Spin transition rates in nanowire superlattices: Rashba spin–orbit coupling effects

Sanjay Prabhakar, Roderick Melnik and Luis L Bonilla

1 M2NeT Laboratory, Wilfrid Laurier University, Waterloo, ON, N2L 3C5, Canada
2 Gregorio Millan Institute, Universidad Carlos III de Madrid, 28911, Leganes, Spain
3 School of Engineering and Applied Sciences, Harvard University, Cambridge, MA 02138, USA

Abstract
We investigate the influence of Rashba spin–orbit coupling in a parabolic nanowire modulated by longitudinal periodic potential. The modulation potential can be obtained from realistically grown superlattices (SLs). Our study shows that the Rashba spin–orbit interaction induces the level crossing point in the parabolic nanowire SLs. We estimate large anticrossing width (approximately 117 µeV) between singlet–triplet states. We study the phonon and electromagnetic field mediated spin transition rates in the parabolic nanowire SLs. We report that the phonon mediated spin transition rate is several order of magnitude larger than the electromagnetic field mediated spin transition rate. Based on the Feynman disentangling technique, we find the exact spin transition probability. For the case wave vector \( k = 0 \), we report that the transition probability can be tuned in the form of resonance at fixed time interval. For the general case (\( k \neq 0 \)), we solve the Riccati equation and find that the arbitrary values of \( k \) induces the damping in the transition probability. At large value of Rashba spin–orbit coupling coefficients for (\( k \neq 0 \)), spin transition probability freezes.

1. Introduction

Low-dimensional semiconductor nanostructures such as quantum dots, quantum wells and quantum wires can be formed in the plane of two-dimensional electron gas (2DEG) with the application of externally applied gate potentials, have attracted significant interest for building robust spintronics logic devices and other applications [1–9]. Single electron spins in these nanostructures can be manipulated by several parameters such as the gate controlled electric fields in the lateral direction and externally applied magnetic fields. The Rashba and Dresselhaus spin–orbit couplings provide another efficient way to control the single electron spins in these nanostructures [1, 6, 10]. The Rashba spin–orbit coupling arises due to structural inversion asymmetry in the crystal lattice along the growth direction [11]. The Dresselhaus spin–orbit coupling arises due to bulk inversion asymmetry in the system [12].

Accurate estimation of the spin transition rate, mediated by phonons and electromagnetic fields, is of great interest for the design of optoelectronic devices [7, 13, 14]. Long spin relaxation rates, approximately 0.85 ms in GaAs quantum dots and 20 ms in InGaAs quantum dots, have been measured by utilizing several different experimental techniques such as pulsed relaxation and optical orientation methods [15, 16]. In these experiments, it is confirmed that the transition rate is dominated by the spin–orbit coupling with respect to the environment [2, 17, 18]. Because of the spin–orbit coupling, the electron spin qubits in the nanowire quantum dots localized in a transmission line resonator can be manipulated, stored and read out with the application of the gate controlled electric fields [13, 19]. In this paper, we investigate the energy spectrum of the parabolic nanowire modulated by realistically grown superlattices (SLs) in the longitudinal direction [20–22]. We focus on the study of the crossing of the energy spectrum of the nanowire SLs accounting for the Rashba spin–orbit coupling. The crossing point can be achieved with the accessible values of the strength of the Rashba spin–orbit coupling.

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with the Rashba spin–orbit coupling under the influence of electromagnetic field radiation [23, 24], phonons [18] and Dyakonov–Perel (DP) [25] mechanisms. We can write the momentum as a classical variable in the DP mechanism under the Markovian process [25–27] and estimate the transition probability by utilizing the Feynman disentangling technique method [2, 28, 29]. The DP mechanism corresponds to the spin splitting of the conduction band in zinc blende semiconductors at finite wave vectors which is equivalent to the presence of an effective magnetic field that causes the precession of an electron spin [25, 26].

The paper is organized as follows: in section 2, we develop a theoretical model that allows us to find the crossing of the energy spectrum of the parabolic nanowire SLs with the Rashba spin–orbit coupling. In this section, we also develop the theoretical model that allows us to find the spin transition rate. In section 3, we plot the dispersion relation (see figure 1) of the parabolic nanowire modulated by longitudinal periodic potential. In figures 2 and 3, we plot the spin transition rate of the nanowire SLs with the Rashba spin–orbit coupling via electromagnetic field radiation, phonons and DP mechanisms. Finally, in section 4, we summarize our results.

2. Theoretical model

The total Hamiltonian of the quasi-one-dimensional parabolic nanowire formed in the plane of 2DEG with the Rashba spin–orbit coupling in the presence of longitudinal modulation potential (see figure 1 for experimental set up) can be written as [4, 30–33]

\[
H = H_{xy} + H_z + H_R, \tag{1}
\]

\[
H_{xy} = \frac{p_y^2}{2m} + \frac{1}{2}m\omega_0^2 y^2 + \varepsilon_v(k), \tag{2}
\]

\[
H_z = \frac{p_z^2}{2m} + V(z), \tag{3}
\]

\[
H_R = \frac{\alpha}{\hbar} (p_x\sigma_y - p_y\sigma_x), \tag{4}
\]

where \(H_z\) is the Hamiltonian of the electrons along the \(z\)-direction and \(H_R\) is the spin–orbit Hamiltonian associated with the Rashba coupling. The full descriptions of \(H_z\) and \(H_R\) will be discussed shortly. In the above Hamiltonians \(p_x, p_y\) and \(p_z\) are the momentum operator, \(m\) is the effective mass, \(\alpha\) is the strength of the Rashba spin–orbit coupling and \(\omega_0 = \hbar/m\ell_0^2\) is the confinement frequency of the parabolic potential with \(\ell_0\) being the oscillator strength. \(\varepsilon_v(k)\) provides the periodic longitudinal modulation potential along the \(x\) direction in the form of: [4, 34, 35]

\[
\varepsilon_v(k) = \frac{\Delta_1}{2} (1 - \cos kl), \tag{5}
\]

where \(\Delta_1\) is the first miniband width and \(l\) is the SL period [21, 36]. The second term in (1) represents the Hamiltonian of the electron along the \(z\)-direction where \(V_z\) is the asymmetric triangular quantum well confining potential along the \(z\)-direction. Usually, the asymmetric triangular quantum well potential can be found by solving the Schrödinger–Poisson equations self-consistently [1, 37]. The potential along the \(z\)-direction can be chosen as \(V_z = eE_z\) for \(z \geq 0\) and \(V_z = \infty\) for \(z < 0\) [38]. The ground state wavefunction \(\Psi_{0z}(z)\) of \(H_z\) can be written in the form of Airy function (Ai) as [1, 37, 38]

\[
\Psi_{0z}(z) = 1.4261q^{1/2}Ai(qz + \varphi_1), \tag{6}
\]

where \(\varphi_1 = -2.3381\) is the first zero of the Airy function and

\[
q = \left[ \frac{2mE_g^{1/2}}{\hbar^2} \right]^{1/3}. \tag{7}
\]

We will make use of an average momentum squared in the state (6), \(\langle p_z^2 \rangle = 0.78(\hbar q)^2\), and the average position \(\langle z \rangle = 1.56/q\) to estimate the thickness of the 2DEG. The structural inversion asymmetry in \(V_z\) leads to the Rashba spin–orbit coupling (see equation (4)) and the Rashba coefficient \(\alpha\) can be written as [39]

\[
\alpha = \frac{\gamma_R e(E)}{\hbar}, \quad \gamma_R = \frac{\hbar^2 \Delta (2E_g + \Delta)}{2mE_g (E_g + \Delta) (3E_g + 2\Delta)}, \tag{8}
\]

where \(\Delta\) stands for the spin–orbit splitting in the valence band and \(E_g\) is the band gap. For InAs material, we adopt the value \(\gamma_R = 110\ \text{Å}^2\).

Since, \([p_z, H_{xy}] = 0\), we consider \(p_z\) is the good quantum number and the eigenvalue of \(p_z\) can be written as [30, 31, 35]

\[
p_z = \frac{m}{\hbar} \frac{d\varepsilon_v(k)}{dk} = \frac{ml}{2\hbar} \Delta_1 \sin kl. \tag{9}
\]

The Hamiltonians (2) and (4) can be written in terms of annihilation and creation operators as

\[
H_{xy} = (a^\dagger a + \frac{1}{2}) \hbar \omega_0 + \varepsilon_v(k), \tag{10}
\]

\[
H_R = -\frac{\alpha m l}{2\hbar^2} \Delta_1 \sin kl \sigma_x + \frac{i\alpha}{\ell_0 \sqrt{2}} (a^\dagger - a) \sigma_x, \tag{11}
\]

To find the energy spectrum of the above Hamiltonian, it is convenient to rotate the Hamiltonian \(H_{xyR} = H_{xy} + H_R\) by \((i\pi \sigma_z/4)(H_{xy} + H_R) \exp (i\pi \sigma_z/4)\) so that the eigenvalue
of $p_r$ couples to $\sigma_z$. The new Hamiltonian can be written as $H_{xy} = H_0 + H_1$, where $H_0$ is the diagonal part and $H_1$ is the non-diagonal part [4]:

$$H_0 = \left( a^\dagger a + \frac{1}{2} \right) \hbar \omega_0 - \frac{\Delta_1}{2} \xi \sin kl \sigma_z + \epsilon_v(k),$$

$$H_1 = \frac{i\alpha}{\hbar \sqrt{8}} \left( a^\dagger - a \right) \sigma_x + \text{H.c.},$$

where $\xi = \hbar^2/(am)$ is the spin-precession length, $\sigma_\pm = \sigma_z \pm i\sigma_y$ and H.c. stands the Hermitian conjugate. From equation (13), it is clear that the non-diagonal part couples the $c$ and $c^\dagger$ of $H_{xy}$. The energy spectrum of the nanowire can be written as

$$\varepsilon_{n,\pm/2} = \left( n + \frac{1}{2} \right) \hbar \omega_0 - \frac{\Delta_1}{2} \xi \sin kl + \varepsilon_v(k),$$

$$+ \frac{\alpha^2 \xi}{8 \hbar^2} \left[ \frac{n}{\hbar \omega_0 \xi - \Delta_1 \sin kl} - \frac{n + 1}{\hbar \omega_0 \xi + \Delta_1 \sin kl} \right],$$

$$\varepsilon_{n,-1/2} = \left( n + \frac{1}{2} \right) \hbar \omega_0 + \frac{\Delta_1}{2} \xi \sin kl + \varepsilon_v(k),$$

$$+ \frac{\alpha^2 \xi}{8 \hbar^2} \left[ \frac{n}{\hbar \omega_0 \xi + \Delta_1 \sin kl} - \frac{n + 1}{\hbar \omega_0 \xi - \Delta_1 \sin kl} \right].$$

We now turn to the calculation of spin–flip transition rate in parabolic nanowire SLs with electromagnetic field radiation. Following [7], the interaction between electron and piezo-phonon can be written as [18, 42–44]

$$u_{q \sigma}^\text{se}(r, t) = \sqrt{\frac{\hbar}{2 \rho V \omega_{q\sigma}}} e^{i(q \cdot r - \omega_{q\sigma} t)} e^\text{A}_{q\sigma} b_{q\sigma}^\dagger + \text{H.c.}$$

Here, $\rho$ is the crystal mass density, $V$ is the volume of the nanowire SLs, $b_{q\sigma}$ creates an acoustic phonon with wave vector $q$ and polarization $\sigma$, where $\sigma = \sigma_x, \sigma_y, \sigma_z$ are chosen as one longitudinal and two transverse phonon modes. Also, $A_{q\sigma}$ is the electric field created by phonon strain, where $\alpha = l, t, l, t$ are chosen as a classical variable whose dependence on the position $r$ and time $t$. The vector potential $A(r, t)$ of the electromagnetic field radiation is written as

$$A(r, t) = \frac{\hbar}{2 e \epsilon_0 V} \hat{e}_{q\lambda} b_{q\lambda} e^{i(q \cdot r - \omega_{q\lambda} t)} + \text{H.c.},$$

where $\omega_{q\lambda} = c |q|$, $b_{q\lambda}$ annihilate photons with wave vector $q$, $c$ is the velocity of light, $V$ is the volume of the nanowire and $\epsilon_x$ is the dielectric constant of the nanowire. The polarization vector holds the relation as $\hat{e}_{q\lambda} = (\sin \phi, -\cos \phi, 0)$ and $\hat{e}_{q\sigma} = (\cos \phi \cos \phi \sin \phi, -\cos \phi \sin \theta)$ because we express $q = q(\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)$. The above polarization vectors holds the relation as $\hat{e}_{q\lambda} = \hat{e}_{q\sigma} \times \hat{q}$, $\hat{e}_{q\sigma} = \hat{q} \times \hat{e}_{q\lambda}$ and $\hat{q} = \hat{e}_{q\lambda} \times \hat{e}_{q\sigma}$. Based on the Fermi–Golden Rule, the electromagnetic field mediated spin transition rate (i.e. the transition probability per unit time) in the nanowire modulated by longitudinal periodic potential is given by [40]

$$\frac{1}{T_1} = \frac{V}{(2\pi)^2 \hbar} \times \int d^3q \sum_{\lambda=1,2} |M_{q\lambda}|^2 \delta \left( \hbar \omega_q - \varepsilon_{q,0/-2} + \varepsilon_{q,0/+2} \right),$$

where the matrix element $M_{q\lambda} = \langle n, 1/2 | H_{xy} | n, -1/2 \rangle$ is found perturbatively. The spin transition rate (i.e. $n, -1/2 \rightarrow n, +1/2$) is given by

$$\frac{1}{T_1} = \frac{\alpha^2 e^2 \Delta_1 \sin kl}{4\pi \hbar \xi} \left[ \frac{1}{\varepsilon_{q,0}^2 (\hbar \omega_0 \xi)^2 - (\Delta_1 \sin kl)^2} + 1 \right].$$

2.2. Phonon mediated spin transition rate

We now turn to the calculation of the phonon-mediated spin relaxation rate in parabolic nanowire SLs. Following [7], the interaction between electron and piezo-phonon can be written as [18, 42–44]

$$u_{q\sigma}^\text{se}(r, t) = \sqrt{\frac{\hbar}{2 \rho V \omega_{q\sigma}}} e^{i(q \cdot r - \omega_{q\sigma} t)} e^\text{A}_{q\sigma} b_{q\sigma}^\dagger + \text{H.c.}$$

2.3. Spin-flip transition probability: Feynman disentangling technique

We used the Feynman disentangling technique [2, 28, 29] to find the transition probability of electron spins of the Hamiltonian associated with the Rashba spin–orbit coupling. Under the DP mechanism [25, 26], we consider the momentum $p(t) = m \dot{r}$ as a classical variable whose dependence on time $t$ is generated by a Markovian process [27]. In this case, the Rashba spin–orbit Hamiltonian $\hat{H}_R = \exp(-i\tau \sigma_z/4) \hat{H}_R \exp(i\tau \sigma_z/4)$ can be written as

$$\hat{H}_R(t) = \frac{\xi}{\hbar} \hbar \omega_0 \cos \omega_0 t (s_+ + s_-) - \frac{\Delta_1}{\xi} \Delta_1 \sin kl s_z,$$
where $\xi = \hbar \omega_0 l_0 / \alpha$ is the spin-precession length, $\xi_0$ is the spin-orbital radius and $s_\pm = s_x \pm i s_y$. The spin operators obey the $SU(2)$ algebra, $[s_x, s_z] = 2s_z$, and $[s_x, s_y] = \pm is_y$. The spin evolution operator, $U(0, t) = T \exp (-i/\hbar \int dt \bar{H}_\mu(t))$ can be exactly found by utilizing Feynman disentangling method [2, 29] $U(0, t) = \exp(a(t) s_x) \exp b(t) s_x \exp (c(t) s_y)$. where $a(t), b(t)$ and $c(t)$ are time-dependent functions that can be found exactly. In the disentangled form, the evolution operator can be written as

$$U(t) = \exp(i\mu t), T \exp \left\{ -\frac{i}{\hbar} \int_{t'=0}^t \left[ \frac{\xi_0}{\xi} \hbar \omega_0 \cos \omega_0 t - \vec{\chi} \right] s'_+ \right\},$$

(24)

where $T$ is the time ordering operator and $a(t) = -\frac{i}{\hbar} \int \chi(t') dt'$.

(25)

$$s'_\mu = \exp \left\{ \frac{i}{\hbar} s_\mu \right\} \int \chi(t') dt', \quad s_\mu = \exp \left\{ -\frac{i}{\hbar} s_\mu \right\} \int \chi(t') dt'.$$

(26)

By differentiating equation (26) with respect to 'a' and utilizing the initial condition $s'_\mu(0) = s_\mu$, we find the relations $s'_+ = s_+$, $s'_- = s_0 a + s_z$, $s'_z = s_- - 2s_x a - a^2 s_+$. By substituting these relations in equation (24) and equating the coefficient of $s_+ = 0$, we find the differential equation in the form of

$$\frac{d a}{d t} = -\frac{i}{\hbar} \left\{ \frac{\xi_0}{\xi} \hbar \omega_0 \cos \omega_0 t \left( 1 - a^2 \right) - \frac{1}{\xi} \Delta_1 \sin kl \right\}.$$  

(27)

In an analogous way, we can disentangle $s_0$ and $s_-$ by differentiating equation (26) with respect to 'b' and 'c', respectively. However, a single function $a(t)$ needed to find the transition probability [29]. The differential equation (27) can be solved exactly for the case $k = 0$. Thus, its solution can be written as

$$a(t) = \frac{\exp \left\{ -2i\xi_0 \sin (\omega_0 t) / \xi_0 \right\} - 1}{\exp \left\{ -2i\xi_0 \sin (\omega_0 t) / \xi_0 \right\} + 1}.$$  

(28)

The transition probability between the opposite spin states can be written as

$$\omega_{01/2 \to -1/2} = \frac{|a|^2}{1 + |a|^2} = \sin^2 \left( \frac{\xi_0}{\xi} \sin \omega_0 t \right).$$  

(29)

From equation (29), it is clear that the spin–flip transition probability is enhanced with the Rashba spin–orbit coupling. At large value of Rashba spin–orbit coupling constant, the splitting of the peak value in the transition probability can be achieved due to the fact that the periodicity of the propagating waves in the crystal lattice changes with $\alpha$. For the general case $k \neq 0$, we solve numerically the Riccati equation (27) to find the transition probability. In the disentangling operator scheme, as mentioned before, we write the momentum $(p(t) = mv)$ as a classical variable under the DP mechanism [25, 26], whose dependence on time $t$ is generated by a Markovian process [27]. Thus the Riccati equation (27) can be treated as a non-relativistic case. In such a situation, if a particle with a magnetic moment travels with a relativistic speed in an electromagnetic field whose orbital movement can be regarded as a classical then one might expect a change in the spin behaviour (or in the particle polarization vector) [45]. Thus, from equation (29), one might expect to flip the spin completely (resonance case) [46] if $\sin \varphi = (n+1/2) \pi / \xi_0$ where $\varphi = \omega_0 t$ and $n = 0, 1, 2, 3, \ldots$

3. Results and discussions

In figure 2(a), we have plotted energy versus $k$ of InAs parabolic nanowire SLs in the presence of the Rashba spin–orbit coupling. We find Kramer’s type degeneracy point at $k = \mp \pi / 2l$. Note that this maxima point is also maxima of $p_x$ (see equation (9)). In figure 2(b), we investigate the level crossing point associated with the spin states $|n, -1/2 \rangle$ and $|n + 1, 1/2 \rangle$. The crossing takes place at $k \approx 0.19 \text{ nm}^{-1}$ and $k \approx 0.43 \text{ nm}^{-1}$. Here the width of the anticrossing is approximately estimated as $117 \mu \text{eV}$.

We now turn to the key results of the paper: the spin transition rate via electromagnetic field radiation, phonons and the DP mechanism [18, 24–26].

In figure 3, we plot the spin transition rate versus $k$ between the spin states $|0, -1/2 \rangle$ and $|0, +1/2 \rangle$ under the
influence of electromagnetic field radiation and phonons. It can be seen that the phonon mediated spin transition rate is several order of magnitude larger than the value mediated by electromagnetic field radiation because the electromagnetic field mediated transition rate vanishes like \( \sin kl \) whereas, the phonon mediated spin transition rate vanishes like \((\sin kl)^5\) [5] (see equations (20) and (22)). The dips in the spin transition rate (see figure 2, solid lines) can be seen due to level crossing. The dips in the spin transition rate can be tuned with the application of the Rashba spin–orbit coupling. The cusp-like structure in the spin–flip transition rate was reported by the authors in [47, 48] for quantum dots system. For the case of parabolic nanowires modulated by longitudinal periodic potential, the dips found in the spin transition rate is new.

Finally, in figure 4, we plotted the transition probability versus time. In figures 4(a) and (b), we show that at \( k = 0 \) (see solid lines), the spin transition probability can be tuned with fixed time interval in the form of resonance. From equation (29), we can write the theoretical condition for finding zero transition probability for the case \((k = 0, \text{solid lines})\) in figure 4 as

\[
\sin \varphi = n\pi \frac{k}{\xi_0},
\]

where \( n = 0, 1, 2, 3 \ldots \) Condition (30) is satisfied by solid lines (black) in figure 4 and thus we find the zero transition probability at fixed interval of \( \varphi \). Also, it can be seen that the spin–flip transition probability can be enhanced with the Rashba spin–orbit coupling. Next, we study the influence of the inclusion of the wavenumber \( k \). We find that there is a superposition effect between \( p_x \) and \( p_y \) in the evolution of the spin dynamics (see equations (24) and (27)) which induces the damping effect or spin echo in the transition probability with respect to time. For simplicity in equation (27), we consider

\[
\sin k\ell = \frac{\xi_0 \hbar \omega_0}{\Delta_1 \ell} \cos \varphi.
\]
Here $\cos \varphi$ oscillates between $-1$ to $+1$ and for fixed value of $k$, the above condition (31) is satisfied several times with the variation of $\varphi$. Thus, one can find the zero spin transition probability at $\varphi = n \pi$. Whenever condition (31) is violated (i.e. $\sin k\ell \neq \pm \omega_{\text{Rashba}} \cos (\Delta_1 \ell)$), then we find a superposition or spin echo (see figure 4 for the case $k \neq 0$). At large value of the Rashba coefficient $\alpha$, the third term of equation (27) dominates over the first and second term and we find the spin freezing in the transition probability (see dashed line in figure 4(b)). Recently, similar type of results have been shown in [33].

4. Conclusion

In figure 2, we have demonstrated that the level crossing in parabolic nanowire SLs can be achieved with the accessible values of the strength of the Rashba spin–orbit coupling. The crossing point can be tuned to the lower values of $k$ and vice versa with the application of the Rashba spin–orbit coupling. In figure 3, we have shown that the phonon mediated spin transition rate is several orders of magnitude larger than the electromagnetic field mediated spin transition rate. The dips in the spin transition rate can be found due to level crossing. Based on the Feynman disentangling technique method, in figure 4, we have shown that the transition probability can be tuned in the form of resonance at $k = 0$. For the arbitrary values of $k$, we have shown that there is a superposition effect which induces the damping in the transition probability. At sufficiently large values of the Rashba spin–orbit coupling coefficients, the spin transition probability freezes for the arbitrary values of $k$. It means that one cannot find the spin–flip transition rate at large value of $k$. In other words, manipulation (injection and detection) of spin qubits far away from the gamma point in quantum wires is not the ideal candidate for the purpose of building a solid state quantum computer. It might be possible that our theoretically investigated spin–flip transition rate in the NWSLs can be experimentally measured with current-state-of-the-art technology (see [9] for experimental setup).

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