Spin Precession of Quasi-Bound States in Heterostructures with Spin-Orbit Interaction

G. Isić\textsuperscript{a,b,∗}, D. Indjin\textsuperscript{a}, Z. Ikonić\textsuperscript{a}, V. Milanović\textsuperscript{c}, J. Radovanović\textsuperscript{c} and P. Harrison\textsuperscript{a}

\textsuperscript{a}School of Electronic and Electrical Engineering, University of Leeds, United Kingdom
\textsuperscript{b}Institute of Physics, Belgrade, Serbia
\textsuperscript{c}School of Electrical Engineering, University of Belgrade, Serbia

We use a finite-difference model that is capable of describing the single state spin dynamics in a double-barrier AlGaAs heterostructure. The use of Green’s functions enables a description of the double-barrier structure by a finite matrix while the interaction with contacts is described by appropriate self-energies. To account for interface roughness scattering, a self-energy \( \Sigma_{\text{IR}}(E, k) \) is derived within the random phase approximation. The dominant part is due to in-plane momentum relaxation while a smaller part describing spin-flip scattering is neglected. The former only decreases the state lifetime while the latter can also affect the spin precession frequency.

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1. Introduction

The spin-orbit interaction (SOI) in noncentrosymmetric semiconductors provides means for nonmagnetic control of spin phenomena [1]. The carrier spin responds to its electrostatic environment as moving electrons see an effective magnetic field \( B_{\text{eff}} \) in their reference frame. If a nonzero average momentum of the carrier ensemble is accomplished, \( B_{\text{eff}} \) may be manifested through spin precession of coherently excited carriers allowing its direct measurement [2].

We study the spin precession of an electron injected into the well region of a double-barrier AlGaAs system. States within the GaAs well are quasi-bound due to the coupling to the reservoirs behind AlGaAs barriers, i.e. because there is a finite probability that the electron will tunnel out. In a finite-difference model, the finite lifetime due to tunnelling out is described by a self-energy matrix \( \Sigma_{L}(E, k) \) which enforces the correct boundary conditions at boundaries between the system of interest and the reservoirs [3].

2. Finite-difference model

The problem is defined on a grid \( z_{n} = z_{0} + na, \ n = 0, \pm 1, \pm 2, \ldots \), which amounts to using \( \{ |z_{n}\} \) as the basis set to describe the electron’s state in the structure, Fig. 1. The finite-difference model is obtained by approximating differential operators, e.g. \( p_{z} \), with finite differences and representing them by matrices.

\[ p_{z} |z\rangle = \frac{i\hbar}{2a} (|z + a\rangle - |z - a\rangle), \]
\[ \langle z | p_{z} | z'\rangle = \frac{i\hbar}{2a} (\delta_{z,z' + a} - \delta_{z,z' - a}). \]

With \( k \) being the in-plane wave vector, the system is described by the (retarded) Green function [4]
\[ G(E, k) = (E - \varepsilon_{k} - H + i\eta)^{-1}, \]
\[ \varepsilon_{k} = \frac{\hbar^{2}k^{2}}{2m}, \quad \eta \rightarrow 0^{+}. \]

The infinite matrix \( G(E, k) \) can be folded onto a \( N \times N \) matrix \( G_{0}(E, k) \) by representing the interaction with the left (L) and right (R) contact by self-energies \( \Sigma_{L,R} \) is the z-component of the wave vector in the contact
\[ \Sigma_{L}(E, k) = -\frac{\hbar^{2}}{2ma^{2}} [\exp(ik_{L}a) |z_{1}\rangle \times \langle z_{1}| + \exp(ik_{R}a) |z_{N}\rangle \langle z_{N}|]. \]

The device Green function is [5]:
\[ G_{0}(E, k) = [E - \varepsilon_{k} - H_{0} - \Sigma_{L}(E, k)]^{-1}. \]

\[ \left( 513 \right) \]
3. Spin–orbit interaction

SOI is included up to first order in $k$. The spin coordinate is introduced into $G_0(E, k)$ by [1]:

$$G_0(E, k) \rightarrow G_0(E, k) \otimes I_2,$$

(Kronecker product with the $2 \times 2$ unit matrix). The Dresselhaus and Rashba Hamiltonians are given by

$$H_D = \gamma (\sigma x k_x - \sigma y k_y) \frac{d^2}{dz^2},$$

$$H_R = \alpha (\sigma y k_x - \sigma x k_y),$$

and are included in the total Hamiltonian through the SOI self-energy $\Sigma_{SOI}(E, k)$. This is an exact description in absence of scattering potentials.

SOI is manifested as the splitting of quasi-bound states, which are defined as peaks in the local density of states (LDOS):

$$LDOS(E, k, z) = \frac{|z| A(E, k) |z|}{2\pi},$$

$$A(E, k) = 1 \{ G_0(E, k) - G_0^+(E, k) \},$$

where $G_0^+(E, k)$ (the advanced Green function) is the Hermitian conjugate of $G_0(E, k)$. Numerical calculations of LDOS in a double-barrier structure are shown in Fig. 2.

![Fig. 2. Left part is the LDOS in absence of SOI. Right part, SOI included. Dark is small, light is large. LDOS shown in logarithmic scale. Black lines are the two Al-GaAs barriers, the rest is GaAs. Here $k \parallel |11|$ (maximum splitting) and $\varepsilon_k = 80 \text{ meV}, \gamma = 24 \text{ eV } \AA^3, \alpha = 50 \text{ meV}$ while $E_z = E - \varepsilon_k$.](image)

4. Interface roughness

The self-energy due to interface roughness scattering, $\Sigma_{IR}$, is found using the random phase approximation [6]:

$$\Sigma_{IR}(E, k) = \sum_{z_j} |z_j\rangle \langle z_j| \frac{N_W}{\Omega} (W_{kk'}(z_j)$$

$$+ \sum_{k'} \frac{1}{\Omega} |W_{kk'}(z_j)|^2 \langle z_j| G_0(E, k') |z_j\rangle).$$

The sum runs over interface coordinates $z_j$. For $|W_{kk'}(z)|$ we take

$$|W_{kk'}(z)|^2 = A(z)\pi A^2 \exp\left(-\frac{A^2|k - k'|^2}{4}\right),$$

and $A(z)$ is nonzero only in the vicinity of the interface $z = z_j \pm \frac{a}{2}$.

Now, the Green function, $G_T(E, k)$ that accounts for interface roughness scattering is given by

$$G_T(E, k) = (G_0(E, k)^{-1} - \Sigma_{IR}(E, k))^{-1}.$$

Interface roughness scattering broadens the DOS features, as shown in Fig. 3.

![Fig. 3. The interface roughness scattering broadens the quasi-bound states. The density of states (DOS) is the sum of LDOS over all $z$. Parameters are the same as in Fig. 2 and $A = 10 \text{ nm}, A = 10^4 \text{ eV}^2 \text{ nm}^2$, $N_W/\Omega = 10^{-7} \text{ nm}^{-2}$.](image)

5. Spin precession

Figure 4 shows the numerically calculated temporal evolution of the initial state. To study the spin dynamics in the double-barrier structure, we consider the time dependent state $|\psi_k(t)\rangle$ with the initial conditions at $t = t_0$ of being located at $z_S$ (halfway between the two barriers) with spin-up and in-plane wave vector $k$:

$$|\langle z_S | k \psi_k(t)\rangle|^2 = |\langle z_S | k \psi_k(t)\rangle|^2.$$

![Fig. 4. Probabilities for being in spin-up and spin-down state at $z_S$ (the midpoint of the GaAs well region) as a function of time, $t_0 = 0$. Parameters are the same as in Figs. 2 and 3. Blue, $\Sigma_{IR} = 0$, red $\Sigma_{IR} \neq 0$. The dependence is oscillatory with an exponentially decaying envelope due to finite lifetime.](image)

For $t > t_0$ the $|\psi_k(t)\rangle$ state is given by
\[ |\psi_k(t)\rangle = U(t-t_0,k) |\psi_k(t_0)\rangle , \]

where \( U \) is the time-evolution operator given by [7]

\[
U(t-t_0,k) = \frac{i}{2\pi} \int E \exp \left(-i \frac{E (t-t_0)}{\hbar} \right)
\times G(E,k) dE ,
\]

and \( G(E,k) \) represents \( G_0(E,k) \) or \( G_T(E,k) \), depending on whether interface roughness scattering is included or not.

The spin precession frequency is independent of \( \Sigma_{IR} \) because it does not describe spin-flip scattering (a higher-order effect). Its value is consistent with the splitting of the lowest quasi-bound doublet shown in Fig. 3. For \( t < 0.2 \) ps, the lines are noisy due to the finite accuracy of the numerical Fourier transform. Also, for small times the dynamics is influenced by short-lived higher quasi-bound states.

6. Conclusion

Numerical calculations show that the spin-dependent dynamics in a double-barrier structure can be explained by spin precession of the lowest lying quasi-bound doublet. This is analogous to the case in a quantum well where spin precession has been used to directly measure the SOI induced effective magnetic field [2].

A model to account for interface roughness scattering is described. Its main effect is to broaden the DOS features due to in-plane momentum relaxation. In the present model, it does not affect the spin precession frequency.

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