Rashba spin splitting in semiconductor quantum wires

E. A. de Andrada e Silva
Instituto Nacional de Pesquisas Espaciais–INPE, C.P. 515, 12201-970 São José dos Campos–SP, Brazil

G. C. La Rocca
Scuola Normale Superiore and I.N.F.M., Piazza dei Cavalieri 7, 56100 Pisa, Italy
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A general three-dimensional model for asymmetric semiconductor quantum wires is introduced with exact and analytical solutions for the spin-dependent electronic structure. Simple expressions are obtained for the eigenvalues, wave functions, and spin expectation values, valid in both strong and weak Rashba spin-orbit coupling regimes. For III-V quantum wires, the Rashba interaction is shown to be typically in the weak coupling regime and to lead to considerable spin mixing only near the anticrossings, seen only in narrow-gap quantum wires. For realistic wires, the Rashba splitting is shown to decrease with increasing wire confinement.

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The spin-dependent electronic transport in semiconductor nanostructures has an intrinsic quantum character which is determined by the electronic structure of the system. The ultimate nanostructure for the electronic transport is the so-called quantum wire, i.e., a structure in which the electrons are confined by a two-dimensional quantum potential and free to move along a single direction. These semiconductor quantum wires represent important quasi-one-dimensional systems of broad interest in condensed matter physics. However, despite the success in their fabrication[1] and the growing interest connected to the spintronic technology,[2] the physics of their spin-dependent electronic properties is definitely not well known. In particular, the electronic structure of asymmetric semiconductor quantum wires and the role of the spin-orbit interaction, also in relation to the study of many-body effects,[3,4] have been studied so far only with simplified models.

The spin-orbit splitting in the conduction subbands due to the inversion asymmetry in the mesoscopic potential, also called simply the Rashba effect or splitting,[5] has been extensively studied in semiconductor quantum wells since the advent of the low-dimensional systems.[6] Good agreement between theory and experiment has been obtained. Recently, interest has been much renewed after different proposals for spintronic devices based on such an effect;[7] of particular interest for these devices is the Rashba effect in semiconductor quantum wires. Different groups have investigated the problem theoretically, and it was shown that the conducting states in quantum wires, contrary to the quantum well case, present an intrinsic k-dependent spin mixing, which leads to novel spin-dependent transport properties.[4,8,9] Moroz and Barnes[8] considered electrons in two dimensions, confined by a parabolic potential well; Mireles and Kirczenow,[9] with numerical tight-binding calculations, studied the electron transmission along similar infinite two-dimensional quantum wires; and, more recently, Governale and Zulicke[4] revisited the model studied in Ref. 8 and clarified the nature of the spin mixing. However, the Rashba spin-orbit term in such two-dimensional models is introduced phenomenologically with a constant coupling parameter, connected to the asymmetry in the third (frozen) dimension. This is a good approximation only when the coupling parameter does not vary much with electron energy, which in general is not the case. In the quantum well case, for instance, such a phenomenological approach leads to a Rashba splitting linear in k, while it is known that the spin splitting actually presents a sublinear dependence.[6] In the quantum wire case, when the confinement in the two directions is comparable, the electron dynamics is strongly coupled in all three dimensions, and the spin splitting should definitely be described taking such coupling into account.

In this work, we introduce a simple three-dimensional model of an asymmetric semiconductor quantum wire, in which the Rashba spin-orbit coupling is actually derived from a realistic description of the bulk semiconductor electronic structure. We show that it is possible to obtain exact, analytical, and simple solutions for the spin-resolved electronic structure of actual three-dimensional semiconductor asymmetric quantum wires, within the envelope function approximation based on multiband $k \cdot p$ Hamiltonians. The general solutions apply to multiband models used to describe not only III-V, but also II-VI and IV-VI direct gap semiconductor nanostructures. Here, we present detailed results for the most common case of III-V semiconductors using only well-known material parameters. In the following, we describe the wire model, the theoretical approach, and the solutions obtained. Specific quantitative predictions are made for the spin mixing in III-V structures, including the splitting reduction effect, due to the quantum wire confinement. These predictions will be useful in guiding and interpreting experimental observations of the Rashba splitting in semiconductor quantum wires.

A common way to construct semiconductor quantum wires is to start from a quantum well, e.g., grown along the z direction, and to further confine the electrons along a transverse direction, say, y, with an additional potential, so that the electrons become free to move only along x. Let us consider, for example, rectangular quantum wires with the cross section formed by a small-gap material surrounded by vacuum or larger-gap materials, which can be grown, e.g., by nanolithography as well as self-assembling.[1] The quantum confinement which characterizes such wires is described by

the variation of the band parameters within the plane orthogonal to the wire axis [the (y,z) plane in the present case].

The Rashba splitting in the conduction band can be derived from the 8×8 Kane model for the bulk, including the Γ_6 conduction and Γ_8 and Γ_7 valence bands. This is particularly evident when the corresponding eigenvalue problem is rewritten as an effective Schrödinger equation for the electrons in the conduction band,[10,11] i.e.,

$$H_{eff}(E)\psi=(H_0+H_{so})\psi=E\psi, \tag{1}$$

where

$$\psi=e^{ik_x x}\begin{pmatrix}\psi_\alpha(y,z)\\ \psi_\beta(y,z)\end{pmatrix} \tag{2}$$

is the electron envelope function with $\psi_{\alpha,\beta}$ spin components. The two terms of the effective (and energy-dependent) Hamiltonian are given by the spin-independent

$$H_0(E)=\left[E_c+\frac{\hbar^2k_x^2}{2m}-\frac{\hbar^2}{2}\left(\frac{d}{dy}\frac{1}{m}\frac{d}{dy}+\frac{d}{dz}\frac{1}{m}\frac{d}{dz}\right)\right] \tag{3}$$

and the spin-dependent

$$H_{so}(E)=\left(\frac{d}{dy}\beta\right)k_x\sigma_z-\left(\frac{d}{dz}\beta\right)k_x\sigma_y + i\left[\left(\frac{d}{dy}\beta\right)\frac{d}{dz}-\left(\frac{d}{dz}\beta\right)\frac{d}{dy}\right]\sigma_x, \tag{4}$$

σ_i being the Pauli spin matrices. The effective mass m and the spin-orbit coupling parameter β are given by $\hbar^2/2m(E)=P^2[2/(E-E_c+E_g)+1/(E-E_c+E_g+\Delta_o)]$ and $\beta(E)=P^2[1/(E-E_c+E_g)-1/(E-E_c+E_g+\Delta_o)]$, where E_c stands for the conduction-band edge, E_g for the fundamental band gap, Δ_o for the spin-orbit splitting of the valence band, and P for the Kane interband momentum matrix element. Apart from P which is assumed to be constant, all the band parameters depend on both y and z, according to the material composition of the wire. It is important to note that due to the energy dependence of m and β, H_{so}, as well as H_0, is not separable. For H_0, this corresponds to the well-known coupling between transverse and parallel motion due to nonparabolicity effects, while for H_{so}, it means that the Rashba spin-orbit coupling depends on the three-dimensional dynamics, differently from what assumed in previous two-dimensional models, neglecting the dynamics along z.

Let us consider an asymmetric quantum well along the z direction, composed by a thin layer, of width L, of a III-V semiconductor (material I) between two different semi-infinite ones with larger energy gap (see inset in Fig. 1). To simplify, we assume that one of these two barrier materials have a much larger energy gap, so that it can be approximated by an infinite barrier. The other finite-barrier material, which we call material II, is taken as a lattice-matched semiconductor of similar band structure in accordance with the assumptions of the envelope function approximation. For the potential along y, we assume a square infinite-barrier quantum well of width d, so that the wave function is not zero

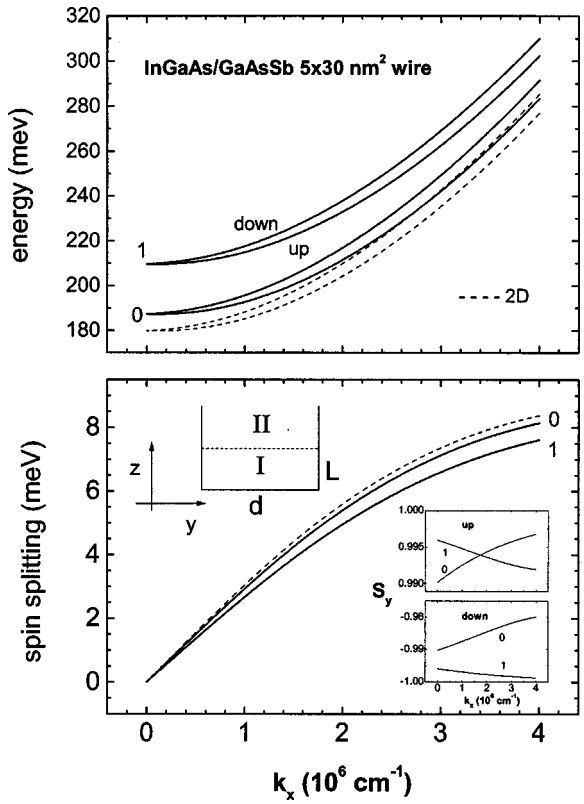

FIG. 1. Rashba spin-orbit split conduction subbands in a rectangular $In_{0.53}Ga_{0.47}As/GaAs_{0.5}Sb_{0.5}$ quantum wire, with $L=5$ nm and $d=30$ nm. In the upper panel is shown the dispersion relations of the lowest (0) and first excited (1) subbands. In the lower panel is plotted the spin splitting as a function of the electron wave vector along the axis of the wire. With dashed lines, it is shown also the 2D or quantum well limit. The wire symmetry and the obtained expectation value of the y spin component are also shown in the insets. The band parameters used were $E_g^I=0.75$ eV, $\Delta_o^I=0.36$ eV, $m_I(0)=0.041m_e$, $E_g^{II}=0.81$ eV, $\Delta_o^{II}=0.75$ eV, and $V=0.360$ eV.

only in the material I (which defines the $L\times d$ rectangular quantum wire) and in the corresponding region of material II (due to wave function penetration in the finite barrier of height V).

The spin-resolved electronic structure of such rectangular (flatband) asymmetric quantum wires is now shown to present general analytical solutions. In each material, β is constant, $H_{so}=0$ and the solutions of Eq. (2) are plane waves. The general solution for the confined states with energy $E(<V)$, vanishing at the interfaces with an infinite barrier and being continuous across the interface between materials I and II, can then be written as

$$\psi=e^{ik_x x}\sum_{n=1}^{\infty}\sin\left(\frac{n\pi}{d}y\right)\begin{pmatrix}A_n\\ B_n\end{pmatrix}\begin{cases}\sin(k_n z) & \text{in I,}\\ \sin(k_n L)e^{-\rho_n(z-L)} & \text{in II,}\end{cases} \tag{5}$$

with

$$k_n=\sqrt{\frac{2m_I}{\hbar^2}E-k_x^2-\left(\frac{n\pi}{d}\right)^2} \tag{6}$$

and

$$\rho_n = \sqrt{\frac{2m_{II}}{\hbar^2}(V-E)+k_x^2+\left(\frac{n\pi}{d}\right)^2}, \tag{7}$$

where we have set $E_c^I=0$ and $E_c^{II}=V$, and $m_{I,II}$ correspond to the energy-dependent effective mass calculated in each material.

The final solution is obtained from the remaining boundary conditions which are obtained integrating Eq. (2) across the interface. In the present case, they have a simpler form when the spin quantization axis is set along y and read

$$\begin{pmatrix} -\frac{\hbar^2}{2m}\frac{d}{dz}-\beta k_x & -\beta\frac{d}{dy} \\ \beta\frac{d}{dy} & -\frac{\hbar^2}{2m}\frac{d}{dz}+\beta k_x \end{pmatrix} \times \begin{pmatrix} \psi_\alpha \\ \psi_\beta \end{pmatrix} \quad \text{continuous across the I-II interface.} \tag{8}$$

The corresponding infinite set of linear equations obtained for the coefficients $\{A_n, B_n\}$ can be written as

$$\left[\frac{k_n}{m_I}\cos(k_nL)+\left(\frac{\rho_n}{m_{II}}+\frac{2\Delta\beta}{\hbar^2}k_x\right)\sin(k_nL)\right]A_n + \frac{2\Delta\beta}{\hbar^2}\sum_{m=1}^{\infty}\left(\frac{m\pi}{d}\right)b_{n,m}\sin(k_mL)B_m=0, \tag{9}$$

for $n=1,2,\ldots,\infty$, where

$$b_{n,m}=\frac{2}{\pi}\frac{m}{m^2-n^2}[1-(-1)^{n+m}]$$

and zero if $n=m$, plus similar equations obtained interchanging A and B, and changing the sign of $\Delta\beta$ $(=\beta_I-\beta_{II})$. In actual calculations, one truncates the system of equations at n_{max} and has then $2n_{max}$ equations for the same number of unknown coefficients $\{A_1,B_1,A_2,B_2,\ldots,A_{n_{max}},B_{n_{max}}\}$. For a given k_x, solutions are found only for a discrete set of energies, which are the roots of the characteristic equation.

In the two-dimensional (2D) or quantum well limit, obtained when $d\to\infty$, it is easy to see that the usual Rashba effect, described by an effective magnetic field perpendicular to both growth and $\vec{k}_\parallel$ directions, is recovered. In the strong confinement or thin wire limit, convergence is obtained with a small n_{max}, which gives the number of transverse subbands included. In narrow wires and for values of $k_x \leqslant 3\times10^6$ cm^{-1}, lowest subband spin splittings accurate whithin a few percent are already obtained with $n_{max}=2$. This two-transverse-subband approximation already allows the study of subband spin mixing and leads to simple and useful analytical expressions for the electronic structure of thin semiconductor quantum wires. In this approximation, Eq. (9) turns into two independent sets of two coupled equations for $\{A_1,B_2\}$ and $\{A_2,B_1\}$, respectively, corresponding to eigenvalues, satisfying

$$F_1^+F_2^- = \left(\frac{8}{3d}\right)^2\left(\frac{2\Delta\beta}{\hbar^2}\right)^2, \tag{10}$$

and a similar equation with interchanged subband indices, where we have defined

$$F_n^{\pm}=\frac{k_n}{m_I}\frac{1}{\tan(k_nL)}+\frac{\rho_n}{m_{II}}\pm\frac{2\Delta\beta}{\hbar^2}k_x. \tag{11}$$

The expectation value of the spin components can also be easily calculated and one finds $\langle\sigma_x\rangle=\langle\sigma_z\rangle=0$ and, for the first set of states with $\{A_1,B_2\}\neq0$,

$$\langle\sigma_y\rangle=\frac{c_1|A_1|^2-c_2|B_2|^2}{c_1|A_1|^2+c_2|B_2|^2}, \tag{12}$$

with

$$c_n=L-\frac{\sin(2k_nL)}{2k_n}+\frac{\sin^2(k_nL)}{\rho_n}. \tag{13}$$

The results shown in the figures and discussed below are all obtained from Eqs. (10) and (12) above.

As an example, we show in Fig. 1 the dispersion relation and the Rashba spin splitting of the lowest (0) and first excited (1) spin-orbit split conduction subbands obtained for an $In_{0.53}Ga_{0.47}As/GaAs_{0.5}Sb_{0.5}$ (material I/material II) lattice matched quantum wire. Its dimensions are $L=5$ nm and $d=30$ nm and, for comparison, we have also plotted the results in the 2D quantum well limit, i.e., for infinite d. The Rashba splitting in the wire is smaller than in the quantum well, and the splitting in the excited one-dimensional subband is smaller than that in the lowest one, contrary to the asymmetric square quantum well case. As a matter of fact, the extra energy in the wire derives from the transverse confinement and does not correspond to a larger barrier penetration along z; thus, the resulting reduction of the spin splitting is due to the fact that the Rashba coupling parameter β decreases with electron energy. In Fig. 2, we show that, indeed, a stronger confinement, i.e., a shorter d, leads to a smaller Rashba spin splitting. This splitting reduction effect, explained by the coupled three-dimensional dynamics, is contrary to the common expectation of larger splittings in smaller systems.

With respect to the quantum well, the main qualitatively new physics in the quantum wire Rashba effect concerns the subband spin mixing, which can be measured with the expectation value of σ_y. In the quantum well, it is always 1 for spin up (along y) and -1 for spin down, independent of k_x or L. The inset of Fig. 1 shows the obtained $S_y=\langle\sigma_y\rangle$ for the split states, which we still denote ''up'' and ''down'' even though they are not completely polarized, of both the lowest and first excited subbands of the $In_{0.53}Ga_{0.47}As/GaAs_{0.5}Sb_{0.5}$

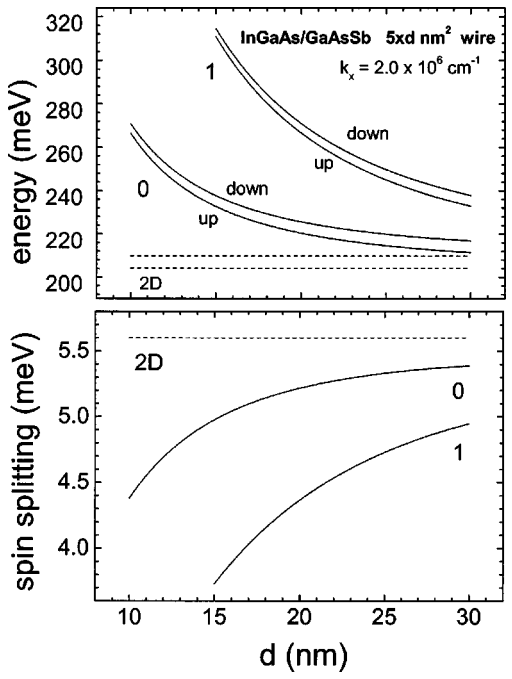

FIG. 2. Rashba splitting reduction effect. The energy of the allowed states and the Rashba splitting for an electron with $k_x = 2 \times 10^6$ cm^{-1} in a $L = 5$ nm $In_{0.53}Ga_{0.47}As/GaAs_{0.5}Sb_{0.5}$ quantum wire are plotted as a function of the lateral confinement length d.

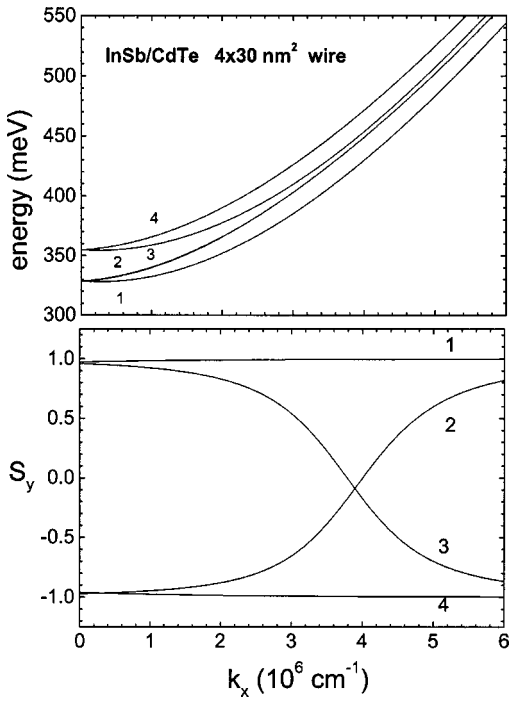

FIG. 3. Dispersion relation and average spin for the first conducting subbands in a $L = 4$ and $d = 30$ nm InSb/CdTe quantum wire, with an anticrossing between states 2 and 3 and the corresponding subband spin mixing. The parameters used in this case were $E_g^I = 0.24$ eV, $\Delta_o^I = 0.81$ eV, $m_I(0) = 0.015 m_e$, $E_g^{II} = 1.59$ eV, $\Delta_o^{II} = 0.8$ eV, and $V = 0.55$ eV.

quantum wire. We note that the average spin is always approximately ± 1 as, for a not too large k_x, the spin splitting in the subbands of the quantum wire is much smaller than their energy difference, preventing any sizable spin mixing. Nevertheless, we can note a tendency of spin mixing between the first subband ''up'' and lowest subband ''down'' states, which are those that eventually would cross at a much larger k_x. The other two states tend instead to pure spin-up and -down states. With increasing confinement, due to the larger energy separations, the mixing is further inhibited. These results imply that for realistic III-V wire structures the Rashba spin-orbit interaction is typically in the weak coupling regime.

From the quantitative point of view, a strong subband spin mixing occurs only near level anticrossings as in the example shown in Fig. 3, where the dispersion relation and the corresponding S_y for the first conduction subbands, in a InSb/CdTe $L = 4$ and $d = 30$ nm quantum wire, are shown. In fact, we see that the states 2 and 3 (respectively, lowest subband ''down'' and first subband ''up'' states at small k_x) have opposite S_y before and after the anticrossing.[4] At such large values of k_x, however, it is expected that, for a quantitative evaluation of the spin mixing in these III-V quantum wires, it will be important to consider also the so-called bulk k^3 spin-orbit contribution, which derives from higher-order terms not included in the Kane model and is due to the lack of inversion symmetry in the zinc-blende crystal.[12] In first-order perturbation theory, the k^3 contribution to the spin-orbit splitting in the quantum wire of Fig. 1 can be estimated assuming an average k^3 coupling parameter (constant across the interface) of value $\gamma = 75$ eV Å^3.[13] A k^3 contribution is obtained which is of the order of 30% of the Rashba splitting at small k_x and reaches 50% at $k_x \sim 3 \times 10^6$ cm^{-1}. The inclusion of the bulk k^3 term in a quantitative evaluation of the spin-orbit effects in III-V semiconductor quantum wires is then still more important than in the quantum well case. In quantum wires made of semiconductors with inversion symmetry, like the lead-salt IV-VI compounds, the spin-orbit splitting, which is solely given by the Rashba contribution, can be precisely calculated with the present solution (including more than two subbands if necessary), using the appropriate parameters and $k \cdot p$ expressions.[14]

In summary, we have demonstrated the existence of general analytical solutions for the Rashba spin-split (and mixed) subbands in three-dimensional semiconductor quantum wires, applicable to strong and weak coupling regimes and to wires made of different compounds described by Kane-like $k \cdot p$ models. In particular, for the III-V semiconductor quantum wires, we have shown that the Rashba spin-orbit interaction is typically in the weak coupling regime, it decreases with increasing wire confinement, and that the bulk k^3 contribution should be taken into account in a precise evaluation of the spin-orbit effects in these wires.

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