Time Dependent Configuration Interaction Study of Anisotropic Spin Exchange in Laterally Coupled Quantum Dots

Michał P. Nowak†, Bartłomiej Szafran

†mnowak@novell.ftj.agh.edu.pl

Faculty of Physics and Applied Computer Science, AGH University of Science and Technology,
Al. Mickiewicza 30, 30-059 Kraków, Poland

We perform a time-dependent simulation of the spin exchange process in laterally coupled quantum dots. The calculation is based on configuration interaction scheme – a numerically exact approach. Noninteracting electrons exchange their spins in a manner that can be understood by the interdot tunneling associated with the spin precession in the effective spin-orbit-induced magnetic field which results in anisotropic spin swap. The Coulomb interaction blocks the electron transfer between the dots, but the spin transfer and its precession is still present. We also show a possibility of restoration the isotropy of the spin exchange.

Introduction

One of proposals for realization of a solid state quantum computer employs spins of electrons confined in quantum dots [1]. In order to implement an universal quantum gate one has to perform both single and two qubit operations including single spin rotations and spin swaps. The spin swaps occur due to the exchange interaction between electrons confined in adjacent dots.
Spin-orbit (SO) coupling changes the way the spins of confined electrons evolve. As a consequence the exchange interaction possesses an anisotropic part [2]. Previous work [2, 3] on the role of SO coupling for the exchange interaction focused on stationary states. The purpose of the present work is to study the spin exchange process and the way it actually takes place in time in the presence of the SO coupling.

Theory

The model system : laterally coupled dots:

$$V(x,y) = -\frac{V_0}{\left(1+\left[\frac{x^2}{R_x^2}\right]^{10}\right)\left(1+\left[\frac{y^2}{R_y^2}\right]^{10}\right)} + \frac{V_b}{\left(1+\left[\frac{x^2}{R_b^2}\right]^{10}\right)\left(1+\left[\frac{y^2}{R_y^2}\right]^{10}\right)} \quad (1)$$

with $V_0 = 50$ meV, $V_b = 10$ meV – interdot barrier, $2R_x = 90$ nm and $2R_y = 40$ nm , and $2R_b = 10$ nm the interdot barrier width and the material parameters taken for $In_{0.5}Ga_{0.5}As$.

Stationary states calculation: diagonalization of two-electron Hamiltonian

$$H = h_1 + h_2 + \frac{e^2}{4\pi\epsilon\epsilon_0|\mathbf{r}_1 - \mathbf{r}_2|} \quad (2)$$

in the basis of eigenstates of one-electron, two-dimensional Hamiltonian

$$h = \left(\frac{\hbar^2\mathbf{k}^2}{2m^*} + V(r)\right)\mathbf{1} + H_{SIA} + H_{BIA}, \quad (3)$$

that are determined in a multicenter Gaussian basis [4]. The Hamiltonians

$$\begin{aligned} H_{SIA} &= \alpha(\sigma_x k_y - \sigma_y k_x) + H_{diag}, \\ H_{BIA} &= \beta\left(\sigma_x k_x - \sigma_y k_y\right) + H_{cub}, \end{aligned} \quad (4)$$

stands for Rashba (resulting from inversion asymmetry of the nanostructure) and Dresselhaus (resulting from inversion asymmetry of the crystal lattice) spin-orbit interactions respectively.

Spin swap simulation: time evolution described by the Schrödinger equation $i\hbar\frac{\partial\Psi}{\partial t} = H\Psi$, with solution of the form $\Psi = \sum_m c_m e^{\frac{-iE_m t}{\hbar}}\Psi_m$, c_m determined by the initial condition – the electrons localized in separate dots with opposite spin orientations in a chosen direction.

Effective SO magnetic field: precession of a single electron spin described by the Bloch equation $\frac{d\langle\mathbf{s}\rangle}{dt} = g\mu_b\langle\mathbf{B}_{SO}\times\mathbf{s}\rangle$. The $\mathbf{B}_{SO}$ is the spin-orbit-induced magnetic field [5]

$$\mathbf{B}_{SO} = \frac{2\alpha}{g\mu_B}\begin{pmatrix} k_y \\ -k_x \\ 0 \end{pmatrix} + \frac{2\beta}{g\mu_B}\begin{pmatrix} k_x \\ -k_y \\ 0 \end{pmatrix}. \quad (5)$$

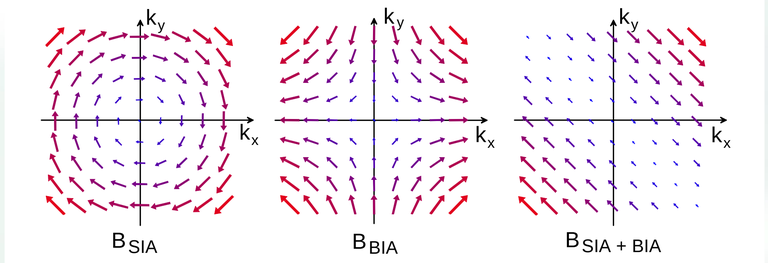

Figure 1. *Effective spin-orbit magnetic field B_{SO} originating from: B_{SIA} – Rashba, B_{BIA} – Dresselhaus coupling and $B_{SIA+BIA}$ – both the interactions with $\alpha = \beta$.*

Results

We first assume that the nanostructure is perfectly symmetric in the growth direction which implies $\alpha = 0$ – pure Dresselhaus coupling ($\beta = 10.8$meV nm).

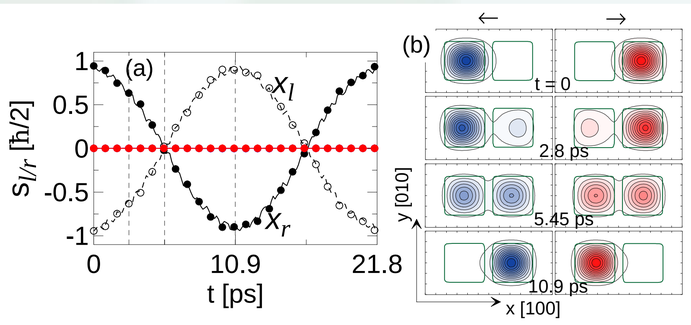

Figure 2. *(a) Black lines – the x component of the spin stored in quantum dots for pure Dresselhaus coupling and electrons spins oriented initially antiparallel in the x direction. The circles – results obtained without SO coupling.(b) Spin-left and spin-right densities.*

- Without the SO interaction the swap [dots in Fig. 2(a)] is independent of the initial spin orientation and is exact at $\tau = 10.9$ ps.
- With Dresselhaus interaction included exchange process as depicted with dots in Fig 2(a) is obtained for spins initially antiparallel in the x direction (lines in Fig. 2(a) [for z direction see Fig. 3(c)].

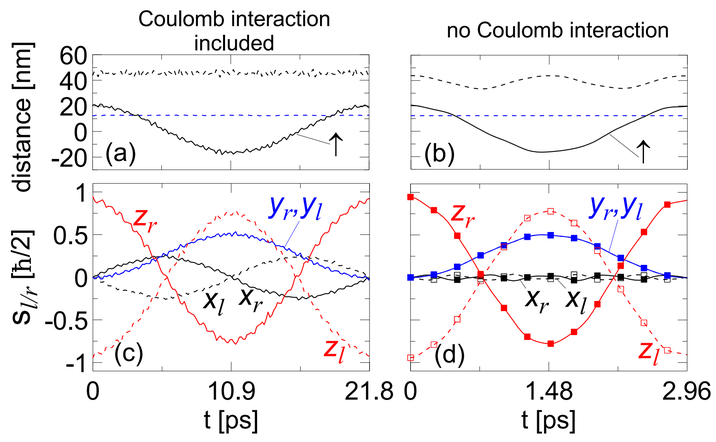

Figure 3. *Pure Dresselhaus coupling and the electrons spins initially set antiparallel in the z direction. (a,b) The average position of the spin-up density (black solid line). The electron-electron distance (dashed lines) in the x (black), and y (blue) directions. (c,d) The spin components. Squares in (d) obtained from one-electron calculation.*

- In the presence of SO coupling both the spin swap result and the process itself distinctly depend on the initial spin orientation [comp. Fig. 2(a), Fig. 3(c)]. Orientation of the spin is tilted during the exchange process.
- The Coulomb interaction blocks the electron interdot transfer [comp. dashed curves in Figs. 3(a) and (b)]. The spin packet motion between the dots is still observed – solid curve in Fig. 3(a,b).

With Coulomb interaction neglected the two-electron results are reproduced by the sum [dots in Fig. 3 (d)] of two one-electron cases in which the electron is initially placed in the left(right) dot and tunnels to the adjacent one [see Fig. 4(g,h,i)].

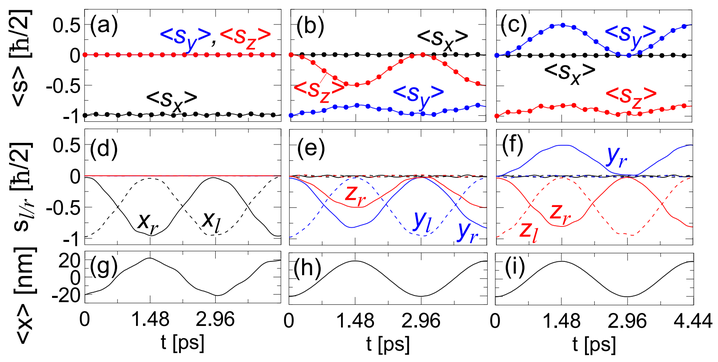

Figure 4. *Single electron and pure Dresselhaus coupling. (a,b,c) curves – average values of spin components, circles – results obtained from the Bloch equation. (d,e,f) The spin stored in the quantum dots. (g,h,i) The average x position of the electron packet.*

- Motion of the electron is accompanied with tilt of its spin orientation (curves in Fig. 4(d-f)) – the spin precesses in effective SO magnetic field as described by the Bloch equation – dots in Fig. 4(a-c).
- If the spin is set along the B_{SO} direction, no precession is observed [Fig. 4(a)] – with agreement with the case of Fig. 2(a).

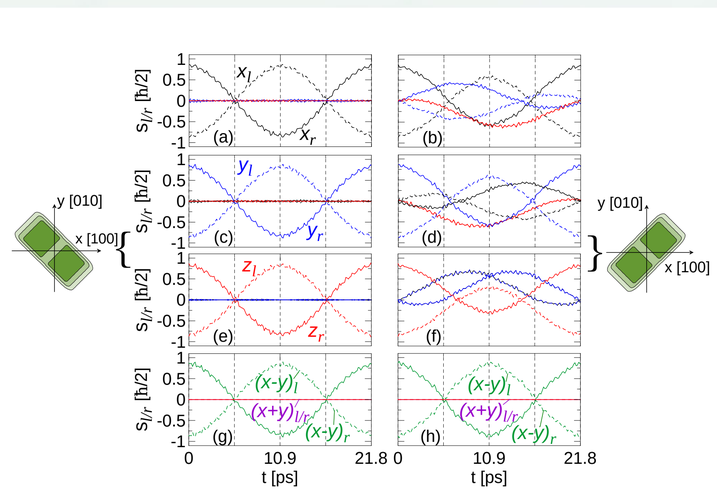

Figure 5. *Two interacting electrons with equal linear Dresselhaus and Rashba constants – $\alpha = \beta = 10.8$ meV nm.*

For $\alpha = \beta$ and the dots aligned along the $[1\bar{1}0]$ crystal direction (for which case $B_{SO} = 0$) no influence of initial spin orientation on spin swap is observed [Fig. 6(a,c,e,g)] – the spin exchange is isotropic, contrary to [110] alignment [Fig. 6(b,d,f,h)].

Conclusions

- The spin swap involves **motion of spin packets** that undergo precession in the effective spin-orbit-induced magnetic field.
- In presence of the SO coupling generally the swap is accompanied by a **tilt of the spin orientation**.
- The process is **anisotropic** unless the initial orientation of the spins **is aligned with the effective magnetic field vector**.
- The **isotropy** of the spin swap **is reinstated for equal Rashba and Dresselhaus constants** provided that the dots are aligned in the $[1\bar{1}0]$ crystal direction.

Acknowledgements

This work was supported by MPD Programme operated within the Foundation for Polish Science and co-financed by the EU European Regional Development Fund. Calculations were performed in ACK–CYFRONET–AGH on the RackServer Zeus.

References

[1] D. Loss and D.P. DiVincenzo, Phys. Rev. A **57**, 120 (1998).

[2] K. V. Kavokin, Phys. Rev. B **64**, 075305 (2001).

[3] S. Gangadharaiah, J. Sun, and O. A. Starykh, Phys. Rev. Lett. **100**, 156402 (2008); F. Baruffa, P. Stano, and J. Fabian, Phys. Rev. Lett. **104**, 126401 (2010).

[4] M.P. Nowak and B. Szafran, Phys. Rev. B **81** 235311 (2010).

[5] L. Meier et al., *Nature Physics* **3**, 650 (2007).

INNOVATIVE ECONOMY
NATIONAL COHESION STRATEGY

FNP Foundation for Polish Science

EUROPEAN UNION
EUROPEAN REGIONAL
DEVELOPMENT FUND