Spin-orbit splitting of electronic states in semiconductor asymmetric quantum wells

E. A. de Andrada e Silva
Instituto Nacional de Pesquisas Espaciais, CP515, 12201 São José dos Campos, São Paulo, Brazil

G. C. La Rocca and F. Bassani
Scuola Normale Superiore and INFM, Piazza dei Cavalieri 7, I-56100 Pisa, Italy

(Received 12 November 1996)

The spin-orbit splitting in the dispersion relation for electrons in III-V semiconductor asymmetric quantum wells is studied within the standard envelope-function formalism starting from the eight-band Kane model for the bulk. The Rashba spin-orbit splitting in the different subbands is obtained for both triangular and square asymmetric quantum wells. It is shown, for example, that the Rashba splitting in AlAs/GaAs/$Ga_{1-x}Al_xAs$ square quantum wells is of the order of 1 meV and presents a maximum as a function of the well width. The splitting of the excited subband in square and triangular quantum wells is shown to be bigger and smaller than the splitting in the first subband, respectively. A simple single-band approach, employing spin-dependent boundary conditions and approximate coupling parameters, is also introduced and its range of validity assessed. The discussion presented clarifies the treatment of abrupt interfaces, the Ando argument against the splitting, and the use of common approximations such as neglecting the barrier penetration or the energy-dependent corrections to the parameters. Good agreement is found with available experimental data. [S0163-1829(97)00120-3]

I. INTRODUCTION AND MOTIVATIONS

Contrary to the case of holes, the existence of a spin-orbit splitting for the conducting electrons confined in semiconductor heterostructures has been a controversial issue for more than 20 years.[1–4] New experiments probing spin-dependent static and dynamic properties of these structures have recently renewed the interest on the problem, which is also known as the zero-field spin-splitting problem.[5–10] However, questions like the so-called Ando argument, the role of the interface electric field or the treatment of abrupt interfaces, and the connection between the phenomenological Rashba and the multiband effective mass Hamiltonians have not been totally clarified yet.[8,9,11,12]

It is now recognized that the splitting for asymmetric III-V semiconductor quantum wells presents two distinct contributions. One contribution is due to the inversion asymmetry of the bulk host material and is well known.[13] The other one, which is the controversial one, comes from the asymmetry in the macroscopic confining potential and is described by the so-called Rashba term.[14] This term, derived from general symmetry arguments, has been used to interpret the results of different experiments with asymmetric quantum wells.[14–16] There are many reasons to believe that this term gives the dominant contribution to the splitting in the case of narrow-gap heterostructures.[16–20] In general, though, both terms are present and their interplay brings about a characteristic anisotropy of the spin-orbit splitting.[21,8] Different groups have recently suggested that the Rashba term is important also in GaAs heterostructures, where it was believed to be negligible.[8–10,20] However, comparison of the experimentally determined coupling parameters with microscopic theory has not been easy.[8,11] In the following, we present a study of the problem in the standard envelope-function approximation aimed at bridging the gap between the experiments and the Rashba model and at clarifying a few controversial theoretical arguments.

The spin-orbit coupling parameter in the Rashba term is usually taken to be proportional to the average effective electric field $\langle E\rangle=\langle -(1/e)(d/dz)(E_c+V)\rangle$, where E_c stands for the conduction-band-edge profile, V for the space charge and/or applied electrostatic potential energy, and z is the growth direction. This is, however, not correct. It is easy to see that the band-edge profile E_c and the electrostatic potential V do not play a similar role. As will be shown below, in general the Rashba spin-orbit term in a heterostructure has two different contributions. The introduction of two coupling parameters, instead of one, is helpful. A detailed calculation of the splitting in triangular (as in a heterojunction) and square (as when left and right barrier are different) asymmetric quantum wells, together with an analysis of simple approximations, will help to illustrate the difference between the two contributions to the Rashba term in a semiconductor quantum well. The difficulties behind the determination of the Rashba spin-orbit coupling parameter are closely connected with the controversy around the breakdown of Ando's argument against the splitting.

In view of the first experimental attempts to estimate the spin-orbit splitting in the conduction subband of narrow-gap semiconductor heterostructures, which led to values much smaller than those predicted theoretically,[2,3] a qualitative argument was put forward by Ando and attracted much attention [see footnote in Ref. 4]. It questioned the first calculations and seemingly justified the early experimental results. The argument points out essentially that the splitting—since it results from the relativistic effect in which a moving electron with nonzero wave vector k sees in its reference frame the interface electric field transformed into a magnetic field—should be very small (zero in first-order perturbation theory): the reason being the fact that the confined electrons

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see an average effective electric field (or force) equal to zero.

Such explanation was later criticized as oversimplified, partly in view of subsequent more accurate measurements in which large splittings were observed with different techniques and in different structures.[8,15–18] It has then been suggested that the Ando argument breaks down because the average effective electric field felt by a localized electron is nonzero when the effective mass is not constant across the interface.[19,22] The usual unperturbed effective-mass Hamiltonian allowing for changes in the effective mass along the growth direction, reads

$$H=-\frac{\hbar^2}{2}\frac{d}{dz}\frac{1}{m^*(z)}\frac{d}{dz}+E_c(z)+V(z), \tag{1}$$

where $m^*(z)$ is the conduction-band-edge effective mass, which changes from semiconductor to semiconductor. The discontinuity in the effective mass leads at the interface to an impulsive force. The force balance for the confined states, which is given by $\langle[H,p_z]\rangle=0$, leads then to a nonzero expectation value for the effective electric field [i.e., $\langle E\rangle=\langle-(1/e)(d/dz)(E_c+V)\rangle\neq 0$]. But this did not solve the problem because the evaluation of the interface electric field is not unambiguous;[8,11] some confusion has arisen, in particular, when trying to argue whether to use E_c or E_v in the band-edge discontinuity contribution to E (E_v standing for valence-band edge).

It is shown below that Ando's argument fails firstly because there is a spin-orbit correction coming from a change in the boundary conditions which goes beyond the above approach; and secondly because the main spin-orbit splitting term in the conduction band due to the interaction with the valence band is not simply proportional to the effective electric field.

Next, after presenting in some detail the standard envelope-function treatment of the spin-orbit splitting in the conduction subband (Sec. II), we show results (Sec. III) for the Rashba splitting in both triangular and square (also known as flat band) asymmetric quantum wells. In Sec. IV we present a perturbation expansion of the model and derive approximate expressions for the coupling parameters in a simple one-band model. In the conclusions we summarize the results and discuss possible experiments and applications of this simple one-band model in the study of spin-dependent properties of the semiconductor heterostructures.

II. THE THEORETICAL MODEL

To explain our approach, we start noting that the eigenvalue problem associated with the effective-mass Hamiltonian (1) above is exactly equivalent to that with the corresponding bulk effective-mass Hamiltonian in each material plus the Ben-Daniel Duke boundary conditions at the interfaces. To work with the bulk effective-mass Hamiltonian in each layer plus appropriate boundary conditions for the envelope functions at the interfaces is the spirit of the effective-mass theory for the semiconductor heterostructure problem.[23] Generalized (energy dependent) Ben-Daniel Duke boundary conditions for the envelope functions in different models have been derived matching the total wave function and its derivative at the interface.[24,25]

Hamiltonian (1) has indeed been successfully applied to describe a wide range of structures with materials of nearly the same interband matrix elements.[26] It can be derived from a two-band $k\cdot p$ effective-mass model for the bulk with a simple projection into the conduction band. One method of deriving the boundary conditions is to integrate the multiband effective-mass Schrödinger equation across the interface.[23,26] The Ben-Daniel Duke conditions result from the two-band model. To include the spin-orbit interaction, however, one has to start from an eight-band kp model (or six band in the case of strong spin-orbit coupling), considering the top valence and split-off bands and the conduction band.

The eight-band Kane model for III-V semiconductor inversion layers in the infinite barrier approximation was treated in detail recently.[20] Besides leading to simple and useful analytic expressions for the coupling parameters the model was also shown to be quite accurate for the description of the spin-dependent properties of heterostructures with intermediate gap materials like InAs and GaSb.[20] We here consider a finite barrier height and extend the treatment to include effects from the interface and barrier penetration. A more sophisticated model for GaAs quantum wells including higher conduction bands was recently considered in Ref. 10.

With the same notation and basis functions as in Ref. 20, the Schrödinger-like equation for the two components of the conduction-band envelope function, with allowance for the z dependence of the band parameters, becomes [see also Ref. 12]

$$\left[-\frac{\hbar^2}{2}\frac{d}{dz}\frac{1}{m(z,\varepsilon_\pm)}\frac{d}{dz}+\frac{\hbar^2k^2}{2m(z,\varepsilon_\pm)}+E_c(z)+V(z)\mp\left(\frac{d\beta}{dz}(z,\varepsilon_\pm)\right)k-\varepsilon_\pm\right]f_\pm=0, \tag{2}$$

with

$$\frac{1}{m(z,\varepsilon_\pm)}=\frac{P^2}{\hbar^2}\left(\frac{2}{\varepsilon_\pm-V(z)-E_v(z)}+\frac{1}{\varepsilon_\pm-V(z)-E_v(z)+\Delta(z)}\right) \tag{3}$$

and

$$\beta(z,\varepsilon_\pm)=\frac{P^2}{2}\left(\frac{1}{\varepsilon_\pm-V(z)-E_v(z)}-\frac{1}{\varepsilon_\pm-V(z)-E_v(z)+\Delta(z)}\right). \tag{4}$$

The $\pm$ sign refers to spin up and down along the y direction. The parallel wave vector k is set along x and the linear in k term corresponds to the Rashba term (proportional to $\vec{\sigma}\cdot\vec{k}\times\hat{z}$). The momentum matrix element, taken to be independent of z,[25] is denoted by P, Δ stands for the spin-orbit splitting in the valence band, and $\varepsilon_\pm$ are the spin-dependent eigenenergies; $|\varepsilon_+-\varepsilon_-|$ being the spin-orbit splitting.

A. Boundary conditions

Let us now consider at $z=0$ an interface between two semi-infinite layers of semiconductors 1 and 2, so that we may write

$$\frac{1}{m}=\frac{1}{m_1}\,\theta(-z)+\frac{1}{m_2}\,\theta(z) \tag{5}$$

and

$$\beta=\beta_1\theta(-z)+\beta_2\theta(z). \tag{6}$$

From integration across the interface we obtain as boundary conditions $f_\pm$ *continuous* and

$$-\frac{\hbar^2}{2m}\frac{df_\pm}{dz}\mp\beta k f_\pm \ \ continuous. \tag{7}$$

The two-spin components always remain decoupled. As the basis functions for the spin states are those pointing along the y direction, if we call Ψ the spinor with components f_+ and f_-, the boundary conditions can be given as Ψ *continuous* and

$$\frac{\hbar^2}{2m}\frac{d}{dz}\,\psi+\sigma_y\beta k\psi \ \ continuous, \tag{8}$$

where σ_y is the usual Pauli spin matrix. This simpler form shows transparently the cross product symmetry in the Rashba term (remember that k is along x).

The boundary conditions above are equivalent to those obtained in Refs. 10 and 26–28. The decoupling of the spins and the consequent simplicity in the expressions above occur because here we set the spin-quantization direction along the $\vec{k}$-dependent effective magnetic field. The boundary conditions above reduce to the generalized Ben-Daniel Duke boundary conditions when k or Δ goes to zero. Note also that in the case of symmetric quantum wells the mirror reflection will take the spin-up condition into the spin-down one and vice versa, so that the Rashba splitting is exactly zero.

When considering the dependence of β on z in Eq. (2), two contributions to the Rashba spin-orbit splitting can be identified: the first is related to the discontinuity in the band parameters and the second is related to the space charge and/or external electrostatic field. The former brings about the spin-dependent boundary condition of Eqs. (7) or (8), the latter gives a spin-dependent term in the effective-mass Hamiltonian. These two contributions to the Rashba term have been identified also in a previous estimation of the Rashba coupling parameter.[12] In order to clarify the difference between the two contributions, and the correct way to calculate them, we will consider next asymmetric quantum wells where one or the other contribution dominates.

III. RESULTS

The band-edge discontinuities and the space charge and/or external electrostatic potential would contribute to the Rashba term in a similar way only if the edge discontinuities were all the same, as in a single potential step. In real samples, though, the contributions are of a different character and they are both present. It is instructive to look at the splitting in two basic types of asymmetric quantum wells: triangular and square. In the infinite-barrier approximation for a heterojunction the splitting depends exclusively on the space-charge field while in a square asymmetric flat-band quantum well the splitting is only due to the band-edge discontinuities. We start with the latter.

A. Asymmetric square quantum well

Let us consider the problem of the stationary states of electrons confined in semiconductor quantum wells of the type $Al_xGa_{1-x}As/GaAs/Al_yGa_{1-y}As$ with $x\neq y$. The eigenvalues $\varepsilon_\pm$, for every value of k parallel, are obtained by solving Eq. (2). In this flat-band well case one proceeds as usually, i.e., writes down plane-wave solutions for $f_\pm$ in the different regions and matches the solutions at the interfaces with the appropriate boundary conditions [Eq. (7)]. The solutions are obtained from the equality

$$\left(\frac{\hbar^2k_w}{2m_w}\right)^2-\frac{\hbar^2k_w}{2m_w\tan(k_wL)}\left[\frac{\hbar^2}{2}\left(\frac{q_r}{m_r}+\frac{q_l}{m_l}\right)+(\beta_r-\beta_l)k\right]$$
$$=\left(\frac{\hbar^2q_r}{2m_r}+(\beta_r-\beta_w)k\right)\left(\frac{\hbar^2q_l}{2m_l}-(\beta_l-\beta_w)k\right), \tag{9}$$

where r, l, and w refer to the barrier on the right, to the one on the left, and to the well material, respectively; the wave vectors in the growth direction are given by

$$q_i=\sqrt{(2m_i/\hbar^2)(E_{c,i}-\varepsilon)+k^2}, \quad i=r,l \tag{10}$$

and

$$k_w=\sqrt{(2m_w/\hbar^2)(\varepsilon-E_{c,w})-k^2}, \tag{11}$$

and m_j and β_j are given by Eqs. (3) and (4) with the corresponding band parameters. L is the well width and $\varepsilon_\pm$ is the energy ε that satisfies Eq. (9) above with $\pm\beta_j$.

Particularly large splittings are obtained with a pure AlAs barrier in one side of the GaAs quantum well. The conduction-band-edge profile, the density of probability of the first bound state and its energy in a 50 Å-wide $AlAs/GaAs/Al_{15}Ga_{85}As$ quantum well, for example, are as shown in Fig. 1. In Fig. 2 we plot the splitting at a fixed parallel wave vector $k=0.02$ Å$^{-1}=2.0\times10^6$ cm^{-1} as a function of the well width. Note that the splitting presents a maximum as a function of L. Starting from large values of L, the splitting first increases with decreasing well width up to when it is close to the critical width for another bound state, where the competition between confinement and barrier penetration effects produces the maximum. A similar behavior is observed in the well-width dependence of the binding energy of excitons in quantum wells.

One should also note that the splitting is bigger in the excited subband due to the larger amplitude of the envelope function at the small barrier interface that, in accord to the spin-dependent boundary conditions [Eq. (7)], leads to a larger spin-orbit effect. We should also mention that the splitting initially grows both with k and with the aluminum concentration x. The quantized subband energy, however, should remain below the AlAs X state in the conduction band to prevent Γ-X mixing effects, which are not included in the model.

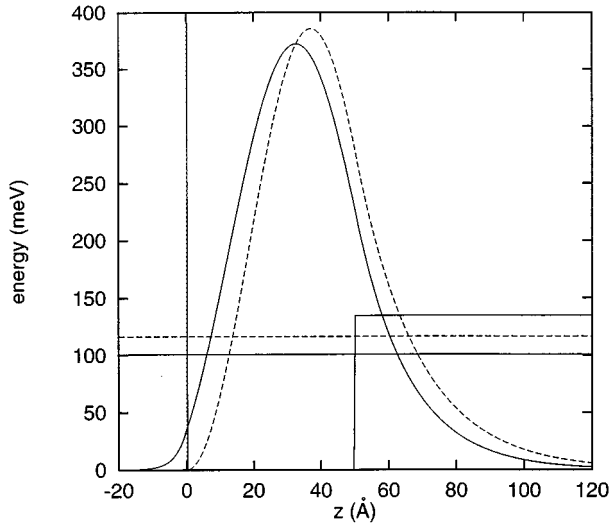

FIG. 1. Conduction-band-edge profile of an AlAs/GaAs/$Al_{0.15}Ga_{0.85}As$ asymmetric square quantum well. The density probability and the energy of the lower-bound state is shown with continuous lines. The dashed lines show the infinite-barrier approximation, where there is no barrier penetration. The band parameters used for the alloy were $E_g=(1.519+1.247x)$ eV and $\Delta=(1.859+1.115x+0.37x^2-E_g)$ eV. For the conduction-band offset we used the 72% rule for $x<0.4$ and 1 eV for a pure AlAs barrier.

In order to evaluate the role played by the large barrier interface, we compare the results above with those obtained in the infinite-barrier approximation, when no wave-function penetration is allowed in the AlAs barrier. The solution in this case is simpler and given by

$$-\frac{\hbar^2}{2m_r}k_r+\beta_r k=+\frac{\hbar^2}{2m_w}\frac{k_w}{\tan(k_wL)}+\beta_w k. \qquad (12)$$

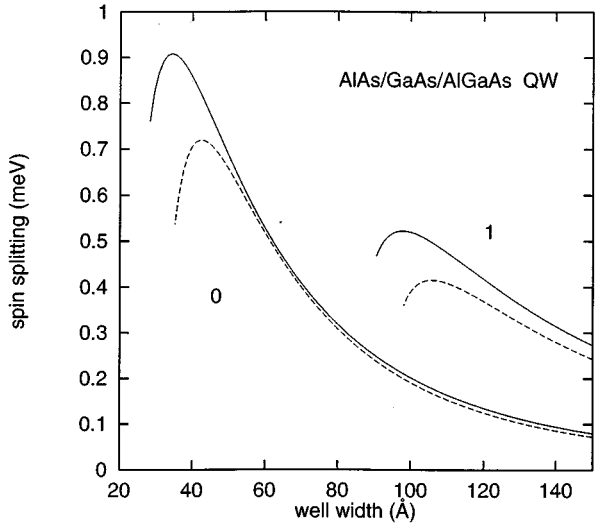

FIG. 2. Rashba spin-orbit splitting in the ground (0) and first excited (1) subbands of the asymmetric AlAs/GaAs/$Al_{0.15}Ga_{0.85}As$ quantum well, as a function of the well width. The results within the infinite-barrier approximation are plotted with dashed lines. The lines, for small L, end at the respective critical values for another bound state in the well and $k=2.0\times10^6$ cm^{-1}.

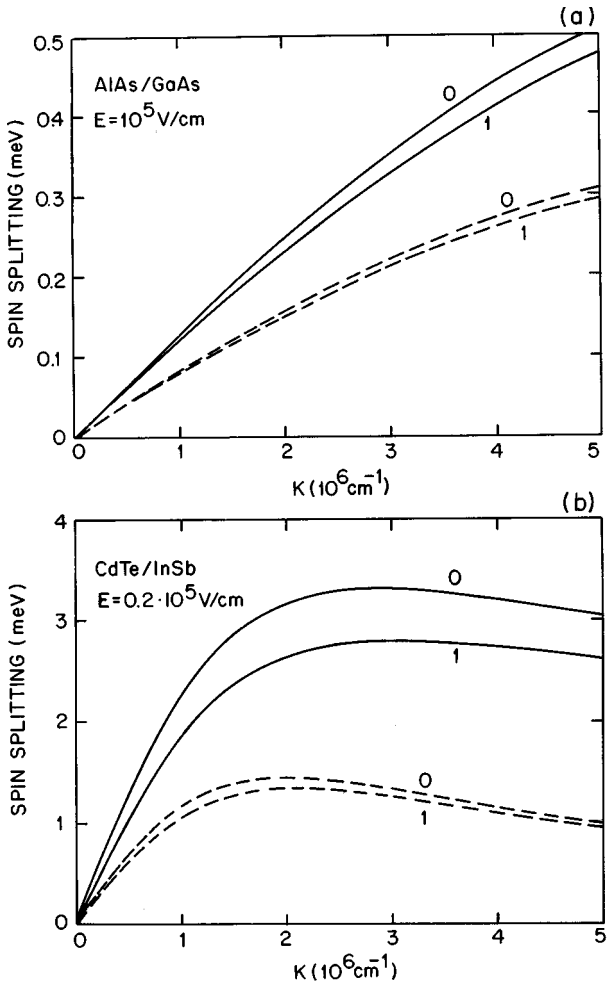

FIG. 3. Rahsba spin-orbit splitting for a triangular asymmetric quantum well. The upper panel (a) shows the obtained splittings in the first two subbands of the model AlAs/GaAs heterojunction as a function of parallel wave vector, both with (dashed lines) and without (solid lines) the infinite-barrier approximation. The interface electric field is fixed $E=10^5$ V/cm. In the lower panel (b) we plotted similar results using the parameters of a CdTe/InSb heterojunction ($m^*=0.015m_e$, $E_g=0.24$ eV, and $\Delta=0.81$ eV for InSb, and $E_g=1.59$ eV and $\Delta=0.8$ eV for CdTe).

The results are shown with the dashed lines in Figs. 1 and 2. One should note that the penetration, when small, contributes very little to the splitting and does not cause the drastic reduction one would expect following Ando's reasoning.

B. Triangular quantum well

Here, as a model for a heterojunction, we consider a triangular quantum well formed by a heterointerface plus a constant electric field in the small-gap material, which is proportional to the carrier concentration ($E=en_s/\varepsilon_{sc}$) and confines the electrons near the interface. Equation (2) in this case is integrated numerically. In Fig. 3 we show the results using typical parameters for two different heterojunctions: AlAs/GaAs and CdTe/InSb. Figure 3(a) shows the obtained splittings in the ground (0) and first excited (1) subbands as a function of parallel wave vector for the case of an AlAs/GaAs heterojunction with an interface electric field $E=10^5$ V/cm. We first note that, in accord with other multi-

band calculations,[29–32] the splitting grows linearly with k only in the small-k limit. Contrary to the square well case, we see that the splitting in the excited subband of a triangular quantum well is close to the splitting in the first subband but smaller. The reason is that, in this case, the splitting is mainly due to the z dependence of the electrostatic potential V (or the electric field), which is the same for both subbands. In accord to the expression for β [Eq. (4)], due to nonparabolicity effects, a larger energy subband will have a smaller spin-orbit effect, as observed in the figure.

As before, it is instructive to check the infinite-barrier approximation. Again, contrary to what one would expect from Ando's reasoning, one gets bigger splittings by allowing wave-function barrier penetration. This is a direct result of the spin-dependent boundary conditions, which adds to the total splitting. The effect is bigger in the triangular case since the electrons are pushed towards the interface and the amplitude of the envelope function there is bigger than in the square well case when the density of probability peaks at a larger distance from the interface. The subband quantization energy increases less than 10% in the infinite barrier approximation so that the nonparabolicity reduction in this case is much smaller than in the excited subband case and contributes very little.

The spin-orbit effects in the conduction band are known to be bigger in the smaller gap semiconductors. In Fig. 3(b) we show the results for the above triangular quantum-well model made of CdTe as barrier and InSb as well, with a conduction-band discontinuity of 550 meV. The spin splitting in such heterojunction has been investigated in Ref. 18. Here we want to call attention to two facts. First, as shown in the figure, note that the infinite-barrier approximation for the conduction-band offset is worse in this case, due to both the smaller band offset and the smaller gap. And second, note that the splitting, instead of saturating for increasing k, reaches a maximum splitting and then decreases. This last fact may be used for optimizing the spin-dependent properties of possible heterostructure devices.

C. Perturbative expansion: simple one-band model

Different perturbation expansions can be used, depending on the structure and on the kind of band alignment, in order to make the model simpler and more transparent. Here we are interested in the reduction to a one-band model to make contact with the Rashba model Hamiltonian that has been used to describe different experimental results. When the conduction bands in the barrier and in the well are parabolic and the band offset is somewhat smaller than the gaps, as in GaAs/$Ga_{1-x}Al_xAs$ heterostructures, a good expansion parameter to use is

$$\delta=\frac{\varepsilon_{\pm}-V-E_c}{E_g+\Delta}, \tag{13}$$

where E_g is the band gap and to simplify the notation we have not indicated the z dependence. For GaAs/$Ga_{1-x}Al_xAs$ quantum wells, for example, δ is of the order of 0.05, both in the well and in the barrier.

A perturbative series is obtained by expanding the energy-dependent parameters as

$$\frac{1}{m}=\sum_{n=0}^{\infty} c_n\delta^n \quad \text{and} \quad \beta=\sum_{n=0}^{\infty} b_n\delta^n. \tag{14}$$

The zeroth-order approximation, when all terms involving δ are neglected, corresponds to the parabolic approximation. The effective-mass Hamiltonian [Eq. (2)] becomes

$$H=-\frac{\hbar^2}{2}\frac{d}{dz}\frac{1}{m^*(z)}\frac{d}{dz}+\frac{\hbar^2k^2}{2m^*(z)}+E_c+V(z), \tag{15}$$

where m^* is the conduction-band-edge effective mass that depends only on z and in each material is given by

$$m^*=\frac{\hbar^2}{P^2}\frac{E_g(E_g+\Delta)}{3E_g+2\Delta}. \tag{16}$$

In zeroth order $\beta=b_0$ and we get

$$\beta=\frac{\hbar^2}{2m^*}\frac{\Delta}{3E_g+2\Delta}. \tag{17}$$

It is important to realize that, even in this parabolic approximation, the boundary conditions are spin dependent [$f_{\pm}$ and $-(\hbar^2/2m^*)(df_{\pm}/dz)\mp\beta k f_{\pm}$ continuous]. In this approximation, the contribution to the splitting from $V(z)$ is only indirect through the value of the wave function at the interface.

To better compare the two contributions we go to the next order. Including the next term in the expansions above we obtain an approximate effective Hamiltonian of the form

$$H=-\frac{\hbar^2}{2}\frac{d}{dz}\frac{1}{m(\varepsilon_{\pm},z)}\frac{d}{dz}+\frac{\hbar^2k^2}{2m(\varepsilon_{\pm},z)}+E_c+V(z)$$
$$\mp\alpha_{so}k\frac{dV}{dz}, \tag{18}$$

where

$$\alpha_{so}=\frac{\hbar^2}{2m^*}\frac{\Delta}{E_g}\frac{2E_g+\Delta}{(E_g+\Delta)(3E_g+2\Delta)} \tag{19}$$

is the same Rashba spin-orbit coupling parameter obtained in Ref. 20. The energy dependence that appears in both m and β $(=b_0+b_1\delta)$ corresponds to nonparabolicity corrections which in GaAs/$Ga_{1-x}Al_xAs$ systems are small due to the smallness of δ. Neglecting these small corrections, the boundary conditions remain the same. In Table I we list the values of the coupling parameters α_{so} and β for different semiconducting III-V compounds.

TABLE I. Spin-orbit coupling parameters α_{so}, Eq. (19), and β, Eq. (17), for different III-V semiconductor compounds. The bulk parameters used are those from the *Numerical Data and Functional Relationships in Science and Technology*, edited by O. Madelung, M. Schultz, and M. Weiss, Landolt-Börnstein, New Series Group III, Vol. 22, Pt. a (Spring-Verlag, Berlin, 1982).

	GaAs	GaSb	InAs	InSb
α_{so} (Å^2)	4.4	33	110	500
β (eV Å^2)	3.7	18	31	96

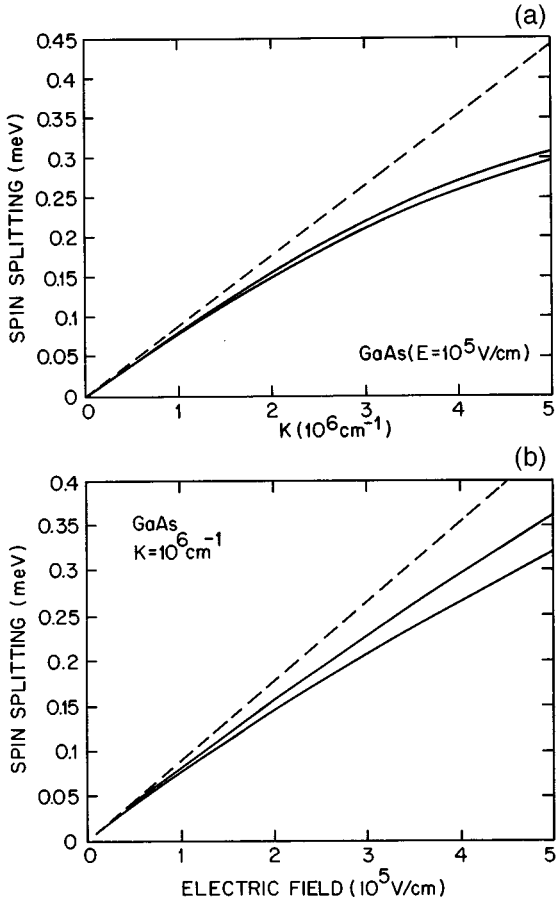

FIG. 4. Comparison between the splittings obtained in the multiband and one-band (dashed lines) models. The spin-orbit splitting in the first two subbands of a GaAs infinite-barrier heterojunction is plotted in the upper panel (a) as a function of k for a fixed electric field and in the lower panel (b) as a function of the electric field for a fixed $k=10^6$ cm^{-1}. See text for the discussion.

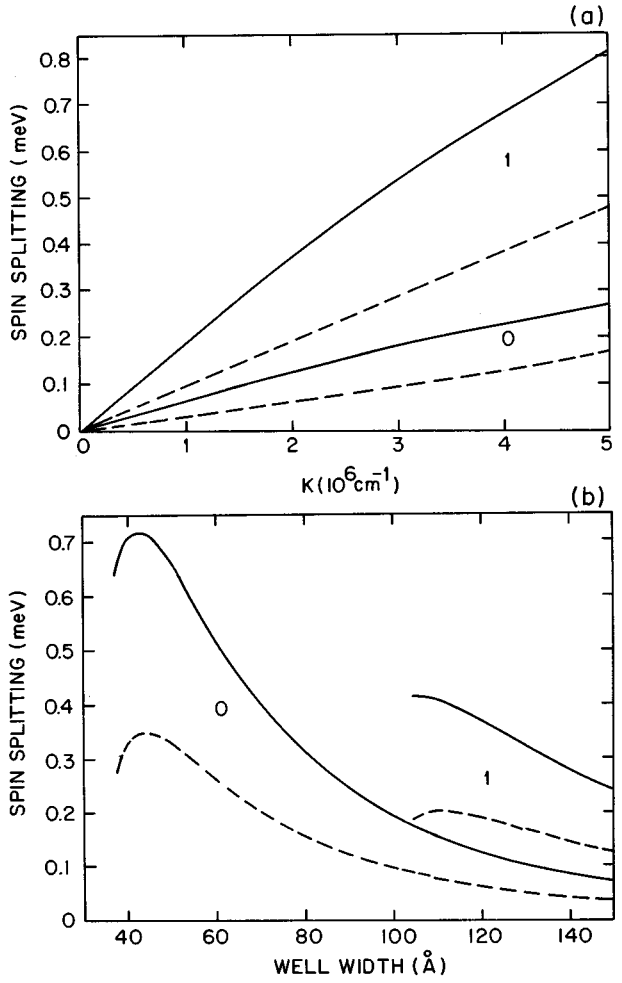

FIG. 5. Comparison between the multiband and one-band (dashed lines) splittings in the case of asymmetric square quantum wells. The splittings in the first two subbands of an AlAs/GaAs/$Al_{0.15}Ga_{0.85}As$ quantum well are plotted on top as a function of k ($L=120$ Å) and below as a function of the well width ($k=2.0\times10^6$ cm^{-1}); the infinite-barrier approximation is employed on the AlAs side.

In the infinite-barrier approximation the splitting in the triangular quantum well can then be approximated by $|\varepsilon_+ - \varepsilon_-| = 2\alpha_{so}kE$ (linear with both k and E, and independent of the subband). The small parameter in the perturbation expansion in this case increases both with k and with E. The limits of applicability of the one-band model can then be evaluated from Fig. 4. There we compare the complete numerical solution of Eq. (2) with the solution neglecting nonparabolicity corrections, i.e., the solution of Eq. (18) with m and α_{so} given by Eqs. (16) and (19), respectively. We can see that the simple one-band model gives an upper bound value for the Rashba splitting. In a GaAs heterojunction, the approximation gives very accurate values for $k \leqslant 10^6$ cm^{-1} when $E \sim 10^5$ V/cm or for $E \leqslant 10^5$ V/cm when $k \sim 10^6$ cm^{-1} (recall, for example, that in a GaAs heterojunction with $n_s = 5.0\times10^{11}$ cm^{-1} we have $E \sim 0.8\times10^5$ V/cm and $k_F \sim 1.7\times10^6$ cm^{-1}).

The one-band (first order in δ or ''parabolic'') approximation is less effective in the asymmetric square quantum well problem. In Fig. 5, where the dashed lines give the one-band approximation, we see that it gives sensibly smaller splittings down to low values of k and large values of the well width. Here we see a partial breakdown of the perturbation expansion, due to the nonlinear sensibility of the splitting to the envelope-function value at the interface and to the energy. The simple model nevertheless reproduces all the major features besides giving quite reasonable estimates of the splitting.

More experiments would be needed in order to fully test the present approach. We limit ourselves here to a few comments on very recent experiments. In the Raman scattering experiment of Ref. 8, a Rashba contribution of $2\alpha k$ with $\alpha = -6.9\pm0.4$ meV Å was extracted from different measurements of the spin splitting in a sample consisting of an asymmetrically doped thick GaAs quantum well, with small barrier penetration. In the simplest one-band or Rashba model we set $\alpha = \alpha_{so}e\langle E\rangle$, where $\langle E\rangle$ is average space-charge electric field in the well, which in this case was inferred to be -1.06×10^5 V/cm. We then obtain $\alpha_{so} = 6.5\pm0.4$ Å^2. The theoretical value in Table I corresponds to the splitting in the infinite-barrier approximation which is, as discussed above, 35–40 % smaller. Considering the uncertainties both in the experiment and in the material parameters entering the theoretical value, we obtain here a very good agreement between theory and experiment.

A quantitative description of recent antilocalization data was given with the same one-band model in Ref. 9. Good agreement with other experimental data was shown also in Ref. 10, whose calculation with a larger Hamiltonian gave splittings 35–40 % larger than those obtained before[20] with the simplest model discussed above, i.e., in the infinite barrier approximation and in first order in δ. In view of the present results we can say that the difference comes mainly from the barrier penetration and from the spin-dependent boundary conditions.

IV. CONCLUSIONS

We have presented a detailed study of the so-called Rashba spin-orbit splitting in the spectrum of the two-dimensional electron gas in asymmetric semiconductor quantum wells. A few theoretical issues much debated in the literature, like the treatment of abrupt interfaces, the Ando argument, and simpler approximations have been discussed and clarified. A simple one-band model with spin-dependent boundary conditions and approximate coupling constants has been suggested. The model can be used as a starting point for the calculation of spin-dependent effects in the quantum transport of small semiconductor heterostructure.[33] The spin-orbit splitting in the conduction subband plays an important role also in the luminescence polarization studies of the exciton and of the electron ultrafast spin dynamics.[33] The splitting in the different subbands of both triangular and square asymmetric quantum wells have been investigated. The splitting in the excited subband was shown to be bigger in the square well and smaller in the triangular well, which can be explained in view of the two different contributions to the Rashba term in semiconductor heterostructure plus nonparabolicity corrections. Good agreement was found with available experimental data, but more experiments are needed in order to fully test the theory presented here. In particular, the well-width dependence of the splitting in $AlAs/GaAs/Al_xGa_{1-x}As$ asymmetric quantum wells and the k dependence of the splitting in InSb heterojunctions, both exhibiting a nonmonotonic behavior, are still to be tested experimentally.

Finally, we want to point out that for a quantitative comparison with the experiment one should add the k^3 contribution, as explained in Ref. 20, and use a self-consistent electrostatic potential. The model and the procedure, including the boundary conditions, are, however, as explained above and the simple one-band approximation can be used to obtain semiquantitative estimates and the qualitative dependence on different parameters.

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