# Effective one-band approach for the spin splittings in quantum wells

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The spin-orbit interaction of two-dimensional electrons in quantum wells grown from the III-V semiconductors consists of two parts with different symmetry: the Bychkov-Rashba and the Dresselhaus terms. The last term is usually attributed to the bulk spin-orbit Hamiltonian which reflects the $T_d$ symmetry of the zincblende lattice. While it is known that the quantum well interfaces may also contribute to the Dresselhaus term, the exact structure and relative importance of the interface and bulk contributions are not well understood. To deal with this problem, we perform tight-binding calculations of the spin splittings of the electron levels in [100] GaAs/AlGaAs quantum wells. We show that the obtained spin splittings can be adequately described within the one-band electron Hamiltonian containing, together with the bulk contribution, the two interface contributions to the Dresselhaus term. The magnitude of the interface contribution to the spin-orbit interaction for sufficiently narrow quantum wells is of the same order as the bulk contribution.

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## I. INTRODUCTION

The spin-orbit interaction of two-dimensional (2D) electrons in the heterostructures based on the noncentrosymmetric cubic semiconductors has been extensively investigated during the last three decades [1–3]. However, there is still no complete understanding of the physical nature and magnitude of different contributions to the spin-orbit interaction even in the conventional GaAs/AlGaAs heterostructure systems.

For the bulk III-V semiconductors the general form of the one-band effective mass electron Hamiltonian with the spin-orbit terms and the effective-mass anisotropy terms was established from a symmetry consideration [4,5]. The magnitudes of these terms can be derived from the many-band Kane $\mathbf{k}\cdot\mathbf{p}$ models [5–7] or obtained in microscopic calculations [8,9].

The spin-orbit interaction of 2D electrons in the heterostructures grown from the III-V semiconductors consists of two parts with different symmetry: the Bychkov-Rashba and Dresselhaus terms. The isotropic part of the spin-orbit interaction (the Bychkov-Rashba contribution) is induced by the electric field along the growth direction. It consists of two contributions: the bulk contribution, associated with the smooth part of the electric field along the normal, and the interface contribution, associated with the strong atomic field at the well interfaces [10]. Analogously, the anisotropic part of the spin-orbit interaction of 2D electrons (the Dresselhaus term) contains the bulk contribution, related to the spin-orbit interaction in the zincblende lattice, and the interface contribution, determined by the atomic structure of the interfaces.

For the first time, the effect of sharp interfaces on the electron and hole states in the III-V semiconductor heterostructures was noticed in tight-binding calculations in the 1980s in Refs. [11–13]. It was shown that the low $C_{2v}$ symmetry of the interface produces heavy-light hole mixing in [001] grown heterostructures. However, for some time this phenomenon has been neglected in the literature. Later, the interface anisotropic terms in the effective mass Hamiltonian for holes were proposed in Refs. [14,15] to explain the nature of the anisotropic exchange splitting of excitonic levels in type II GaAs/AlAs superlattices. The magnitudes of the interface anisotropic terms were estimated in the tight-binding model [16], from the experimental data [17], and in pseudopotential calculations [18].

In Refs. [19,20] it was shown that the mixing of heavy and light holes at the interfaces also leads to a spin-orbit interface anisotropic term in the one-band electron Hamiltonian. This term induces a contribution to the electron spin splitting, in addition to the bulk contribution. Later, it was noticed [21] and confirmed by tight-binding calculations [22,23] that the interface-induced spin splitting can be observed alone, without the admixture of the bulk contribution, in the heterostructures grown from diamond lattice semiconductors. More recently, two interface anisotropic spin-dependent terms, one of which coincides with the term proposed in Refs. [19,20], were introduced in the electron effective Hamiltonian in Refs. [24,25] in an attempt to describe the lateral anisotropy of 2D electron $g$ factors recently observed in the [100] GaAs quantum wells [26–28]. Similar interface terms were derived in Ref. [29] from the $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian containing infinite number of bands. The analysis of the experimental data from Refs. [26–28] shows that the contributions to the $g$-factor anisotropy from the quantum well interfaces and from the bulk regions are of the same order of magnitude [24]. Recently, it was demonstrated within the framework of the 14-band Kane model that the interface spin-orbit terms are substantial in the Luttinger $4 \times 4$ Hamiltonian for 2D holes in GaAs quantum wells [30].

It should be mentioned that, at present, there is strong controversy concerning the value of the bulk spin-orbit constant $\gamma$ in various semiconductors [7,31–34]. For example, it was concluded in Ref. [31] from measurements of the spin splittings of electron dispersion in GaAs quantum wells that the bulk spin-orbit constant $\gamma$ in GaAs is approximately half of the value which was previously accepted in the literature [7,32]. However, in the interpretation of the experimental data in Ref. [31], the presence of anisotropic spin-orbit terms localized at the interfaces was not taken into account. Recent discovery of a giant linear spin splitting of 2D holes [35] shows that one should be extremely careful when transferring spin physics of the bulk semiconductors to low-dimensional systems. Some novel ways to determine the bulk spin-orbit Dresselhaus parameter from the experiments on bulk semiconductors

subjected in homogeneous and inhomogeneous magnetic field were discussed in Refs. [36–39].

The tight-binding approach is the method which is able to take into account both the bulk and the interface contributions to the spin-orbit interaction of 2D electrons by a rigorous uniform way. Tight-binding calculations of the spin splittings of 2D electrons in [110] quantum wells grown from III-V semiconductors were recently performed in Refs. [40,41].

In this paper we perform tight-binding calculations of spin splittings of the electron energy spectrum in [100] GaAs quantum wells subjected to an electric field along the growth direction. We compare the obtained dependencies of the spin splittings on the quantum well width and the electric field with the analytic expressions derived within the one-band electron Hamiltonian containing the bulk [4] and the two interface [24,25] spin-orbit terms. From the comparison, we extract the values of the bulk and interface parameters in the one-band electron Hamiltonian. The analytical one-band calculations perfectly reproduce the tight-binding numerical calculations for different quantum wells. As a result, we estimate the magnitudes of the two interface terms and prove the importance of the interface contributions to the spin splitting of the 2D electron spectrum in GaAs quantum wells.

## II. TIGHT-BINDING CALCULATIONS

We use the standard $spds^*$ tight-binding model which is explained in detail in Ref. [42]. In this method, the electron wave function $\psi(\boldsymbol{r})$ is written as a linear combination

$$\psi(\boldsymbol{r}) = \sum_{i,\alpha} C_{i\alpha}\Psi_\alpha(\boldsymbol{r}-\boldsymbol{r}_i) \tag{1}$$

of localized atomic-like functions $\Psi_\alpha$, which are assumed to be orthogonal [43], at atoms $i$ with coordinates $\boldsymbol{r}_i$.

Since we are interested in the in-plane dispersion of free electrons in a heterostructure, we impose periodical boundary conditions in the interface plane (001). Because of the periodicity in the [100] and [010] directions, we can introduce the in-plane wave vector $\boldsymbol{k}$ and, for a given value of $\boldsymbol{k}$, construct the tight-binding Hamiltonian with a discrete spectrum. For the sake of numerical simplicity and to avoid spurious solutions at the boundaries, we also use periodic boundary conditions along the growth direction [001] taking the barrier layers thick enough to exclude the influence of their thickness on the calculated energies.

The Hamiltonian in this basis is a matrix of the size $10\times 2\times n$, where 10 stands for basis functions $\alpha = s, s^*, p_x, p_y, p_z, d_{yz}, d_{zx}, d_{xy}, d_{x^2-y^2}, d_{3z^2-r^2}$, 2 stands for the spin index, and $n$ is the number of atoms in elementary cells for periodic structures. The explicit form of matrix elements of the Hamiltonian may be found in [44] or [45]. In the empirical variant of the method, the parameters are fitted to reproduce the band structure of the bulk materials, we use the standard parametrization of Jancu *et al.* [42]. The matrix of the Hamiltonian is the sparse matrix with blocks $20\times 20$ corresponding to atoms and chemical bonds between them. Iterative methods allow [46,47] the fast and efficient solution of eigenproblems even for very large systems.

We consider a GaAs quantum well between $Ga_{0.7}Al_{0.3}As$ barriers. The alloy is treated in the virtual crystal approximation: the tight-binding parameters are taken as a weighted linear combination of the corresponding GaAs and AlAs parameters

$$\kappa(Ga_{0.7}Al_{0.3}As) = 0.7\kappa(GaAs) + 0.3\kappa(AlAs)\,, \tag{2}$$

where $\kappa$ stands for the tight-binding parameters of the corresponding material (in brackets). This approximation does not include the possible effects of bowing, which is almost absent in the AlGaAs ternary alloy, and disorder, which is averaged out in optical and transport properties. For other ternary alloys a more sophisticated approximation might be necessary [48].

To calculate the spin splitting we choose small wave vector $\boldsymbol{k}$ and change its direction in the (001) plane. At finite $\boldsymbol{k}$, the (double) degeneracy of quantum-confined electron states is lifted, with the splitting proportional to $|\boldsymbol{k}|$. For each lateral direction of $\boldsymbol{k}$, we calculate the splitting $\Delta(\boldsymbol{k})$ and the vector $\boldsymbol{s}$ of the mean value of the electron spin for the lower spin branch as explained in Ref. [40].

The electric field $E_z$, applied along the growth direction and causing the quantum well asymmetry, is taken into account in the framework of the standard procedure [49] by shifting the diagonal energies due to the local potential at atomic sites. The electrostatic potential is chosen in the form

$$U_{TB}(z) = \begin{cases} -eE_z a/2, & z < -a/2, \\ eE_z z, & -a/2 < z < a/2\,, \\ eE_z a/2\,, & z > a/2, \end{cases} \tag{3}$$

where $E_z$ is the electric field, $e>0$ is the absolute value of the electron charge, and $a$ is the quantum well width.

The spin-orbit part of the effective Hamiltonian for an electron in quantum well can be written as

$$\hat{H}_{\rm SO}(\boldsymbol{k}) = \beta(k_x\hat{\sigma}_x - k_y\hat{\sigma}_y) + \alpha(k_y\hat{\sigma}_x - k_x\hat{\sigma}_y). \tag{4}$$

The solution of this one-band Hamiltonian gives us the energy splitting between the two states:

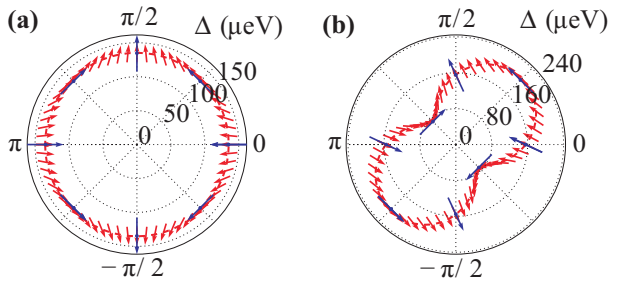
$$\Delta(\boldsymbol{k}) = 2\sqrt{(\beta^2+\alpha^2)k^2 + 4\alpha\beta k_x k_y}, \tag{5}$$

and the mean values of the spin projections for the lower energy state:

$$s_x = -\frac{\beta k_x + \alpha k_y}{\Delta(\boldsymbol{k})}, \quad s_y = \frac{\beta k_y + \alpha k_x}{\Delta(\boldsymbol{k})}. \tag{6}$$

The splittings and the spin direction as functions of the lateral wave vector angle are extracted from tight-binding calculations and fitted with Eqs. (5) and (6). The fit is shown in Fig. 1. This allows us to extract the Dresselhaus and Rashba constants $\beta$ and $\alpha$ directly from the tight-binding calculations.

With the help of the tight-binding approach, we have calculated the absolute values of the spin splitting constants as functions of the well width in the range from 1 to 20 nm, and the electric fields $E_z$ in the range from 0 to $10^5$ V/cm. The results of this calculation as well as their analysis are presented in Sec. IV. Here we only mention that, in accordance with symmetry consideration, the parameter $\alpha$ vanishes at zero electric field, when the quantum well is symmetric, and then increases linearly with $E_z$. The Dresselhaus parameter $\beta$ depends on the electric field $E_z$ in a weaker manner: it starts




$\alpha = -2.341\times10^{-10}$ (eV Å) $\quad$ $\alpha = 6.593\times10^{-3}$ (eV Å)

$\beta = 1.352\times10^{-2}$ (eV Å) $\quad$ $\beta = 1.413\times10^{-2}$ (eV Å)

FIG. 1. 2D electron spin splittings and direction of the spin as a function of the angle of the lateral wave vector $\boldsymbol{k}$ for the quantum well width equal to 30 atomic layers and $|k| = 5\times10^{-3}$ Å$^{-1}$. The direct results of the tight-binding calculations (blue arrows) are shown together with the results of fitting of the tight-binding calculations by Eqs. (5) and (6) (red dashed curve for the spin splitting and red arrows for the spin directions). Left and right panels show the results for the electric fields $E_z = 0$ and $E_z = 1\times10^5$ eV/cm, respectively.

to deviate significantly from the zero-field value only when the variation of electrostatic potential $-eE_z z$ from the electric field $E_z$ in the interface region is comparable with the quantum confinement energy $E_0$.

## III. ONE-BAND HAMILTONIAN APPROACH TO SPIN SPLITTINGS OF 2D ELECTRONS

For a quantum well grown along the [001] direction from the zincblende semiconductors, the bulk cubic spin-orbit term in the one-band electron Hamiltonian [7] takes the form

$$\hat{H}_{\rm BIA} = \frac{d}{dz}\gamma(z)\frac{d}{dz}(k_x\hat{\sigma}_x - k_y\hat{\sigma}_y). \tag{7}$$

This term corresponds to the linear approximation in the electron lateral wave vector $\boldsymbol{k} = (k_x, k_y)$. Here $\gamma(z)$ is the bulk spin-orbit parameter, which depends on the layer material.

In addition to the bulk contribution (7), the spin-orbit interaction of an electron in a quantum well with abrupt interfaces also has interface contributions [20–25,29]. They have the same symmetry as the bulk term (7), but contain, instead of the operator $d^2/dz^2$, the $\delta$ function and its derivative localized at the well interfaces [24,25]:

$$\hat{H}_{\rm int} = \sum_{\nu=l,r}(\hat{H}_{{\rm int},0,\nu} + \hat{H}_{{\rm int},1,\nu}),$$
$$\hat{H}_{{\rm int},0,\nu} = \zeta_\nu\delta(z-z_\nu)(k_x\hat{\sigma}_x - k_y\hat{\sigma}_y),$$
$$\hat{H}_{{\rm int},1,\nu} = \xi_\nu\delta'(z-z_\nu)(k_x\hat{\sigma}_x - k_y\hat{\sigma}_y). \tag{8}$$

The parameters $\zeta_{l,r}$ and $\xi_{l,r}$ are determined by the structure of the chemical bonds of the atoms on the interface. Equations (8) assume continuity of the wave-function derivative at the interfaces of the quantum well.

Also note that the definition of the bulk contribution (7) is not completely unambiguous: e.g., one might use terms proportional to $[\gamma(z)\,d^2/dz^2 + d^2/dz^2\gamma(z)]/2$ or $[\gamma(z)]^{1/2}d^2/dz^2[\gamma(z)]^{1/2}$, this would lead to the renormalization of interface parameters in Eq. (8). Our choice is based on the simplicity of Eq. (7).

Let $u(z)$ be the electron wave function of the ground level $E_0$ of space quantization within the one-band electron Hamiltonian. Projection of the operators (7) and (8) onto the first subband leads to the anisotropic spin-orbit interaction of 2D electrons [the first term in Eq. (4)]:

$$\hat{H}_D = \beta\,(k_x\hat{\sigma}_x - k_y\hat{\sigma}_y), \quad \beta = \langle u|\hat{\beta}|u\rangle \equiv \langle\hat{\beta}\rangle,$$
$$\hat{\beta} = \frac{d}{dz}\gamma(z)\frac{d}{dz} + \sum_{\nu=l,r}[\zeta_\nu\delta(z-z_\nu) + \xi_\nu\delta'(z-z_\nu)]. \tag{9}$$

We consider a rectangular quantum well. The function $\gamma(z)$ in this structure is a step-like function with the two different values in the well and in the barrier layers:

$$\gamma(z) = \begin{vmatrix}\gamma_b, & z<0,\ z>a,\\ \gamma_w, & 0<z<a.\end{vmatrix}$$

In zero electric field the symmetry of the quantum well $D_{2d}$ leads to the relations between the coefficients $\zeta_\nu$ and $\xi_\nu$ for the left and right interfaces: $\zeta_l = \zeta_r$, $\xi_l = -\xi_r$. If an electric field $E_z$ is applied along the normal to the quantum well, the relations $\zeta_l = \zeta_r$, $\xi_l = -\xi_r$ are retained, but the wave function $u(z)$ is not symmetric with respect to the quantum well center. The result is

$$\beta = \beta_b + \beta_{{\rm int},0} + \beta_{{\rm int},1},$$
$$\beta_b = -\int_{-\infty}^{\infty} dz\,\gamma(z)[u'(z)]^2,$$
$$\beta_{{\rm int},0} = \zeta\,[u(z_l)^2 + u(z_r)^2],$$
$$\beta_{{\rm int},1} = \xi\,\{[u(z_l)^2]' - [u(z_r)^2]'\}. \tag{10}$$

The potential energy of an electron in an empty rectangular quantum well in zero electric field, $E_z = 0$, is

$$U(z) = \begin{vmatrix}0, & -a/2<z<a/2,\\ U_0, & z<-a/2,\ z>a/2.\end{vmatrix} \tag{11}$$

For a nonzero electric field $E_z$ the electron potential energy is the sum of the quantum well potential (11) and the potential (3) due to the applied electric field: $\tilde{U}(z) = U(z) + U_{TB}(z)$.

The wave function $u(z)$ of the ground state corresponding to the potential $\tilde{U}(z)$ is expressed via the Airy functions in the well region:

$$u(z) = c_A{\rm Ai}\left(\frac{z - E_0/eE_z}{d}\right) + c_B{\rm Bi}\left(\frac{z - E_0/eE_z}{d}\right), \tag{12}$$

and the exponents in the barriers:

$$u(z) = \begin{vmatrix}c_l e^{\kappa_l z}, & z<-a/2,\\ c_r e^{-\kappa_r z}, & z>a/2.\end{vmatrix} \tag{13}$$

Here $d = (2meE_z/\hbar^2)^{-1/3}$ is the characteristic localization length due to the electric field, $\kappa_{l,r} = \sqrt{2m(U_0 \mp eE_z a/2 - E_0)}/\hbar$. The coefficients $c_A$, $c_B$, $c_l$, $c_r$, and the eigenenergy $E_0$ were calculated as the functions of

the quantum well width $a$ and the electric field $E_z$ by use of the standard methods.

## IV. RESULTS

In this section we present, compare, and discuss the results of the tight-binding and the one-band calculations of spin splittings of 2D electrons in GaAs quantum wells. We consider quantum wells in the typical heterostructures $Ga_{0.7}Al_{0.3}As/GaAs/Ga_{0.7}Al_{0.3}$ with the following $\mathbf{k}\cdot\mathbf{p}$ parameters: $U_0 = 300$ meV and $m = 0.067m_0$. In Fig. 2 we present the results of calculations of the bulk and the interface spin-orbit parameters in the one-band 2D electron Hamiltonian according to Eqs. (10)–(13).

In Fig. 2(a) we show the magnitudes of the bulk and interface contributions to the spin-orbit interaction as functions of the quantum well width $a$ for a zero electric field $E_z = 0$. The dependencies $\beta_i(a)$, $i = b,(\text{int},0),(\text{int},1)$, are nonmonotonic. The origin of this fact is most transparent for the bulk contribution $\beta_b$. Indeed, if we neglect the difference between $\gamma_b$ and $\gamma_w$, the value $\beta_b$ is proportional to $\langle k_z^2\rangle$ [see Eq. (10)]. It is easily seen that the value $\langle k_z^2\rangle$ tends to zero as $1/a^2$ for the thick quantum wells and as $a^2$ for the thin quantum wells. In between, the coefficient $\beta_b(a)$ has a maximum at quantum well widths $a \simeq 1/\kappa_0 \simeq 2$ nm when $E_0 \sim U_0$ (here $\kappa_0 = \sqrt{mU_0}/\hbar$). One can show from Eqs. (10) that the dependencies of the interface contributions to the magnitude of spin splittings, $\beta_{\text{int},0}(a)$ and $\beta_{\text{int},1}(a)$, also exhibit the power behavior in the region of large and small widths $a$. So, for the case $E_z = 0$ we have[1]

$$\beta_b \sim a^{-2}, \quad \beta_{\text{int},0} \sim a^{-3}, \quad \beta_{\text{int},1} \sim a^{-3} \tag{14}$$

at $a \to \infty$, and

$$\beta_b \sim a^2, \quad \beta_{\text{int},0} \sim a, \quad \beta_{\text{int},1} \sim a^2 \tag{15}$$

at $a \to 0$.

Now let us discuss the case of a nonzero electric field. The bulk contribution $\beta_b$ is proportional to $\langle k_z^2\rangle$, and the value $1/\sqrt{\langle k_z^2\rangle}$ is of the order of the electron localization length. The last value is defined by the minimum of the two values: the quantum well width $a$ and the length of localization due to the electric field $d$. In the case of small electric fields we have $a \ll d$, while for enough large well widths we arrive at the opposite inequality $a \gg d$. The transition between these two regimes occurs at the electric fields $E_0(E_z = 0) \sim eE_z a$.

In Fig. 2(b) we show the bulk and the interface contributions to the spin-orbit parameter $\beta$ as a function of the electric field $E_z$ for the infinitely wide quantum well, $a \to \infty$. The absolute values of $\beta_b$ and $\beta_{\text{int},0,1}$ increase with the electric field $E_z$ in the region from $E_z = 0$ up to $E_z \sim U_0\kappa_0/e$. At small electric fields, the contributions to $\beta$ depend on the electric field $E_z > 0$ as[2]

$$\beta_b \sim (E_z)^{2/3}, \quad \beta_{\text{int},0} \sim E_z, \quad \beta_{\text{int},1} \sim E_z. \tag{16}$$

In large electric fields, $E_z > U_0\kappa/e$, the energy level $E_0$ becomes resonant. This is illustrated in Fig. 2(b) by blurring and broadening of the graphic lines.

To extract the interface parameters in the one-band Hamiltonian (8), we fit the dependence $\beta(a)$ obtained in the tight-binding calculations for the electric field $E_z = 10^5$ V/cm with the analytical dependence (10) using the least-squares method. We take into account that the bulk spin-orbit Dresselhaus parameter $\gamma$ is different in the well and in the barrier regions of the heterostructure, thereby fixing the ratio of the spin-orbit bulk parameters in the well and in the barrier: $\gamma_b/\gamma_w = 0.7$. From Fig. 3(a) it is seen that as calculated in the tight-binding approximation, dependence $\beta(a)$ is very well reproduced by the analytical formula (10) with the three fitting parameters $\gamma = \gamma_w$, $\xi$, and $\zeta$. From the fitting procedure we obtain the following values of the bulk and interface parameters: $\gamma = \gamma(\text{GaAs}) = -23$ eV Å$^3$, $\xi = -1.5$ eV Å$^3$, $\zeta = 6.5 \times 10^{-6}$ eV Å$^2$. This result for the coefficient $\xi$ corresponds by the order of magnitude to the estimations of $\xi$ within the multiband $\mathbf{k}\cdot\mathbf{p}$ Hamiltonians performed in Refs. [20,50]. The obtained value of $\gamma$(GaAs) is consistent with the value usually accepted in the literature [7,32]. Existence of the terms $\hat{H}_{\text{int},0,v}$ and the magnitude of $\zeta$ appear to be pertinent to the discussion of GaAs quantum wells.

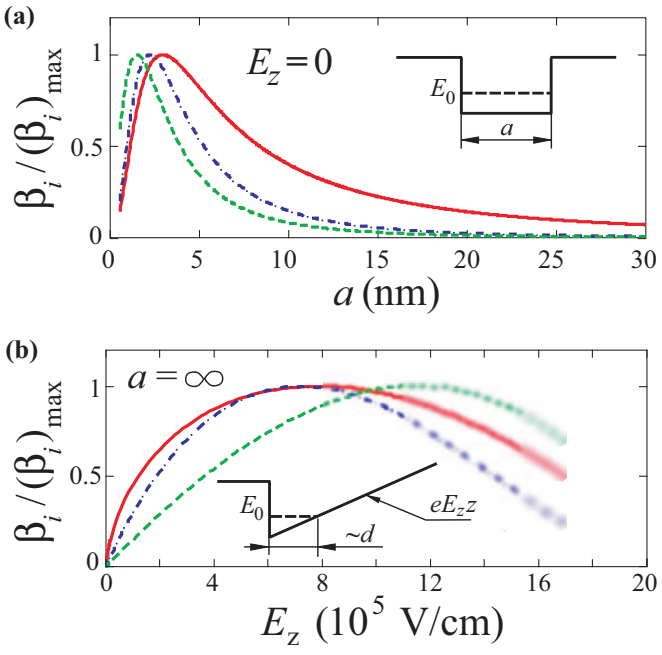



FIG. 2. Different contributions $\beta_i$, $i = b$, (int,0), (int,1), to the anisotropic part of the 2D electron spin-orbit interaction (a) as functions of the quantum well width for zero electric field and (b) as functions of electric field for the infinitely large quantum well width. Red solid lines correspond to the bulk contribution $\beta_b$, blue dash-dot and green dash lines correspond to the interface contributions $\beta_{\text{int},0}$ and $\beta_{\text{int},1}$.

[1]The asymptotic behavior $\beta_b \sim \langle k_z^2\rangle \sim a^2$ at $a \to 0$ may be hardly seen in tight-binding calculations, as the dependence $\langle k_z^2\rangle(a)$ starts to deviate from $a^2$ at widths $\sim 3$ Å and for thicker quantum wells the dependence is close to linear.

[2]Note that the electric field in infinitely wide quantum wells cannot be treated perturbatively as long as the perturbation approach relies on the inequality $eE_z a \ll U_0$, which is not satisfied for very wide quantum wells.

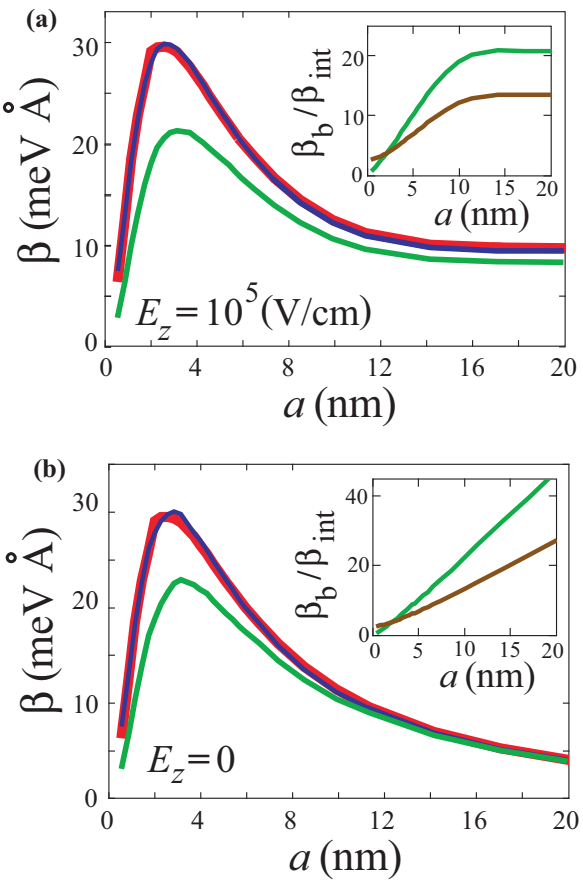



FIG. 3. 2D electron spin splitting parameter $\beta$ as a function of the quantum well width. Panel (a) presents $\beta$ for the electric field $E_z = 10^5$ V/cm, while panel (b) corresponds to $E_z = 0$. Red and blue lines demonstrate the results of calculations within the tight-binding approach and the one-band approach, respectively. Green curves show the bulk contributions $\beta_b$ to the one-band result for $\beta$. Insets present the ratios $\beta_b/\beta_{\text{int},0}$ (brown curve) and $\beta_b/\beta_{\text{int},1}$ (green curve).

We also check that for the obtained parameters $\gamma$, $\xi$, and $\zeta$ the analytical one-band dependencies $\beta(a)$ for the electric field $E_z$ in the interval from 0 up to $10^5$ V/cm reproduce the results of the tight-binding calculations of $\beta(a)$. In Fig. 3(b) we compare the results of the tight-binding calculations with the analytical one-band results for $E_z = 0$. The agreement is perfect, without changing the parameters $\gamma$, $\xi$, and $\zeta$. This proves that the description of the electron spin-orbit interaction in GaAs quantum wells with abrupt interfaces within the one-band Hamiltonians (7) and (8) is adequate. It is clear from Fig. 3 that the bulk contribution dominates for the wide wells, while for the narrow wells the bulk and the interface contributions have the same order.

The functional dependencies of the bulk and the interface contributions are quite similar. Thus, below we discuss in details the possibility to distinguish them.

To this end, we draw the parametric plots $(\beta_b, \beta_{\text{int,j}})$ as a function of quantum well parameters. The regions in these plots where the parametric curve may be approximated with the straight line starting at the origin indicate the intervals of the parameters where it is hard to distinguish the bulk and interface

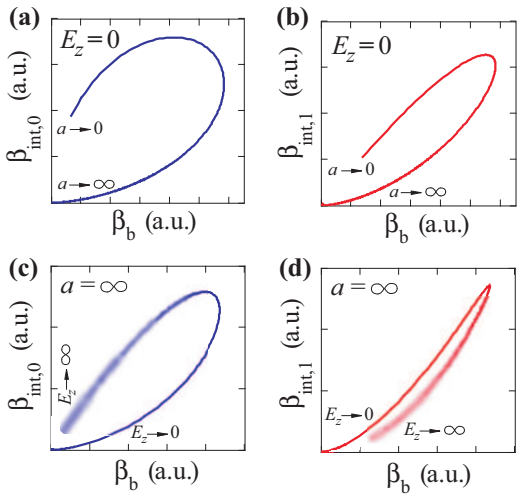



FIG. 4. Parametric plots of the bulk $\beta_b$ and the interface $\beta_{\text{int,j}}$, $j = 0,1$, contributions to the anisotropic part of the 2D electron spin-orbit interaction. Panels (a) and (b) demonstrate the positions of the points $(\beta_b, \beta_{\text{int,j}})$ at zero electric field using quantum well width $a$ as a parameter. Panels (c) and (d) show the positions of $(\beta_b, \beta_{\text{int,j}})$ for the infinitely large quantum well width using electric field $E_z$ as a parameter.

contributions as long as they are approximately proportional each other. In contrast, the regions where this curve is directed perpendicular to the straight line starting at the origin are most favorable for the measurement of the relative strength of different contributions.

In Figs. 4(a) and 4(b) we show parametric plots $(\beta_b, \beta_{\text{int},0})$ and $(\beta_b, \beta_{\text{int},1})$ at zero electric field $E_z = 0$ using the quantum well width $a$ as a parameter. We see that all contributions $\beta_{\text{int},0}(a)$, $\beta_{\text{int},1}(a)$, and $\beta_b(a)$ are almost proportional in the wide intervals of the values of quantum well width $a$. There is relatively small region of quantum well widths $a$ where the contributions are easy to distinguish, around the position of maximum for the bulk contribution $\beta_b$. This implies that if we have in hand the experimental or the numeric (e.g., tight-binding) dependence $\beta(a)$ of the total spin splitting, which has some uncertainty $\delta\beta(a)$, we can establish the relative magnitudes of the bulk $\beta_b(a)$ and the interface $\beta_{\text{int},0,1}(a)$ contributions in this dependence $\beta(a)$ only for rather small values of the uncertainty, $\delta\beta(a) \ll \beta(a)$.

In Figs. 4(c) and 4(d) we present the parametric plots $(\beta_b, \beta_{\text{int},0})$ and $(\beta_b, \beta_{\text{int},1})$ for the infinitely wide quantum well using the value of the electric field $E_z$ as a parameter varying from zero to $\sim U_0\kappa/e$. It is clear from the plot, that the functions $\beta_b(E_z)$, $\beta_{\text{int},0}(E_z)$, and $\beta_{\text{int},1}(E_z)$ are almost linearly dependent.

## V. CONCLUSION

In conclusion, we show that the results of atomistic calculations of spin splittings of the 2D electron spectrum in GaAs quantum wells can be perfectly described in the framework of a one-band effective-mass model by adding the two interface spin-orbit terms in the one-band Hamiltonian. The developed one-band description allows us to conclude that the interface-induced anisotropy contributes significantly

to the value of the spin-orbit Dresselhaus parameter $\beta$ in the 2D electron Hamiltonian.

Our calculations are made within the one-electron picture which is suitable for low densities of 2D electrons. We demonstrated that separation of the bulk and the interface contributions to the spin splittings in experiments is complicated by the fact that all these contributions have very similar functional dependencies on the quantum well width and the applied electric field. However, based on qualitative arguments, we expect that this is not the case for the quantum wells with high electron densities in which the 2D electron charge significantly affects the profile of the heterostructure potential $U(z)$. Due to the Coulomb repulsion, electrons are "pushed" from the center of quantum well to the regions near the interfaces (see, for example, Ref. [24]). Therefore the significance of the interface effects substantially increases and depends on the 2D electron density.

In quantum wells with nonzero electron densities there also exists a contribution to the observed magnitude of the spin-orbit interaction from the electron-electron interaction [51]. The strength of the corresponding renormalization of the constant $\beta$ depends on the geometry of the quantum well and the electron density. This fact further complicates the interpretation of the experimental data on the absolute value of the spin-orbit coupling in quantum wells.

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