Time-dependent tunneling of spin-polarized electrons in coupled quantum wells

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Abstract. We have solved the in-plane momentum-dependent effective-mass nonlinear Schrödinger equation for a spin-polarized electron wave packet in a InAs double quantum well system with an interlayer voltage. Considering a time-dependent Hartree potential, we have calculated the spin-polarized nonlinear electron dynamics between both quantum wells at different in-plane momentum values and applied bias. The spin-splitting caused by the Rashba effect is combined with the level matching between the spin dependent resonant tunneling levels making possible the observed local spin density oscillations which depend on the applied bias value. The filtering efficiency has been studied using time-dependent calculations.

1. Introduction
Dynamics of spin-polarized electrons in semiconductor structures has been a field of growing interest during the last years. Spin-related effects in transport form the basis of the emerging field of spintronics.[1]-[4] The extra degrees of freedom provided by electron spins, in addition to those provided by electron charges, are expected to play an important role in future devices.[5]
One key to realizing such spin devices is the spin-orbit interaction caused by the Rashba effect in semiconductor structures. The Rashba effect, i.e., spin-orbit coupling due to electric field in a quantum well potential, is believed to be the most prominent tuning force. A weak electric field $F$ applied perpendicular to the quantum well plane can vary the spin-splitting substantially in the Rashba effect.[4] Thus, the subband energies of both up(+) and down(-) spin states are[6, 7]

$$\varepsilon_{\pm} = \varepsilon_0 + \varepsilon_{\|} \pm \alpha |k_{\|}|$$  \hspace{0.5cm} (1)

where $\varepsilon_0$ is the edge of the ground subband, $k_{\|}$ is the momentum in the 2D plane, $m^*$ is the effective-mass, $\varepsilon_{\|} = \hbar^2 k_{\|}^2 / 2m^*$ is the kinetic energy in the semiconductor layer plane and $\alpha$ is the parameter for the Rashba spin-orbit splitting which is linear in $k_{\|}$.

The values of the Rashba coupling constant using weak antilocalization analysis as a function of the structural inversion asymmetry have been investigated by Koga et. al.[6, 7] They also studied an electronic spin-filter device composed by a triple barrier resonant tunneling diode which can generate a spin-polarized current without using magnetic properties of materials.[6]
Such a device combines the spin-split tunneling levels induced by the Rashba interaction and the spin blockade phenomena between two regions separated by a barrier. The matching of spin-dependent tunneling levels was performed by controlling the bias voltage between both coupled...
quantum wells. The possibility of having local spin density oscillations in a bilayer system as a function of the electronic sheet density has been recently demonstrated.[8]

In view of such recent spin-polarized devices and theoretical models, one remaining key question is the theoretical analysis of spin effects in coupled quantum well systems, in particular the quantum tunneling in a bilayer system considering extra degrees of freedom provided by electron spins and applied bias. In this work, we study the time-dependent evolution of a spin-polarized charge density in a double quantum well system when an external bias is applied. The method of calculation is based on the discretization of space and time for the carrier wave functions. We study a spin-filter tunneling device, that uses a InAs double quantum well, which can generate an oscillating spin-polarized tunneling current between both electron layers when a voltage bias is applied. In such a device, the combination of the spin-splitting phenomena, caused by the Rashba effect, with the level-matching between the spin-dependent resonant tunneling levels, leads to spin-polarization dependent oscillations between both quantum wells which depend on the applied bias value.

2. Model
Let us now consider our previous simpler model[8] with static Hartree potential. In such a case, and due to the mirror symmetry for up and down spins, there is a symmetric charge distribution for each case, and due to the mirror symmetry for up and down spins, there is a symmetric charge density oscillation. We study a spin-filter tunneling device, that uses a InAs double quantum well, which can generate an oscillating spin-polarized tunneling current between both electron layers when a voltage bias is applied.

A spin-polarized charge density in a double quantum well system when an external bias is applied. In such a device, the combination of the spin-splitting phenomena, caused by the Rashba effect, with the level-matching between the spin-dependent resonant tunneling levels, leads to spin-polarization dependent oscillations between both quantum wells which depend on the applied bias value.

An electron with a wave vector \( k_\parallel \) can transmit through the barrier if the resonant tunneling level in the left quantum well (denoted as \( \varepsilon_r \)) matches that in the right quantum well (denoted as \( \varepsilon_l \)) in the absence of the Rashba effect or when parallel momentum is null. If parallel momentum is not null and the Rashba effect is present, the tunneling levels \( \varepsilon_r \) and \( \varepsilon_l \) experience the level splitting: \( \varepsilon_{r,l}^\pm \rightarrow \varepsilon_{r,l}^\pm \pm \alpha_r \parallel k_\parallel \), where \( \alpha_r \parallel \) is the Rashba parameter value \( \alpha(z) \) in the right and left layers and the plus and minus signs correspond to the resonant levels for different spin states, which we denote as up (+) and down (-) spins, respectively. The sign for the value of \( \alpha_l \) is opposite to that of \( \alpha_r \) because of the mirror symmetry in the present device about the middle barrier, while their absolute values are almost equal. Thus, the resonant tunneling levels in the left quantum well \( \varepsilon_l^\pm \) will not match the ones in the right quantum well \( \varepsilon_r^\pm \) (Fig. 1) if the Rashba effect is present and \( k_\parallel \neq 0 \). In such a case, the total wave function has the form \( \Psi(r, t) = \phi(k_\parallel, z, t)e^{ik_\parallel r} \) and in order to remove an \( \varepsilon_\parallel \) term in the Schrödinger equation, we have taken \( \phi(k_\parallel, z, t) = \psi(k_\parallel, z, t)e^{-i\varepsilon_\parallel t} \). Assuming the conservation of \( k_\parallel \) across the device,[6, 8] the wave function \( \psi^\pm \) will be given by the \( k_\parallel \)-dependent nonlinear Schrödinger equation

\[
\frac{i\hbar}{\partial t} \psi^\pm(k_\parallel, z, t) = \left[ -\frac{\hbar^2}{2m^*} \frac{\partial^2}{\partial z^2} + V_H(z, t) + V_{qw}(z) + V_{bias}(z) \pm \alpha(z)k_\parallel \right] \psi^\pm(k_\parallel, z, t) \tag{2}
\]

where \( m^* \) is the InAs electron effective mass, \( V_{qw}(z) \) is the double quantum well potential, \( V_{bias}(z) \) is the external bias potential and \( \pm \alpha(z)k_\parallel \) is the effective potential energy for up(+) and down(-) spins, respectively.[6] The \( V_H \) term is the self-consistent Hartree potential and is given by the Poisson’s equation.
Figure 1. A schematic illustration of the proposed spin device in absence of external applied bias. Conduction band potential profile ($V_H + V_{qw}$) and the spin-dependent energy levels. The downward and upward arrows denote the clockwise and counterclockwise spin states, respectively.

\[
\frac{\partial^2}{\partial z^2} V_H(z, t) = -\frac{e^2}{\varepsilon} [n(z, t) - N_D(z)], \tag{3}
\]

\[n(z, t)\] being the electron density, \(\varepsilon\) the InAs dielectric constant and \(N_D(z)\) the density of positive donor charges, which are assumed to be located far from the quantum wells. The \(z\)-dependent electron density is calculated from

\[
n(z, t) = \int \rho_0^+ f(\varepsilon_\parallel^+) |\psi_\parallel^+(k_\parallel, z, t)|^2 d\varepsilon_\parallel^+ + \int \rho_0^- f(\varepsilon_\parallel^-) |\psi_\parallel^-(k_\parallel, z, t)|^2 d\varepsilon_\parallel^- \tag{4}
\]

once the wave functions are obtained by solving Eq. (2) numerically. In Eq. (4) \(f(\varepsilon_\parallel^\pm)\) is the Fermi-Dirac distribution function. At zero temperature, \(f(\varepsilon_\parallel^\pm) \rightarrow \Theta(\varepsilon_F - \varepsilon_\parallel^\pm)\) and \(n_s = \varepsilon_F (\rho_0^+ + \rho_0^-)\) approaches the two-dimensional sheet density. \(\Theta\) is the step function, \(\varepsilon_F\) is the Fermi energy and \(\rho_0^\pm = m^*/2\pi\hbar^2\) is the two-dimensional, single-spin density of states. The Fermi energy \(\varepsilon_F\) is given by the electron sheet density value in the bilayer system.

The \(V_H\) potential is a quantity that depends on the wave function form in Eq. (3), see Eq. (4), where \(V_H\) depends on the different \(k_\parallel\)-dependent wave function forms. Now we discretize time by a superscript \(\vartheta\), \(k_\parallel\) by a subscript \(\xi\) and spatial position by a subscript \(j\). Thus, \(\psi \rightarrow \psi_{j,\xi}^\vartheta\). The various \(z\) values become \(j\delta z\) in the conduction band, where \(\delta z\) is the mesh width. Similarly, the time variable takes the values \(\vartheta \delta t\) and \(k_\parallel\) takes the values \(\xi \delta k\), where \(\delta t\) and \(\delta k\) are the time and momentum step, respectively. The time evolution is calculated with the split-step method.[9] In the split-step approach, the wave packet is advanced in time steps \(\delta t\) short enough that the algorithm \(e^{-i\vartheta T_H/2} e^{-i\Delta t U} e^{-i\vartheta T_H/2}\) can be applied to the generator. \(T_H\) and \(U\) are the
Figure 2. Effective conduction band potential ($V_H + V_{qw} \pm \alpha k_\parallel + V_{bias}$) and spin wave function amplitudes $|\psi^- (k_\parallel, z, t)|^2$ at $t=1\text{ps}$ and $t=0\text{ps}$. We have taken an initial 2D electron sheet density equal to $n_s = 3 \times 10^{12}$ cm$^{-2}$ and $\epsilon^\pm = 0.5\epsilon_F$ at $V_{bias} = 45\text{mV}$.

Hamiltonian kinetic and potential terms. In each time step $\delta t$, the algorithm propagates the wave packet freely for $\delta t/2$, applies the full potential interaction, then propagates freely for the remaining $\delta t/2$. The split-step algorithm is stable and norm preserving and it is well suited to time-dependent Hamiltonian problems.[10, 11] In each time step $\delta t$, the algorithm propagates the different $k_\parallel$-dependent wave packets to obtain the $z$-dependent electron sheet density in the bilayer system. Then, the Poisson’s equation associated with $V_H$ is solved using a tridiagonal numerical method for each $t$ value.[12]

We have taken two added Gaussian wave packets, each of them centered in one of the quantum wells, as our initial wave function. In this way, the different wave packets $\psi^\pm (k_\parallel, z, 0)$ are initially symmetric wave functions in our model (Fig. 2). The initial wave function is identical for all $k_\parallel$ states. However, and as time passes, we shall obtain different $k_\parallel$ wave functions due to the dependence of the potential in $k_\parallel$. The width parameter of the gaussians is 53Å. In Fig. 2 we have plotted the conduction band potential ($V_H + V_{qw} + V_{bias}$) and the effective conduction band potential, respectively. We have integrated numerically Eqs. (2) and (3) using an electron sheet density $n_s = 3.0 \times 10^{12}$ cm$^{-2}$. Then, the equations are solved using a spatial mesh size of 0.5Å, a time mesh size of 0.2 a.u and a momentum mesh size of $10^{-3}$ a.u. and a finite box (4000Å) large enough to neglect border effects. We have considered a InAs/In$_{0.75}$Al$_{0.25}$As double quantum well system which consists of two 100Å-wide InAs quantum wells separated by a barrier of thickness equal to 20Å. The barrier height is taken to be 450 meV.
3. Results and discussion

The numerical integration in time allows us to obtain the probability of finding the charge density $P_{l_1,l_2}^\pm$ inside a quantum well region $[l_1, l_2]$ at any time $t$

$$P_{l_1,l_2}^\pm(\epsilon, t) = \int_{l_1}^{l_2} |\psi^\pm(k, z, t)|^2 dz$$  \hspace{1cm} (5)$$

where $[l_1, l_2]$ and $[l_3, l_4]$ are the left and right quantum well limits, respectively. We have plotted the probability density $P_{l_1,l_2}^-$ in left quantum well versus time in Fig. 3 at $V_{bias} = 45mV$. The total probability density in both quantum wells has been taken to be 1. We have taken an initial 2D electron sheet density equal to $n_s = 3.0 \times 10^{12} \text{ cm}^{-2}$. Thin line: $\epsilon^- = 0.1\epsilon_F$. Thick line: $\epsilon^- = 0.6\epsilon_F$. The existence of tunnelling oscillations between the two quantum wells is clearly shown in Fig. 3. We can notice that the density oscillations shown in Fig. 3 have two periods. These rapid small oscillations can be described as the collisions of the particle with the barriers of each quantum well.\[8\] Because of the mirror symmetry in the present device about the middle barrier, $P_{l_1,l_2}^-$ and $P_{l_3,l_4}^+$ are almost equal.

In absence of Rashba effect, a maximum for the amplitude of the tunneling oscillations at $V_{bias} = 45mV$ is obtained (resonant condition) for our structure parameters. This is because the electron energy levels of both wells are exactly aligned at $V_{bias} = 0mV$ and $\epsilon = 0$ (in absence of Rashba effect). Therefore, if $V_{bias} \sim 0$ the conduction band potential between the two semiconductor layers will be shifted by a quantity equal to $eV_{bias}$ and the charge density will oscillate between both wells with a certain tunnelling period. If $V_{bias}$ is increased, the
amplitude of the oscillations will also be increased due to the field-induced tunnelling process between both wells. However, we know that if the potential difference between both wells is higher than the level splitting, the resonant condition is not obtained, and then the tunnelling process is not allowed. As a consequence, a maximum for the amplitude of the oscillations is obtained at $V_{bias} = 45 mV$ and $\varepsilon_\parallel = 0$.

In Fig. 4, we have plotted the averaged amplitude value of the tunnelling oscillations versus $\varepsilon_\parallel$ for different spin states at $V_{bias} = 45 mV$. We have used an electron density $n_s = 3.0 \times 10^{12} \text{ cm}^{-2}$. It is found that the amplitude of the tunnelling oscillations is decreased as we increase $\varepsilon_\parallel$ for both spin orientations. This is because the resonant condition of both wells is at $\varepsilon_\parallel = 0$ in absence of Rashba effect. Therefore, if $\varepsilon_\parallel \sim 0$ the conduction band potential between the two semiconductor layers will be shifted by a quantity equal to $\pm \alpha(z) k_\parallel$ and the resonant condition is now not allowed. Thus, the charge density will oscillate between both wells with a lower amplitude. Such an effect is clearly shown in the numerical data plotted in Fig. 4.

In Fig. 5, we have plotted the averaged amplitude value of the tunnelling oscillations versus $\varepsilon_\parallel$ for different spin states at $V_{bias} = 15 mV$. We have also used an electron density $n_s = 3.0 \times 10^{12} \text{ cm}^{-2}$. For spin down states, we have obtained that the amplitude of the tunnelling oscillations is increased as we increase $\varepsilon_\parallel$ up to a certain value of the energy. In the spin up case, the amplitude decreases with increasing $\varepsilon_\parallel$. This is because the resonant condition is not obtained at $\varepsilon_\parallel = 0$ due to the applied bias is lower than the resonant condition ($V_{bias} = 45 mV$). However,
Figure 5. Amplitude of the tunnelling oscillations versus parallel energy, $E_r = \varepsilon^- / \varepsilon_F$ at $V_{bias} = 15mV$. The amplitudes have been obtained using Eq. (5). $E_r$ has not dimensions. We have considered both spin up and spin down electrons.

If $\varepsilon^- \sim 0$ the conduction band potential between the two semiconductor layers will be shifted by a quantity equal to $\alpha z k_\parallel$ in the spin down case and the resonant condition can again be obtained. Such an effect is clearly shown in the numerical data plotted in Fig. 5 for spin down states. We have found the existence of oscillations up to a certain value of the parallel energy (resonant $\varepsilon^-_\parallel$ value).

In both Figs. 4 and 5, it is clearly shown that spin-down tunneling is much more important than the spin-up case. Such an effect is given by the applied bias direction. To study the spin-down current we can introduce a simple quantity that summarizes the global behavior of the tunneling oscillations associated with one particular spin. We can define the averaged amplitude of the oscillations $< A^\pm >$ for each subband, i.e.,

$$< A^\pm > = \frac{\int \rho^\pm_0 f(\varepsilon^\pm_\parallel) A^\pm(\varepsilon_\parallel) d\varepsilon^\pm_\parallel}{\int \rho^\pm_0 f(\varepsilon^\pm_\parallel) d\varepsilon^\pm_\parallel}$$

(6)

where ratio gives the averaged amplitude considering all $\varepsilon_\parallel$ energies. Fig. 6 shows $< A^- >$ and the amplitude of the tunneling oscillations in absence of Rashba effect ($\varepsilon_\parallel=0$) versus applied bias. The most prominent feature of Fig. 6 is the existence of important oscillations for all applied bias in the $< A^- >$ spin down case. In addition, we can also notice that the $< A^- >$ curve maximum is lower than in the $\alpha = 0$ case. In Fig. 7, we have plotted the filtering efficiency $E^-$, i.e.,
Figure 6. Squares: Averaged amplitude of the tunneling oscillations $<A^->$ versus applied bias (V). Triangles: Amplitude of the tunneling oscillations in absence of Rashba effect.

$$E^\pm = \frac{<A^\pm> - <A^{\mp}>}{<A^+> + <A^->}$$  \hspace{1cm} (7)

versus applied bias. We have obtained a smoothed curve for the efficiency of the device. Also at high bias voltage, the efficiency curve never reaches zero. In addition, $E^-$ is never maximum (i.e., $E^- = 1.0$) at low values. Using a time-independent scheme, values higher than 0.99 were predicted for the spin-filtering efficiency at resonant values.[6]

Finally, we think that these oscillations can be observed experimentally. In the tunnelling experiments, the potential difference between both semiconductor quantum wells can be controlled independently by two different gate voltages. If an interlayer voltage $V_{bias}$ is applied, the conduction band potential between the two InAs semiconductor layers is shifted by a quantity equal to $eV$. If the potential difference between both wells is much higher than the level splitting, the tunneling process is not allowed and there result two initial independent electron sheet densities in both quantum wells. In such a case, we have a symmetric charge distribution of spin-up and spin-down electrons and the local spin density in each single quantum well practically vanishes at $t=0$. However, if low interlayer voltage $V \sim 0$ is applied, we have a coupled quantum well system as shown in Fig. 2, and the induced spin-polarized current which depend on the applied bias direction can be seen before scattering processes destroy coherence of the oscillating wave packets.[8] Then, the filtering efficiency could be measured.

In summary, in this work we have integrated a $k_{||}$-dependent nonlinear effective-mass Schrödinger equation in a InAs double quantum well system. Electron-electron interaction effects have been considered through a time-dependent Hartree potential. We have studied a
A spin device which can generate an oscillating spin-polarized tunneling current between both electron layers when an external voltage is applied. The spin-splitting caused by the Rashba effect is combined with the level matching between the spin dependent resonant tunneling levels making possible the observed local spin density oscillations which depend on the applied bias direction. The filtering efficiency of the device has been studied in a time-dependent scheme obtaining a smoothed curve for $E^-$ at low and high bias voltages.

**Figure 7.** Filtering efficiency $E^-$ versus applied bias voltage $V_{bias}(V)$. 

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