are positive for all values of the interdot distance. The differences $A_S - A_A, \ldots$ approach zero as $d \rightarrow \infty$. We will argue below that $A_S = A_A = 1/2$ with the exception of a very small interdot distance (less than 1 nm). There are thus no contributions from the linear spin-orbit couplings to $\delta E_t$ in the second order. Only the cubic Dresselhaus term contributes, either by itself or in combination with the linear Dresselhaus term. Spin-dependent tunneling is greatly inhibited.

Numerical calculation of the corrections to $\delta E_t$ from spin-orbit couplings are shown in Fig [6]. The dominant correction is the mixed $D$-$D3$ term, followed by $D3$-$D3$.

These are the only second order corrections. For GaAs, and our model geometry, these corrections are about 4 and 5 orders of magnitude lower than $\delta E_t$. The corrections, when only linear spin-orbit terms are present, are much smaller since they are of the fourth order. The dramatic enhancement of the corrections from linear spin-orbit terms close to $d = 0$ is due to the transition from coupled to single dots. We will explore this region in more detail later.

We will first show how naive approaches to calculating spin-orbit contributions to tunneling fail to explain the above results. We use the example of the linear Dresselhaus term. The simplest way to include this term is to begin with the two lowest orbital states (that are four states including spin), $g_1^{0,0,\sigma}$ and $g_2^{0,0,\sigma}$. Because of the time reversal symmetry the resulting 4 × 4 matrices $H$ and $S$ from Eq. [21] block diagonalize into two equal 2 × 2 matrices with elements $H_{11} = E_1^{(0)}$, $H_{22} = E_2^{(0)}$, and $H_{12} = (g_1^{0,0,\sigma})|H_D|g_2^{0,0,\sigma}| = -iE_D\alpha de^{-d^2}$; $S$ is the unit matrix now, since the two states are orthogonal due to symmetry. Using the large $d$ limit for $\delta E_t$, Eq. [25] we obtain the perturbed energies $E_{S(A)} = 2E_0 \pm E_0\sqrt{4/\pi + \alpha^2_D de^{-d^2}}$ with the minus (plus) sign for $S$ ($A$). In the second order of $\alpha_D$ the symmetric and antisymmetric level energies have opposite contributions, giving $\delta E_t \approx (4E_0/\sqrt{\pi}) + (E_0\sqrt{\pi}/2)|\alpha^2_D|d\exp(-d^2)$, in contrast to the numerical results where there is no dependence on $\alpha^2_D$ in the second order. Enlarging the basis by the first excited orbital states (all together 12 states including spin), that is, include $g_3^{0,1,\sigma}$, the symmetric and antisymmetric level energies will have the correct limit for the spin-orbit contributions, $-E_0\alpha^2_D/2$, at $d \rightarrow \infty$. At finite values of $d$ the difference from this limit value is less than 2%. That means there are still terms of order $\alpha^2_D$ in $\delta E_t$. Could using a renormalized basis help? We could, for example, use symmetrized states of the separated dots that include spin-orbit terms. It is not difficult to see that this would not work either: the perturbed single dot ground state, for example, contains the spin admixture from the first excited orbital states. This is then similar to using the 12 state basis in the variational approach.

From the previous example one can see that to get a correct spin-orbit contribution to the energy of a state, it is not enough to include just a few terms in the sum in Eq. [9]. Instead we employ the operators $H^{op}$ given in Eqs. [11] and [12]. To get a contribution for a particular state, say $|i\rangle$, we apply the Löwdin perturbation theory. For this one has to identify states $|j\rangle$ which are degenerate with $|i\rangle$ with respect to the perturbation $H_{SO}$ and which have to be treated exactly. The rest of the states can be treated perturbatively. The condition for a degeneracy of two states can be taken as $|E_i^{(0)}| - |E_j^{(0)}| \leq \alpha_{SO,\alpha_{in}}$, when one considers linear and cubic terms respectively. The finite set of the degenerate states will be denoted by $N$. The effective Hamiltonian $H^{eff}$ acting in $N$ is

$$H^{eff}_{ij} = (H_0 + H_{SO})_{ij} + \frac{1}{2} \sum_{k \neq N} \left( (H_{SO})_{ik} (H_{SO})_{kj} - (H_{SO})_{ik} (H_{SO})_{kj} \right).$$

For the example of the linear Dresselhaus term, we can now use Eq. [10] and [13] to obtain

$$H^{eff}_{ij} = (H_0 + H_D)_{ij} - \frac{1}{2} \alpha_D^2 E_0 (1 - \sigma_z l_z)_{ij} + R_{ij},$$

where

$$R_{ij} = \frac{1}{2} (i |H_D P_N H^{op}_D - H^{op}_D P_N H_D |j).$$
First we note that existence of the operator $H_D^{op}$ means that the coupling through $H_D$ between any two states is always much smaller than the difference of the unperturbed energies of these two states, since $(H_D)_{ij} = (E_i^{(0)} - E_j^{(0)}) (H_D^{op})_{ij} \sim (E_i^{(0)} - E_j^{(0)}) \alpha_D$. Then one can partially diagonalize the effective Hamiltonian to eliminate the off-diagonal $H_D$ terms. It turns out, that this leads to a cancellation of the terms $H_D$ and $R$. The effective Hamiltonian is then

$$H_{ij}^{\text{eff}} = (H_0)_{ij} - \frac{1}{2} \alpha_D^2 E_0 (1 - \sigma_z l_z)_{ij}. \quad (28)$$

This completes the way to get Eq. (10) using Löwdin perturbation theory. There are no linear effects on the double dot energy spectrum from linear spin-orbit terms, which explains the absence of spin hot spots even though symmetry allows that.

The spin-orbit interaction can influence the energy only through the operator $l_z$, which is of the representation $\Gamma_3$, from where we get selection rule—the allowed coupling is between functions of representations $\Gamma_1 \rightarrow \Gamma_3$ and $\Gamma_2 \rightarrow \Gamma_4$. Looking at Fig. 4 accidental degeneracies of states with such representations are not present in the lower part of the spectrum. The crossing of $\Gamma_1^{41}$ with $\Gamma_1^{31}$ considered in the discussion to Fig. 4 also does not follow the selection rule, hence why the anti-crossing is of the third order. From the selection rules one can immediately see that also the expectation value of $l_z$ is zero in any state. This result is more general and holds also if the symmetry of the potential is lower (or none), since it follows from the fact that the Hamiltonian $H_0$ is real, so one can choose eigenfunctions to be real. Then the expectation value of any imaginary operator, such as $l_z$, must vanish. We conclude, that apart from degeneracies following from the single dot [that is limits $d \rightarrow 0(\infty)$] and possible accidental degeneracies respecting the selection rule, double dot states are described by an effective Hamiltonian

$$H_{ii}^{\text{eff}} = E_i^{(0)} - \frac{1}{2} E_0 \alpha_D^2. \quad (29)$$

Particularly, the energies of the two lowest states are given by this equation, with an exception for the state $\Gamma_A$ in the region of small $d$ where it is coupled to $\Gamma_4^{41}$ through $l_z$, and we have to describe it here by a $2 \times 2$ effective Hamiltonian.

An illustration of the $l_z$ influence on the spectrum is in Fig. 7, where the linear Dresselhaus spin-orbit contribution to the energy for several states as a function of the interdot distance is shown. One can see at what interdot distances the $l_z$ operator causes the qualitative change between the double dot case (where the functions are characterized by a definite representation $\Gamma_i$ and the energy contribution from the spin-orbit is a uniform shift) and the single dot case (where the functions are numbered according to the orbital momentum and the spin-orbit contribution to the energy depends on $\sigma_z l_z$). This happens when $E_0 \alpha_D^2$ is comparable to the energy difference of the nearly degenerate states. If the criterion for the coupling between the dots is the constant contribution, $-\alpha_D^2 E_0/2$, to the energy, then the double dot region, as far as the spin-orbit coupling is concerned, is between 1 to 100 nm, that is up to 5 times of the confinement length of 20 nm. As an example, for the function $\Gamma_1^{41}$ the coupling in the effective Hamiltonian through $l_z$ to $\Gamma_2^{31}$ is equal to the unperturbed energy difference if $\alpha_D^2 \sim d^3 e^{-d^2}$, giving $d \approx 3$, corresponding to the interdot distance of 60 nm. Due to the exponential, this result is insensitive to $\alpha_D$.

The Bychkov-Rashba term can be treated analogously. The effective Hamiltonian is $H_D^{op} = [H_0 - (\alpha_{BR}^2/2)E_0(1 + \sigma_z l_z)]_{ij}$. The absence of a linear influence on the energy was based on the existence of $H_D^{op}$. Since we found a case where $H_{D3}$ causes linear anti-crossing (see discussion to Fig. 4), it follows that $H_D^{op}$ can not exist for our double dot potential. However, if one approximates $E_i - E_k \approx E_j - E_k$ in (25), one can use $H_D^{op}$ to simplify the mixed D-D3 correction. This, according to Fig. 4, is the dominant spin-orbit correction for the tunneling energy $\delta E_i$. One gets an analogues expression as Eq. (25), where the needed commutator is stated in Eq. (13). Concluding, if we neglect the mixed D3-D3 term, we can write the spin-orbit contribution to the energy for the lowest orbital states to be $(i = S, A)$

$$\delta E_i^{SO} = -E_0 (\alpha_D^2 + \alpha_{BR}^2)/2 + \alpha_D \alpha_{D3} E_0 l_0^2(k^2)i_i. \quad (30)$$

One note to the eigenfunctions: The matrix elements of
the effective Hamiltonian are computed using the eigenfunctions of $H_0$. But the functions that correspond to the solutions are transformed by the same unitary transformation that leads from $H_0$ to $H^{\text{eff}}$. The sum rule can be used also here to express the influence of $H_{\text{lin}}$ on the eigenfunctions of $H_0$. If $H_0 \Gamma_i = E_i \Gamma_i$, the eigenfunctions corresponding to the effective Hamiltonian, Eq. (26), are

$$\delta \Gamma_i = \sum_{j \not\in \mathcal{N}} (H_{\text{lin}})^{ij} \Gamma_j = -(1 - P_{\mathcal{N}}) H_{\text{lin}}^{op} \Gamma_i.$$  

(31)

Partial diagonalization of the effective Hamiltonian, to go from Eq. (26) to Eq. (28), means we finish the unitary transformation completely and get $\Gamma_{\gamma}' = \Gamma_{\gamma}' - H_{\text{lin}}^{op} \Gamma_{\gamma}'$ for the eigenfunctions corresponding to the effective Hamiltonian, Eq. (28).

C. Finite magnetic field.

The presence of a magnetic field lowers the symmetry of the Hamiltonian without spin-orbit terms. The only nontrivial symmetry operator is the inversion $I$ (see Tab. 11). As a consequence the double dot states fall into two groups (representations of $C_2$): $\Gamma_1$ and $\Gamma_3$ become $\Gamma_S$ (symmetric under $I$) and $\Gamma_2$ and $\Gamma_4$ become $\Gamma_A$ (antisymmetric under $I$). Symmetrized functions $g_i^{n,\mu,\sigma}$ now are

$$g_i^{n,\mu,\sigma} = \Psi_i^{n,d} + D_i \Psi_i^{d,\mu,\sigma},$$

(32)

where the irreducible states $i = S$ and $A$, while the permutation coefficients $D_S = -D_A = 1$. The shifted single-dot wave functions acquire a phase:

$$\Psi_{n,l,\sigma}^{d}(x, y) = \Psi_{n,l,\sigma}(x \pm l_B, y)e^{\pm il_0 \theta y/l_B^2},$$

(33)

depending on which dot they are located.

The double dot energy spectrum of $H_0$ as a function of magnetic field is shown in Fig. 5 for the interdot distance of 50 nm. Indicated are two crossings and one anti-crossing induced by magnetic field. The first crossing is between $\Gamma_1$ and $\Gamma_2$ (notation from the $B = 0$ case). These two states have opposite spins so they are not coupled and there is no level repulsion here. (We will see in the next section that spin-orbit coupling will induce anti-crossing in this case.) The second crossing is between $\Gamma_2$ and $\Gamma_3$, which behave differently under $I$ and so they are not coupled by magnetic field. The actual anti-crossing is between $\Gamma_2$ and $\Gamma_4$, which are both antisymmetric under $I$. This is an example of anti-crossing induced by magnetic field.

In analogy with Eq. (22) we derive analytical expressions for the energies of the lowest symmetric and antisymmetric states in the presence of magnetic field using the LCSDO approximation:

$$E_{S}^{(0)} = \frac{2E_0}{\eta^2} \left( \frac{1 + [1 - d_0(1 - \theta^2)]/\sqrt{\pi} e^{-(d_0)^2(1+\theta^2)}}{1 + e^{-(d_0)^2(1+\theta^2)}} - \frac{d_0(1 - \theta^2)}{\sqrt{\pi} - d_0 e^{-(d_0)^2(1+\theta^2)}} \right)^{1/2} - \frac{d_0(1 - \theta^2)[e^{-(d_0)^2(1+\theta^2)} - d_0 e^{-(d_0)^2(1+\theta^2)}]}{1 - e^{-(d_0)^2(1+\theta^2)}} ,$$

$$E_{A}^{(0)} = \frac{2E_0}{\eta^2} \left( \frac{1 + [1 - d_0(1 - \theta^2)]/\sqrt{\pi} e^{-(d_0)^2(1+\theta^2)}}{1 + e^{-(d_0)^2(1+\theta^2)}} - \frac{d_0(1 - \theta^2)}{\sqrt{\pi} - d_0 e^{-(d_0)^2(1+\theta^2)}} \right)^{1/2} - \frac{d_0(1 - \theta^2)[e^{-(d_0)^2(1+\theta^2)} - d_0 e^{-(d_0)^2(1+\theta^2)}]}{1 - e^{-(d_0)^2(1+\theta^2)}} .$$

(34)

Here $\eta = l_0/l_B = (1 - \theta^2)^{1/4}$. In the limit $d \to \infty$, we can then deduce the tunneling energy in the leading order to be

$$\delta E_{t}^{(0)} = E_0 \frac{4}{\sqrt{\pi}} (1 - \theta^2)^{5/4} e^{-d^2(1+\theta^2)/\sqrt{1-\theta^2}} .$$

(35)

If $\theta = 0$, the above expressions reduce to Eq. (29). On the other hand, if $B \to \infty$, then $\delta E_{t}^{(0)} \sim B^{-5/2} e^{-B^2/B_0}$. Magnetic field suppresses $\delta E_{t}^{(0)}$ by suppressing overlap integrals $\langle \Psi^{-d}|H|\Psi^{d} \rangle$. There are three different effects that magnetic field introduces. First, the wave functions are squeezed by the confinement provided by the vector potential. The natural confinement length is $l_B = l_0(1 - \theta^2)^{1/4}$, present in the exponential decay factors. Second, the gauge phase produces factors $(1 + \theta^2)$ in the exponents of the scalar products $\langle \Psi^{-d}|\Psi^{d} \rangle$. Third, as $B$ increases, the confinement potential $V_C$ becomes less important compared to the confinement of the magnetic vector potential. This gives rise to the factor $(1 - \theta^2)$.

Note that in the limit $B \to \infty$, $\Psi_{n,l,\sigma}^{d}$ is an eigenstate of $H_0$ for any $d$. For reasons explained in last paragraph in the Sec. 41, Eqs. (33) are correct in the limit $d \to \infty$. As $d \to 0$, only $E_{S}^{(0)}$ is correct. The limit value of $E_{A}^{(0)}$ ($d = 0$)/$E_0$ is $4/(1 + \theta^2)$, instead of the exact value of $2(2 - \theta)$.

At a finite magnetic field we have also a new term in the Hamiltonian, the Zeeman term. Since it commutes with $H_0$ the only consequence of this term is a shift of the energy of the states by a value $\sigma \mu g B$ according to their spin $\sigma$. Therefore it introduces new crossings of the states with opposite spin. An example of this can be seen in Fig. 11, where we plot energies of the four lowest states in the region where the Zeeman shift is comparable to the energy differences of the considered states.

D. Effective spin-orbit Hamiltonian

We now study the influence of spin-orbit coupling on the spectrum of double dots in a finite magnetic field. We will see that spin-orbit terms lead to new spin hot spots even at magnetic fields of the order of 1 T, and that linear spin-orbit terms will influence tunneling in the second order.
magnetic field, so that the Zeeman term can be included
\[ \alpha \]
couplings (being now \[ H \]) the analysis of the perturbation theory using operators
\[ \rightarrow \infty \] operators
isism if the Zeeman term is treated as a part of perturbation theory. (For a harmonic potential describing single dots,
\[ \text{enact} \] the energy of state
\[ \text{stant consequence is that the shift can change the number }
\[ \text{any new couplings (non-diagonal terms). But an impor-
\[ \text{case of zero magnetic field, the Zeeman term appears as }
\[ \text{tive Hamiltonians}
\[ \text{Zeeman-spin-orbit term. This means that in the effec-
\[ \text{anti-crossing between} \Gamma_2 \text{and} \Gamma_3 \text{is indicated. In the limit }
\[ B \rightarrow \infty \text{the states merge to Landau levels.}

Although the presence of the Zeeman term complicates the analysis of the perturbation theory using operators \[ H^{\text{op}} \], one can still apply the previously developed formalism if the Zeeman term is treated as a part of perturbation. (For a harmonic potential describing single dots, \[ H^{\text{op}} \] operators \[ H^{\text{fin}} \] have been derived for the case of finite magnetic field, so that the Zeeman term can be included into \[ H_0 \]). Up to the second order in the perturbation couplings (being now \[ \alpha_{SO} \] and \[ \alpha_Z \]), there is no coupled Zeeman-spin-orbit term. This means that in the effective Hamiltonians \[ H^{\text{eff}} \] that we already derived for the case of zero magnetic field, the Zeeman term appears as a shift of the energies on the diagonal without bringing any new couplings (non-diagonal terms). But an important consequence is that the shift can change the number of states we have to include into the basis where the effective Hamiltonian acts, because their energy difference to the considered state is comparable to the spin-orbit coupling.

First, in analogy with Eq. (24), if the energy of a state is far enough from others, we can consider the basis to consist of one term only and the spin-orbit correction to the energy of state \[ |i\rangle \] is
\[ \delta E^{\text{SO}}_i = -E_0 \frac{\alpha_{SO}^2}{2} \langle 1 - \sigma L_z \rangle - E_0 \frac{\alpha_{BR}^2}{2} \langle 1 + \sigma L_z \rangle \]
+ [\[ H^{\text{op}}, H^{\text{D3}} \]],
(36)
where the averaging means the expectation value in the state \[ |i\rangle \] and \[ \sigma \] is the spin of the state. Since the presence of magnetic field lowers the symmetry, the last commutator, \[ |E_{\text{cr}}\rangle \], can not be simplified according to

The symmetry as was the case before in Eq. (30), and, more important, we no longer have \[ L_z = 0 \]. As a result, there are now corrections to the tunneling that are of the second order in the linear spin-orbit couplings. These corrections depend on \[ \alpha^2_{(2)} = \alpha^2_{D} - \alpha^2_{BR} \].

Second, we look how the energies of the four lowest states are changed, using again the example of the linear Dresselhaus term. They are plotted in Fig. 9. Here in the main figure one can see the shift caused by the Zeeman term and the anti-crossing induced by the spin-orbit coupling is magnified in the inset. The anti-crossing states are \[ \Gamma^+_S \] and \[ \Gamma^+_A \]. In the case of zero magnetic field we described each of the four basis states by Eq. (29). Now, in principle, we have to describe them by a \( 4 \times 4 \) effective Hamiltonian Eq. (26). Due to symmetry we can simplify this Hamiltonian into two \( 2 \times 2 \) Hamiltonians, \[ H^{\text{eff}}_1 \], \[ H^{\text{eff}}_2 \], acting in the bases \[ \Gamma^+_S, \Gamma^+_A \] and \[ \Gamma^-_S, \Gamma^-_A \] respectively. The four components of the effective Hamiltonian matrix are
\[ (H^{\text{eff}})_{11} = E^{(0)}_S - E_0 \alpha_{D}^2 \left( 1 - \sigma(L_z)_{11} \right) - \sigma \mu_B B - R_{11} \]
\[ (H^{\text{eff}})_{22} = E^{(0)}_A - E_0 \alpha_{D}^2 \left( 1 + \sigma(L_z)_{22} \right) + \sigma \mu_B B + R_{11} \]
\[ (H^{\text{eff}})_{12} = (H^{\text{eff}})_{21} = (H_D)_{12} \]
(37)
where \( \sigma = -1 \) for \[ H^{\text{eff}}_1 \] and \( \sigma = 1 \) for \[ H^{\text{eff}}_2 \], while indices 1,2 denote the first and the second term in the corresponding basis. Comparing to the case of zero magnetic field the Zeeman term increases the difference of the diagonal elements in \[ H^{\text{eff}}_1 \] and decreases them in \[ H^{\text{eff}}_2 \]. The ground and the fourth excited states which are described by \[ H^{\text{eff}}_1 \] stay isolated, and we can do the perturbative diagonalization to get rid of the off-diagonals. The energy of the two states is then up to the second order in

\[ 2.9 \]
\[ 2.8 \]
\[ 3.1 \]
\[ 3.0 \]
\[ 2.9 \]
\[ 2.8 \]
\[ 3.1 \]
\[ 3.0 \]
\[ 2.9 \]
\[ 2.8 \]
the spin-orbit coupling accurately described by Eq. (36).

Concerning the states \( \Gamma_S^\downarrow \) and \( \Gamma_A^\downarrow \), there is a region in the interdot distance of a few nanometers, where the two states must be described by the two dimensional \( H_{SO}^{2D} \) to account for the anti-crossing, which is caused by the the matrix element \( \langle \Gamma_S^\downarrow | H_D | \Gamma_A^\downarrow \rangle \). LCSDO gives for this element a result correct only in the order of magnitude. This is because even in the limit \( d \to \infty \) this matrix element is of the same order as the neglected coefficients \( c(n,l) \) in the LCSDO approximation, Eq. (34).

The spin-orbit corrections to the energies from \( H_D \) for the four lowest states as functions of the interdot distance are in Fig. 10. Also shown are analytical values computed by Eq. (36), that is, ignoring anti-crossing.

The scale implies that the corrections are of the second order, that is, \( \delta g \) is of the same order as the neglected coefficients \( c(n,l) \) in the LCSDO approximation, Eq. (34).

E. Spin-orbit corrections to the effective g-factor and tunneling frequency

We next analyze spin-orbit corrections to the g-factor, \( \delta g \equiv [\delta E(\Gamma_S^\downarrow) - \delta E(\Gamma_A^\downarrow)]/\mu_B B \), that characterizes the energy cost of a spin flip in the ground state, or the frequency of a spin precession. Another kind of oscillation is electron tunneling, when electron oscillates between the left and the right dot without changing its spin. The frequency of this oscillation, \( \delta E_t/2\hbar \), is given by the energy difference \( \delta E_t = E(\Gamma_A^\downarrow) - E(\Gamma_S^\downarrow) \). Corrections to this energy difference induced by the spin-orbit interaction are denoted in this paper as \( \delta E_t^{SO} \).

First, we take a look at the spin-orbit corrections to the g-factor. Contributions in the second order of the spin-orbit couplings are shown in Fig. 11 as functions of magnetic field at a constant interdot distance. The spin-orbit contribution to the g-factor in the double dot case has the same qualitative dependence on the magnetic field as in the single dot case (see discussion to Fig. 2). However, at finite interdot distances, there is an enhancing effect on the spin-orbit contributions. This can be seen in Fig. 11 where at a certain magnetic field, the spin-orbit contribution to the g-factor is enhanced for a finite \( d \) compared to the case of \( d = 0(\infty) \). We found numerically, that the enhancement can be up to 50% of the value of the correction in \( d = 0 \) at magnetic fields of the order of 1 T.

At the anti-crossing the spin-orbit contributions show cusps. At magnetic fields below the anti-crossing, the dominant spin-orbit contribution is \( D-D \) which reduces the conduction band g-factor by several percent. Contributions \( D-D3 \) and \( BR-BR \) are one order of magnitude smaller. Using Eq. (36), that is ignoring the anti-crossing, we get for the contribution from the linear spin-orbit terms

\[
\delta g(\ln - \ln) = - \frac{E_0}{\mu_B B} \alpha^{(2)} \overline{T_z},
\]

where, in the limit \( d \to \infty \),

\[
\overline{T_z} \approx \theta[1 + (d/\eta)^2 e^{-(d/\eta)^2(1+\gamma^2)}].
\]

From Fig. 11 one can see that the analytical result agrees with numerics.

Finally, we look at the tunneling energy in the presence of both magnetic field and spin-orbit couplings.
spin-orbit corrections, as a function of magnetic field, are shown in Fig. 12. At zero magnetic field there is no contribution from the linear terms (result of the section [AV3]) and the dominant contribution is $D$-$D3$. Similarly to $\delta E_i^{(0)}$, the corrections decay exponentially with increasing magnetic field. Anti-crossing strongly influences the tunneling energy. Using LCSDO for $d \to \infty$ we obtain in the leading order

$$\delta E_i^{\text{lin}} = -E_0 \alpha^2 (d/\eta)^2 e^{-(d/\eta)^2 (1+\theta^2)}. \quad (40)$$

This analytical formula underestimates the corrections from the linear spin-orbit terms by a factor of $\sim 3$. Nevertheless the analytical expression for $D$–$D3$ is reasonably good. In the magnetic field below anti-crossing, the relative change of the tunneling energy stemming from the spin-orbit terms is of order $10^{-3}$.

F. Tunneling Hamiltonian

We now use our results to describe the influence of the spin-orbit interaction on the lower part of the spectrum. We restrict our Hilbert space on the four lowest states $\Gamma^{\pm}_{\pm(A)}$, the eigenstates of the total double dot Hamiltonian. Because of the transformation Eq. (34), these four states have neither definite symmetry with respect to inversion $I$, nor a definite spin in z-direction. In this section we will denote them as spin ‘up’ and spin ‘down’ states. For description of a transport through the double dot it is useful to define the following left and right localized functions

$$L^\sigma (R^\sigma) = \frac{1}{\sqrt{2}} (\Gamma^\sigma_L \pm \Gamma^\sigma_R), \quad (41)$$

where plus and minus holds for $L$ and $R$, respectively. In the limit $d \to \infty$ these functions converge to single dot solutions localized in the left and right dot.

The effective Hamiltonian of our system in the second quantization formalism is

$$H = \sum_{\sigma=L,R} E^\sigma (n_{L\sigma} + n_{R\sigma}) - (\delta E_i^\sigma/2) (a_{L\sigma}^\dagger a_{R\sigma} + a_{R\sigma}^\dagger a_{L\sigma}), \quad (42)$$

where $E^\sigma = (E^\sigma_L + E^\sigma_R)/2$, $\delta E_i^\sigma = E^\sigma_A - E^\sigma_B$, while $a$, and $a'$ are creation and annihilation operators, and $n = a^\dagger a$. We can get both localized and spin-pure states if we diagonalize $\sigma_z$ in a chosen basis. For example, taking $L^\uparrow$ and $L^\downarrow$, we get $L^\text{pure}\uparrow \sim (L^\uparrow + aL^\downarrow)$ and $L^\text{pure}\downarrow \sim (L^\downarrow - a^\dagger L^\uparrow)$, up to normalization $(1 - |a|^2/2)$. That is, the left pure spin state is a linear superposition of both left states with spin ‘up’ and ‘down’. The coefficient $o$ is proportional to $\alpha_{SO}$.

In the following we are interested in the time evolution of localized states given by Hamiltonian Eq. (42). First we note, that due to the non-diagonal terms, the electron which is in a localized state will tunnel into the other localized state after the tunneling time $t_{\text{tun}} = h/\delta E_i^\sigma$, resulting in coherent oscillations. For our parameters $t_{\text{tun}} \approx 1$ ps. In the Hamiltonian there is no mixing between spin ‘up’ and ‘down’ states. However, there will be mixing (or spin-flip) if we work with localized pure spin states. Electron being originally in $L^\text{pure}\uparrow$ will, after the tunneling time $t_{\text{tun}}$, contain $R^\text{pure}\downarrow$ with the probability amplitude

$$c = i \alpha (\delta E_i^\sigma - \delta E_i^\downarrow)/2\delta E_i^\sigma, \quad (43)$$

assuming that the difference in $\delta E_i$ for different spins is much smaller that $\delta E_i$ itself.

In the case of zero magnetic field, because of Kramer’s degeneracy, the tunneling frequencies are the same for both spin orientations. Then whatever is the initial combination of spin ‘up’ and ‘down’ (let it be, for example, $L^\text{pure}\uparrow$), during the time evolution (oscillations) there will be no relative change in the coefficients in this linear combination. Therefore spin-orbit coupling does not lead to spin-flipping and $c = 0$ in Eq. (43).

In a finite magnetic field, the tunneling frequency for spin ‘up’ and ‘down’ are different. The difference is caused only by spin-orbit terms, and is of order $\alpha (d/\eta)^2 = \alpha_{DR}^2$. Equation (40) shows, that the contribution to $\delta E_i^\sigma$ from the linear spin-orbit terms is opposite that of $\delta E_i^\downarrow$ and therefore their difference is twice the expression in Eq. (40). We conclude, that spin-flip during tunneling induced by spin-orbit coupling is proportional to the third power in spin-orbit couplings and depends linearly on the magnetic field if the magnetic field is small ($c \sim \alpha_{\text{lin}}^2 \theta$).

The different tunneling frequency can be exploited for separation of different spin states in a homogeneous magnetic field. Starting with some combination of ‘up’ and ‘down’ states localized in one dot, after time $t_{\text{sep}} = h/(\delta E_i^\uparrow - \delta E_i^\downarrow) = t_{\text{tun}}^2 (\delta E_i^\uparrow/\delta E_i^\uparrow - \delta E_i^\downarrow)$ the part with spin ‘up’ will be localized in the left, and the spin ‘down’ will

FIG. 12: Calculated spin-orbit corrections to the tunneling energy $\delta E_i$ as a function of magnetic field. The interdot distance is 50 nm. Solid lines are numerical data, dashed lines are analytical expressions computed by Eq. (40).
be in the right dot. From Fig. 12 one can see that one needs about $10^3$ coherent oscillations to get the spatial spin separation. Therefore the decoherence time must be longer in order to observe this effect experimentally. We note that the separated states will not be pure spin states, but will contain a small (linearly proportional to $\alpha_{SO}$) admixture of opposite pure spin states.

V. CONCLUSIONS

We have performed numerically exact calculation of the spectrum of a single electron localized by a confining potential in single and double GaAs quantum dots. We have studied the influence of the spin-orbit terms, namely the Bychkov-Rashba and the linear and cubic Dresselhaus terms, on the energy spectrum. In the single dot case we have elaborated on previous results and shown that the spin-orbit interaction has three principal effects on the spectrum: first, the interaction shifts the energy by a value proportional to the second order in the spin-orbit couplings, second, it lifts the degeneracy at zero magnetic field, and, third, the Bychkov-Rashba term gives rise to spin hot spots at finite magnetic fields.

In the double dot case we have addressed the symmetries of the Hamiltonian. For zero magnetic field without spin-orbit terms we have constructed the correlation diagram, between single and double dot states, of the spectrum. We have used properly symmetrized linear combination of shifted single dot solutions as an approximation for a double dot solution and found that for the four lowest states it gives a good approximation for the energy. As for the contributions to the energy from the linear spin-orbit terms, we have found that in zero magnetic field a typical feature of a double dot is a uniform shift of the energy proportional to the second order in the coupling strengths without any dependence on the interdot distance. This is true also if the potential has lower (or none) symmetry (for example biased dots). Therefore, in zero magnetic field, there is no influence on the tunneling frequency up to the second order in the linear spin-orbit couplings and the dominant contribution comes from the mixed linear and cubic Dresselhaus second order term. We found, that spin hot spots in zero magnetic field exist in the double dot, but are solely due to the cubic Dresselhaus term. This means also, that for our potential, for the cubic Dresselhaus term there can not exist a unitary transformation to eliminate its contribution in the first order.

The effective $g$-factor, on the other hand, is influenced by the second order linear spin-orbit couplings even at $B \sim 0$, so the dominant contribution here is the linear Dresselhaus term for GaAs. In finite magnetic fields the uniform shift does not hold any more and there is a contribution to the tunneling frequency in the second order of the linear spin-orbit couplings. We have derived an effective Hamiltonian, using Löwdin’s perturbation theory, with which analytical results up to the second order in perturbations (Zeeman and spin-orbit terms with the exception of cubic Dresselhaus-cubic Dresselhaus contribution) can be obtained provided one has exact solutions of the double dot Hamiltonian without Zeeman and spin-orbit terms. From this effective Hamiltonian we have derived the uniform shift in zero magnetic field. In a finite magnetic field we used linear combinations of single dot solutions to obtain analytical expressions for the spin-orbit contributions to the energy for the four lowest states. We have analyzed them as functions of the interdot distance and magnetic field and compared them with exact numerical values. The spin-orbit relative contribution to the $g$-factor and the tunneling frequency is of the order of $\sim 10^{-2}$ and $\sim 10^{-3}$, respectively. Due to the degeneracy of the energy spectrum at large interdot distance the spin hot spots exist also at smaller magnetic fields compared to the single dot case.

As an application of our results we have constructed an effective Hamiltonian acting in a restricted Hilbert space of four states–electron with spin up and down (these are effective spins in the presence of spin-orbit coupling) localized on either dot. Effectively, there is only spin-conserving tunneling between the localized states, no spin-flip tunneling. In zero magnetic field the spin-orbit interaction does not significantly influence the tunneling frequency, nor it implies spin-flip tunneling. In finite magnetic fields the tunneling frequency is spin dependent, the difference being of second order in linear spin-orbit terms. This leads to a spin flip amplitude proportional to the third power in spin-orbit couplings (it is linear in magnetic field). We propose to use this difference of the tunnelings to spatially separate electron spin in homogeneous magnetic field.

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