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Dynamics of holes wave-packets under Rashba spin-orbit coupling
Dinámica de paquetes de ondas de huecos bajo acoplamiento espín-órbita tipo Rashba

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Resumen

Se estudia la dinámica de un paquete de ondas gaussiano de huecos pesados, en presencia de interacción espín-órbita tipo Rashba, para un sistema semiconductor *cuasi*-unidimensional. Se utiliza un esquema en diferencias finitas, basado en la aproximación de Cayley, y se extiende a la solución de la ecuación de Schrödinger dependiente del tiempo para huecos. Se muestra el fenómeno de la precesión del espín de los huecos, a través de una simulación numérica de la evolución temporal de las componentes del paquete. Es posible evaluar parámetros relevantes, *e. g.* dimensiones y tiempos de inversión de la polarización, en un dispositivo modelado como transistor de efecto campo de espín, que utilice en calidad de portadores a los huecos.

Palabras clave: Espintrónica, acoplamiento espín-órbita, transporte espín polarizado en semiconductores, transistor de efecto campo de espín

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Abstract

The dynamics of a Gaussian wave-packet of heavy holes is studied in the presence of Rashba spin-orbit interaction for a *quasi*-one-dimensional semiconductor system. A finite-difference scheme, based on the Cayley approach, has been extended to solve the time-dependent Schrödinger equation for holes. It is shown the phenomenon of hole-spin precession *via* a numerical simulation of the temporal evolution of the components of the wave-packet. It is possible to evaluate relevant parameters, *e. g.* dimensions and the spin polarization flip-time, when a spin field effect transistor device, is modeled for holes as carriers.

Keywords: Spintronics, spin-orbit coupling, spin-polarized transport in semiconductors, spin field effect transistors

Introduction

The recent interest in the electron spin has opened a new frontier field in Nanosciences named Spintronics (Awschalom and Flatté 2007, 135). One of the more important mechanisms for the spin manipulation in semiconductors systems is the Rashba spin-orbit interaction (SOI-R) (Bychkov and Rashba 1984, 6039). The SOI-R arises as consequence of a potential gradient transversal to the carries movement. It is responsible for carrier spin precession and also breaks the two-fold degeneracy in a typically parabolic dispersion laws. The SOI-R is the key ingredient of the Datta and Das spin field effect transistor (SFET), one of the foundational theoretical works in Spintronics (Datta and Das 1990, 665).

In recent years, SOI-R in quasi-one-dimensional (Q-1D) semiconductors systems become important, due to the abundance of physical phenomena and applications (Guzenko *et al.* 2006, 031202; Sánchez *et al.* 2008, 035315). In addition, the sources of spin dephasing become neglectable when the angular carrier's distribution is restricted to a Q-1D channel (Häusler 2004, 115313). Governale and Zülicke, in a study on the possibility of a non-magnetic spin filter, proposed a Hamiltonian that adequately describes the SOI-R for Q-1D holes systems (Governale and Zülicke 2003, 257).

One of the first numerical works in quantum transport of electronics wave-packets was achieved by Goldberg *et al.* (Goldberg *et al.* 1967, 177). The numerical technique used, based on the Finite Difference Method, allows to solve the time-dependent Schrödinger equation for Hamiltonians without explicit temporal dependence. The Goldberg formalism has been used in the study of the spin-dependent dynamics of electronics (Tung and Lee 1996, 507; Tung and Lee 1996, 2122; Ochoa-Fajardo 2006, 26; Bonfanti-Escalera 2008, 18) and holes (Cuan and Diago-Cisneros 2010, 212) wave-packets. The latter case corresponds to calculation of spin-resolved kinetics coefficients in the scattering on stationary potential barriers under SOI-R.

The aim of this report is to apply the Goldberg formalism to study the time evolution of a holes Gaussian wave-packet under SOI-R in Q-1D systems, described by the Governale and Zülicke Hamiltonian. Also analyze the behavior of the spin components of the packet, mainly the spin precession, in order to obtain useful predictions.

Theoretical Model

For typical experimental parameters, only the first heavy hole sub-band is occupied (Governale and Zülicke 2003, 257; Pala *et al.* 2004, 045304; Winkler *et al.* 2002, 155303), thereby in this theoretical model all non-conducting sub-bands will be neglected. Will be considered, in addition, a strictly one-dimensional system arranged along the *z* axis (positive direction will be assumed as the transport direction). The SOI-R dependent dynamics of the heavy holes on the Bloch representation $D_{3/2}$ of the angular momentum, with the basis $|hh_{\frac{3}{2},+\frac{3}{2}}\rangle$ and $|hh_{\frac{3}{2},-\frac{3}{2}}\rangle$, will be described through the Hamiltonian

$$\hat{\boldsymbol{H}} = \hat{\boldsymbol{H}}_0 + \hat{\boldsymbol{H}}_R = \frac{\hbar^2\gamma}{2m_0}\hat{k}_z^2\boldsymbol{I}_2 + \beta\hat{k}_z\boldsymbol{\sigma}_y, \tag{1}$$

taking the energy reference in the sub-band minimum. In the first term $\gamma = \gamma_1 - (2/5)(2\gamma_2 + 3\gamma_3)$, where γ_i represents the Lüttinger parameters, m_0 is the free electron mass and $\boldsymbol{I}_2$ is the identity matrix (2×2). The second term corresponds to the SOI-R for the one-dimensional heavy hole case (Governale and Zülicke 2003, 257), where β is related with the strength of the SOI-R for the first heavy hole sub-band (Winkler *et al.* 2002, 155303), and $\boldsymbol{\sigma}_y$ is one of the Pauli matrices.

In the energy spectrum for the Hamiltonian (1) appear unfolded branches, one for each spin polarization, in the form

$$E_{\pm}(k_z) = \frac{\hbar^2\gamma}{2m_0}k_z^2 \pm \beta k_z. \tag{2}$$

As a result, both spin components travel with different group velocity.

$$v_{g\pm}(k_z) = \frac{1}{\hbar}\frac{\partial E_{\pm}(k_z)}{\partial k_z} = \frac{\hbar\gamma}{m_0}k_z \pm \beta. \tag{3}$$

Numerical Integration

We assumed the Hartree atomic units system. The time-dependent Schrödinger equation has the form

$$\hat{\boldsymbol{H}}\boldsymbol{\Psi} = \begin{bmatrix} \frac{\gamma}{2}\hat{k}_z^2 & -i\beta\hat{k}_z \\ i\beta\hat{k}_z & \frac{\gamma}{2}\hat{k}_z^2 \end{bmatrix}\boldsymbol{\Psi} = i\frac{\partial}{\partial t}\boldsymbol{\Psi}, \tag{4}$$

where $\boldsymbol{\Psi} = \begin{pmatrix} \Psi_1 \\ \Psi_2 \end{pmatrix}$ is a spinor. Since the Hamiltonian (1) is time independent, the formal solution of (4) can be written as

$$\boldsymbol{\Psi}(z,t) = e^{-i(t-t_0)\hat{\boldsymbol{H}}}\boldsymbol{\Psi}(z,t_0). \tag{5}$$

In order to transform the time evolution equation (5) into a finite difference equation, the temporal variable will be designed by the index *n* and the positional variable by the index *j*, such that $\boldsymbol{\Psi}(z,t) \to \boldsymbol{\Psi}_j^n$. It will then have $z \to j$ò and $t \to n\delta$, with ò and δ as the width of the space and time partitions respectively, $j = 0,1,2,\ldots,J$ and $n = 0,1,2,\ldots,N$, with *J* and *N* the total number of partitions. The equation (5) will take the form

$$\boldsymbol{\Psi}_j^{n+1} = e^{-i\delta\,\boldsymbol{H}_j^n}\boldsymbol{\Psi}_j^n. \tag{6}$$

Using the Cayley approach for the time evolution operator (Goldberg *et al.* 1967, 177)

$$e^{i\delta\boldsymbol{H}} = \frac{\boldsymbol{I}_2 - \frac{1}{2}i\delta\boldsymbol{H}}{\boldsymbol{I}_2 + \frac{1}{2}i\delta\boldsymbol{H}}, \tag{7}$$

the equation (6) take the form

$$\left(\boldsymbol{I}_2 + \frac{1}{2}i\delta\boldsymbol{H}_j^n\right)\boldsymbol{\Psi}_j^{n+1} = \left(\boldsymbol{I}_2 - \frac{1}{2}i\delta\boldsymbol{H}_j^n\right)\boldsymbol{\Psi}_j^n. \tag{8}$$

Since the Hamiltonian (1) is non-diagonal (see equation (4)), the expression (8) leads to a coupled equations system for Ψ_1 and Ψ_2 due to the SOI-R. In order to uncouple the system we propose the orthogonal transformation

$$\boldsymbol{\Phi} = \mathrm{U}\boldsymbol{\Psi} \quad with: \mathrm{U} = \frac{1}{\sqrt{2}}\begin{bmatrix} i & 1 \\ -i & 1 \end{bmatrix}. \tag{9}$$

Substituting in (8) and multiplying by U properly we have

$$\left(\boldsymbol{I}_2 + \frac{1}{2} i\delta \mathrm{H}_j^n\right)\boldsymbol{\Phi}_j^{n+1} = \left(\boldsymbol{I}_2 - \frac{1}{2} i\delta \mathrm{H}_j^n\right)\boldsymbol{\Phi}_j^n, \tag{10}$$

where

$$\mathrm{H} = \mathrm{U}\boldsymbol{H}\mathrm{U}^{\dagger} = \begin{bmatrix} \frac{\gamma}{2}\hat{k}_z^2 - i\beta\hat{k}_z & 0 \\ 0 & \frac{\gamma}{2}\hat{k}_z^2 + i\beta\hat{k}_z \end{bmatrix}. \tag{11}$$

The equations system (10) is now uncoupled for the new spinor $\boldsymbol{\Phi} = \begin{pmatrix} \Phi_1 \\ \Phi_2 \end{pmatrix}$. Hereinafter will be only described the process of solution for Φ_1. The case of Φ_2 could be solve likewise. For simplicity, hereafter the subscripts are omitted accordingly.

Taking into account the form of the *quasi-momenta* operators $\hat{k}_z^2 = -\frac{\partial^2}{\partial z^2}$ and $\hat{k}_z = -i\frac{\partial}{\partial z}$, and the form of the differentials operators in finite difference (Jordan 1950, 164)

$$\begin{aligned} f_j^{''} &= \frac{1}{\grave{o}^2}(f_{j+1} - 2f_j + f_{j-1}), \\ f_j^{'} &= \frac{1}{\grave{o}}(f_j - f_{j-1}), \end{aligned} \tag{12}$$

the recurrence equation for Φ_1 in (10), after a relatively simple algebra, takes the explicit form

$$\Phi_{j+1}^{n+1} + (i\xi - 2 + \eta)\Phi_j^{n+1} + (1-\eta)\Phi_{j-1}^{n+1} = -\Phi_{j+1}^n + (i\xi + 2 - \eta)\Phi_j^n + (-1+\eta)\Phi_{j-1}^n, \tag{13}$$

where $\xi = \frac{4\grave{o}^2}{\delta\gamma}$ and $\eta = \frac{2\grave{o}\beta}{\gamma}$ are dimensionless parameters. The equation (13) can be written as

$$\Phi_{j+1}^{n+1} + \Xi\Phi_j^{n+1} + \Lambda\Phi_{j-1}^{n+1} = \Omega_j^n, \tag{14}$$

with

$$\begin{aligned}
&\Xi = i\xi - 2 + \eta, \\
&\Lambda = 1 - \eta, \\
&\Omega_j^n = -\Phi_{j+1}^n + (i\xi + 2 - \eta)\Phi_j^n + (-1 + \eta)\Phi_{j-1}^n.
\end{aligned}$$

Following the standard procedure (Goldberg *et al.* 1967, 177), it is assumed that the temporal-spatial evolution is given by an expression of the form.

$$\Phi_{j+1}^{n+1} = A_j\Phi_j^{n+1} + B_j^n, \tag{15}$$

where auxiliary functions are defined $A_j = A(z)$ and $B_j^n = B(z,t)$. Substituting (15) in (14) leads to

$$\Phi_j^{n+1} = \frac{-\Lambda}{A_j + \Xi}\Phi_{j-1}^{n+1} + \frac{\Omega_j^n - B_j^n}{A_j + \Xi}. \tag{16}$$

This equation is identical to equation (15) written for $j-1$. Comparing (16) and (15) leads to recurrent expressions for A_j and B_j^n

$$\begin{aligned}
&A_j = -\frac{\Lambda}{A_{j-1}} - \Xi, \\
&B_j^n = \Omega_j^2 - B_{j-1}^n(A_j + \Xi).
\end{aligned} \tag{17}$$

For the initial values in the recurrent equations (17), we suppose that our physical system is in a one-dimensional box of length *L*, such that

$$\Psi(0,t) = \Psi(L,t) = 0 \qquad \forall_t. \tag{18}$$

In our difference scheme we have $z = 0 \to j = 0$ and $L = J$ò. Taking into account(9), the condition (18) is transformed into

$$\boldsymbol{\Phi}_0^n = \boldsymbol{\Phi}_L^n = 0 \qquad \forall_n. \tag{19}$$

With the condition (19) in mind, let us write the equation (14) for $j = 1$

$$\Phi_2^{n+1} = -\Xi\Phi_1^{n+1} + \Omega_1^n. \tag{20}$$

By comparing to (15) we reach

$$\begin{aligned} A_1 &= -\Xi, \\ B_1^n &= \Omega_1^n. \end{aligned} \tag{21}$$

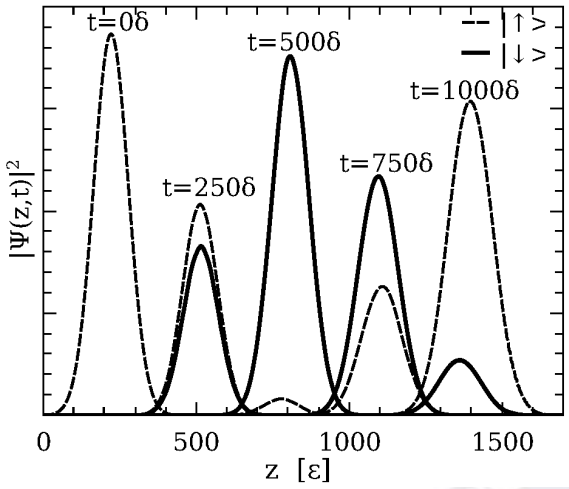

Figure 1 Temporal evolution of the spin components of the wave-packet $\left|\uparrow\right\rangle$ and $\left|\downarrow\right\rangle$ along the *z* direction.

The initial condition $\boldsymbol{\Phi}_j^0; \forall_j$ is easily obtained, considering the transformation (9), from the initial condition of the original problem

$$\boldsymbol{\Psi}(z,0) = \sqrt{\frac{2\pi}{\Delta z}} e^{\frac{(z-z_0)^2}{2\Delta z^2}} e^{ik(z-z_0)} \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \tag{22}$$

where has been considered a Gaussian wave-packet spin-polarized along the positive *z* direction, with spatial dispersion Δz and initial position z_0.

Taking into account (17), (21) and (22) is straightforward to obtain A_j and $B_j^n \; \forall_{j,n}$. Writing (14) in the form

$$\Phi_j^{n+1} = \frac{\Phi_{j+1}^{n+1}}{A_j} - \frac{B_j^n}{A_j} \tag{23}$$

and noting that $\Phi_J^n = 0 \, \forall_n$, it is possible to construct the solution $\Phi_j^n \; \forall_{j,n}$ space traveling back to front: $j = J, j = J-1, \ldots, j = 0$. Once obtained Φ_1 and Φ_2, using the transformation (9), is recovered original solution $\Psi_j^n \; \forall_{j,n}$.

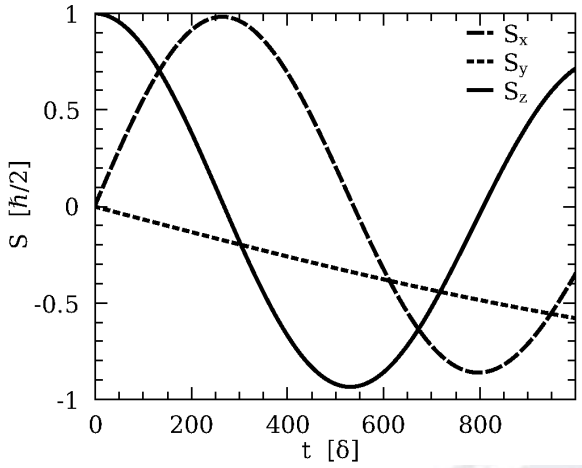

Figure 2 Time dependence of the expected value of the components during the process of spin precession given by the SOI-R.

Numerical Results

In the results shown below, it has been chosen as spatial partition $\grave{o} = 1.89$ *a.u.* and temporal partition $\delta = 7.14$ *a.u.* as well as the physical parameters related to the GaAs (Vurgaftman *et al.* 2001, 5815) $\xi = 0.75$ and $\eta = 0.005$, the latter proportional to the parameter β related to the strength of the SOI-R.

Fig. 1 shows the temporal evolution of the spin components of the wave-packet ($\left|\uparrow\right\rangle = \left\langle \begin{pmatrix} 1 \\ 0 \end{pmatrix} | \Psi \right\rangle$ and $\left|\downarrow\right\rangle = \left\langle \begin{pmatrix} 0 \\ 1 \end{pmatrix} | \Psi \right\rangle$) along the *z* direction. At the first instant of time $t = 0\delta$ only the

component $|\uparrow\rangle$ is nonzero, which is consistent with the choice of the initial condition of the spin polarization of the packet. As the packet travels, *e.g.* $t = 250\delta$, the component $|\downarrow\rangle$ increases while $|\uparrow\rangle$ decreases, as a result of spin precession process induced by the SOI-R. As the spin presses with *t* [see Fig. 2 and 3], it do not represent a well-defined quantum number. Thus, the time-line probabilities shown in Fig.1, by no means can be expected as universal for the present system. This behavior is observed during the whole evolution of the packet. It is further noted that after a time, *e.g.* $t = 1000\delta$, both spin components of the packet are displaced, relative to each other, because they move with different group velocities [see equation (3)]. Despite this spatial shift, it is not possible to obtain a spin-filter behavior (Governale and Zülicke 2003, 257), because there is not any symmetry-breaking mechanism here. The latest exclude the possibility for segregating particles with a defined spin-polarization. Even by placing a dispersive obstacle, *e.g.* a potential barrier, in the transport channel of our system, none filter phenomenon could be detected, for the same reasons commented above. Notice that the packet travels almost without spreading. This could be guarantee by taking the initial and boundary condition using the stationary phase time approach, which has showed the better results dealing with electronic wave-packets (Pereyra and Simanjuntak 2007, 056604).

In order to provide some qualitative comparison, we focus to the total time needed for our hole packet travel the entire system (length 1420 Å), which is similar to that obtained by Tung and Lee (Tung and Lee 1996, 2122), where the dispersion of an electronic wave-packet in a particular potential structure (length 3050 Å) was studied.

It is of particular interest in Spintronics devices as SFET, to know exactly the spin precession of a carrier under SOI-R. Fig. 2 shows the time dependence of the spin expected value

$$S_i = \frac{\hbar}{2}\langle \boldsymbol{\Psi} \,|\, \boldsymbol{\sigma}_i \,|\, \boldsymbol{\Psi} \rangle \qquad being: i = x, y, z, \tag{24}$$

where $\boldsymbol{\sigma}_i$ are the Pauli matrices. Worthwhile noticing, that is possible to evaluate the spin polarization flip-time t_{sf} , which is the time during what a maximum spin *z*-component turns into a minimum one. This occur at $t_{sf} = 530\delta$, *i.e.*, $t_{sf} = 3784.2$ *a.u.*, as can be straightforwardly estimated from Fig.2 [see the time-axis allocation for $S_z \approx$-1 (full line)]. Despite that the

"velocity" of holes are slower than the electrons, the spin polarization flip-time are shorter, *i.e.* the SOI-R is more efficiently for holes (Gvozdic´ and Ekenberg 2006, 377).

It is clearly seen as S_x and S_z oscillate with a certain damping, determined by the decrease of S_y, since they satisfy $\sqrt{S_x^2+S_y^2+S_z^2} \equiv \hbar/2$. This suggests that the spin precession takes place around *y*-oriented axis. The last suitably matches with an effective magnetic field (Bychkov and Rashba 1984, 6039; Datta and Das 1990, 665; Cuan and Diago-Cisneros 2010, 212), whose wave-vector dependence is of the form $\boldsymbol{B}_{eff} \sim \boldsymbol{k} \times \boldsymbol{n}$, being $\boldsymbol{n} = (1,0,0)$ the potential-gradient direction. It is expected that S_x and S_z approach asymptotically to zero as S_y goes to -1 as a result of a conservative requirement, so the spin finally remains on the direction of $\boldsymbol{B}_{eff}$. A clearer description of the spin precession process described above, can be seen in Fig. 3. In this figure, we visualize a parameterized trace of the extreme point for the spin vector $\vec{S} = \vec{S}_x + \vec{S}_y + \vec{S}_z$. Thereby we are graphically showing how evolves each expected value of (24) during the complete temporal interval under consideration. As a bonus, from this 3D-perspective plot, becomes possible to qualitatively verify the fulfillment of the conservation constrain

$$\sqrt{S_x^2+S_y^2+S_z^2} \equiv \hbar/2.$$

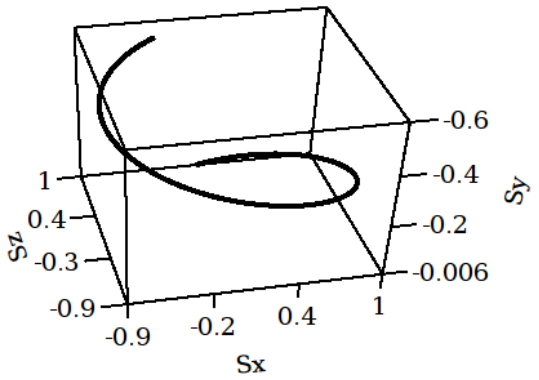

Figure 3 Visualization of the spin precession process from the representation of its components in Fig. 2.

Conclusions

We have successfully extended the formalism of Goldberg *et al.* to study the dynamics of holes wave-packets in *quasi*- one-dimensional systems in the presence of Rashba spin-orbit interaction.

Our numerical model reproduces the expected phenomenology, *i. e.*, the spatial displacement of the spin-up eigen-states respect to the spin-down ones --due to the different group velocity values--, and the spin precession process induced by the SOI-R. Additionally, we were able to estimate the polarization flip-time for the *z*-component of the spin to be approximately 530δ, being similar to the typically founded in the specialized literature which is of the order of $10^{-13}\,s$. We consider the present study could attract interest, whenever a spin field effect transistor device, is modeled for holes as carriers.

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