

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

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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 \mathbf{B}_{eff} in their reference frame. If a nonzero average momentum of the carrier ensemble is accomplished, \mathbf{B}_{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 $\Sigma_{\text{I}}(E, k)$ 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 $z_n = z_0 + na$, $n = 0, \pm 1, \pm 2, \dots$ which amounts to using $\{|z_n\rangle\}$ 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

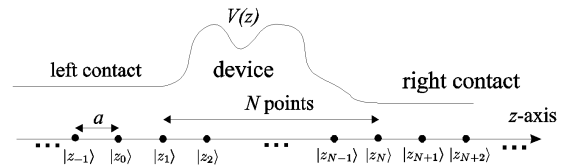


Fig. 1. A schematic of the problem. The device consists of points z_1, z_2, \dots, z_N . In the finite-difference scheme, it is described by Hamiltonian H_0 which is a $N \times N$ matrix.

$$p_z |z\rangle = \frac{i\hbar}{2a} (|z+a\rangle - |z-a\rangle),$$

$$\langle z|p_z|z'\rangle = \frac{i\hbar}{2a} (\delta_{z,z'+a} - \delta_{z,z'-a}). \quad (1)$$

With k being the in-plane wave vector, the system is described by the (retarded) Green function [4]

$$G(E, k) = (E - \varepsilon_k - H + i\eta)^{-1},$$

$$\varepsilon_k = \frac{\hbar^2 k^2}{2m}, \quad \eta \rightarrow 0^+. \quad (2)$$

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 ($k_{\text{L,R}}$ is the z -component of the wave vector in the contact)

$$\Sigma_{\text{I}}(E, k) = -\frac{\hbar^2}{2ma^2} \left[\exp(ik_{\text{L}}a) |z_1\rangle \right.$$

$$\left. \times \langle z_1| + \exp(ik_{\text{R}}a) |z_N\rangle \langle z_N| \right]. \quad (3)$$

The device Green function is [5]:

$$G_0(E, k) = [E - \varepsilon_k - H_0 - \Sigma_{\text{I}}(E, k)]^{-1}. \quad (4)$$

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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]:

$$G_0(E, k) \rightarrow G_0(E, k) \otimes I_2, \quad (5)$$

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

$$H_D = \gamma (\sigma_x k_x - \sigma_y k_y) \frac{d^2}{dz^2},$$

$$H_R = \alpha (\sigma_y k_x - \sigma_x k_y), \quad (6)$$

and are included in the total Hamiltonian through the SOI self-energy $\Sigma_{\text{SOI}}(E, k)$. 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):

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

$$A(E, k) = i (G_0(E, k) - G_0^+(E, k)), \quad (7)$$

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.

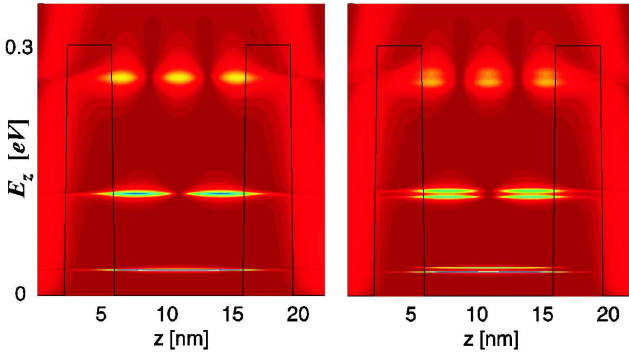


Fig. 2. Left part is the LDOS in absence of SOI. Right part, SOI included. Dark is small, light is large, LDOS shown in logarithmic scale. Black lines are the two AlGaAs barriers, the rest is GaAs. Here $k \parallel [11]$ (maximum splitting) and $\varepsilon_k = 80$ meV, $\gamma = 24$ eV Å³, $\alpha = 50$ meV while $E_z = E - \varepsilon_k$.

4. Interface roughness

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

$$\Sigma_{\text{IR}}(E, k) = \sum_{z_j} |z_j\rangle \langle z_j| \frac{N_{\text{W}}}{\Omega} (W_{kk'}(z_j) + \sum_{k'} \frac{1}{\Omega} |W_{kk'}(z_j)|^2 \langle z_j | G_0(E, k') | z_j \rangle). \quad (8)$$

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

$$|W_{kk'}(z)|^2 = A(z) \pi \Lambda^2 \exp\left(-\frac{\Lambda^2 |k - k'|^2}{4}\right), \quad (9)$$

and $A(z)$ is nonzero only in the vicinity of the interface $z = z_j \pm \frac{a}{2}$. (10)

Now, the Green function, $G_{\text{T}}(E, k)$ that accounts for interface roughness scattering is given by

$$G_{\text{T}}(E, k) = (G_0(E, k)^{-1} - \Sigma_{\text{IR}}(E, k))^{-1}. \quad (11)$$

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

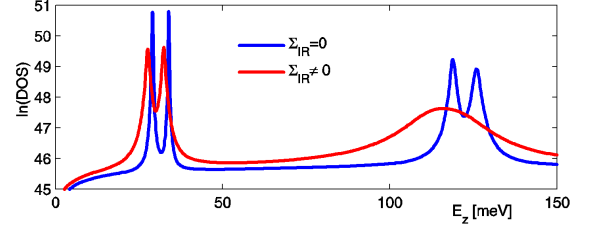


Fig. 3. The interface roughness scattering broadens the quasi-bound states. The density of states (DOS) is the sum of LDOS over all z . Parameters are the same as in Fig. 2 and $\Lambda = 10$ nm, $A = 10^4$ eV² nm², $N_{\text{W}}/\Omega = 10^{-5}$ nm⁻².

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 :

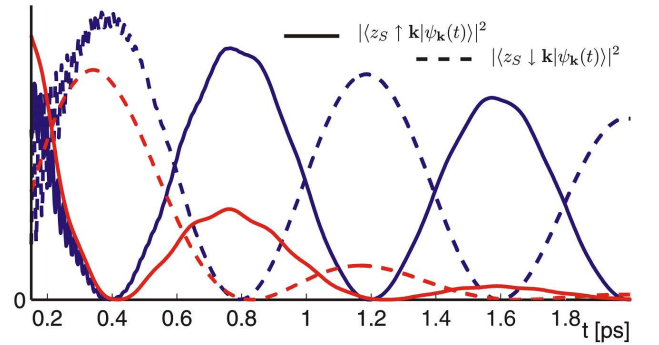


Fig. 4. Probabilities for being in spin-up and spin-down state at z_{S} (the midpoint of the GaAs well region) as a function of time, $t_0 = 0$. Parameters are the same as in Figs. 2 and 3. Blue, $\Sigma_{\text{IR}} = 0$, red $\Sigma_{\text{IR}} \neq 0$. The dependence is oscillatory with an exponentially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

$$|\psi_k(t = t_0)\rangle = |z_{\text{S}} \uparrow k\rangle. \quad (12)$$

For $t > t_0$ the $|\psi_k(t)\rangle$ state is given by

$$|\psi_k(t)\rangle = U(t - t_0, k) |\psi_k(t_0)\rangle, \quad (13)$$

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

$$U(t - t_0, k) = \frac{i}{2\pi} \int_{\mathbb{E}} \exp\left(-i \frac{E(t - t_0)}{\hbar}\right) \times G(E, k) dE, \quad (14)$$

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 Σ_{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.

Acknowledgments

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