# Least-action principle for envelope functions in abrupt heterostructures

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We apply the envelope function approach to abrupt heterostructures starting with the least-action principle for the microscopic wave function. The interface is treated nonperturbatively, and our approach is applicable to mismatched heterostructure. We obtain the interface connection rules for the multiband envelope function and the multiband heterostructure Hamiltonian from the $\boldsymbol{k}\cdot\boldsymbol{p}$ version of the variational principle. The $\boldsymbol{k}\cdot\boldsymbol{p}$ heterostructure Hamiltonian contains the short-range interface terms which consist of two physically distinct contributions. The first one depends only on the structure of the interface, and the second one is completely determined by the bulk parameters. We discover new structure inversion asymmetry terms and new magnetic energy terms important in spintronic applications.

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## I. INTRODUCTION

The envelope function method is a powerful tool which has been widely used to describe and predict various effects in semiconductors. It is normally applicable to materials with translation invariance (allowing for the expansion of the wave function into Bloch functions) and to slowly varying potentials. There are two competing approaches to extending this method to abrupt heterostructures[1] taking into account interface-related effects. The first one is to impose appropriate boundary conditions (interface connection rules) on the envelope wave function at the interface.[2–6] Another possibility is deriving the exact envelope function differential equations which are valid near the interface and which contain the interface-related terms.[7–9] The second approach is more detailed, and it requires a lot more information on the microscopic structure of the interface. Up to now, it has only been applied to the lattice-matched heterostructures where the interface is considered as a small perturbation of a reference periodic crystal (see Ref. 7 for details and review). In this case, it has been shown[1] that connection rules and differential equations are equally valid representations of the interface behavior.

In this paper, we present an extension of the envelope function method which allows to construct the heterostructure Hamiltonian without treating the interface as a small perturbation. It turns out that the best approach to the problem is via the Lagrangian variational principle which encodes the Schrödinger equation. The advantage of this method is that both the Hamiltonian and the boundary conditions at the interface are contained in the averaged variational functional. The resulting $\boldsymbol{k}\cdot\boldsymbol{p}$ heterostructure Hamiltonian coincides with the ordinary $\boldsymbol{k}\cdot\boldsymbol{p}$ Hamiltonians on two sides of the interface. In addition, it contains short-range interface (SRI) terms which are the main subject of our study. We show that the SRI terms consist of two physically distinct contributions. The first one is represented by the Hermitian interface matrix. Its components are directly connected to the boundary conditions for the envelope functions[2] and they are determined by the microscopic structure of the interface. The second contribution is completely determined by the bulk parameters of the materials. It includes new structure inversion asymmetry (SIA) terms and new SRI magnetic terms that are additional to the well-known Rashba SIA terms and to the macroscopic magnetic terms, respectively. Taking them into account is important for various mechanisms of spin polarization, spin filtering, and spin manipulation which play a key role in semiconductor spintronic applications.[10]

The paper is organized as follows. In Sec. II we introduce the $\boldsymbol{k}\cdot\boldsymbol{p}$ variational principle, derive the $\boldsymbol{k}\cdot\boldsymbol{p}$ heterostructure Hamiltonian and the boundary conditions at the interface. In Sec. III we illustrate our method by several examples. Section IV is devoted to the effects of the external magnetic field. We summarize the results in Sec. V.

## II. DERIVATION OF THE $k\cdot p$ VARIATIONAL PRINCIPLE

In this section we consider a model of a semiconductor heterostructure made of two homogeneous semiconductor layers $A$ and $B$ of characteristic length $L$. The layers are joined by a thin boundary region $\Pi$ of the width $d \approx a_A, a_B \ll L$ (see Fig. 1), where $a_A(a_B)$ is the lattice constant in the bulk material $A(B)$, respectively. We work in the single electron approximation, and we denote by $U(\boldsymbol{r})$ the effective po-

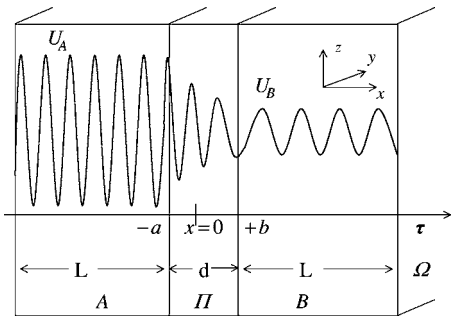


FIG. 1. Sketch of the planar heterointerface between $A$ and $B$ semiconductor layers. $\Pi$ denotes the boundary region. $U_A(U_B)$ is the crystal potential in $A(B)$.

 

tential for electrons. $U(\boldsymbol{r})$ coincides with periodic crystal potentials $U_{A,B}(\boldsymbol{r})$ inside the bulklike regions $A$ and $B$, respectively. To focus on the effects caused by the abruptness of the interface, we do not include any additional long-range interface-induced potentials in our microscopic model.

We start with the microscopic Lagrangian variational principle which encodes the stationary single electron Schrödinger equation. The corresponding Lagrangian density is of the form,

$$\mathcal{L}(\Phi^*,\Phi) = (E - U(\boldsymbol{r}))|\Phi(\boldsymbol{r})|^2 - \frac{\hbar^2}{2m_0}|\nabla\Phi|^2. \tag{1}$$

Here $m_0$ is the free electron mass and $\Phi$ is the microscopic spinor wave function. To simplify the presentation we first neglect the spin-orbit terms in Eq. (1). The variational principle reads,

$$\delta\mathcal{S} = \delta\int_{\Omega} \boldsymbol{d}^3\boldsymbol{r}\mathcal{L}(\Phi^*,\Phi) = 0, \tag{2}$$

where $\delta\Phi$ and $\delta\Phi^*$ are independent variations which vanish at the outer boundaries of the integration region $\Omega = A + \Pi + B$. The variational principle implies the microscopic Schrödinger equation $\hat{H}_{\text{micro}}\Phi(\boldsymbol{r}) = E\Phi(\boldsymbol{r})$ with the Hamiltonian $\hat{H}_{\text{micro}} = (\hat{\boldsymbol{p}}^2/2m_0 + U(\boldsymbol{r}))$, where $\hat{\boldsymbol{p}} = -i\hbar\boldsymbol{\nabla}$ is the momentum operator. The microscopic probability flux density $\boldsymbol{j} = (\Phi^*(\boldsymbol{r})\hat{\boldsymbol{p}}\Phi(\boldsymbol{r}) + \hat{\boldsymbol{p}}^*\Phi^*(\boldsymbol{r})\Phi(\boldsymbol{r}))/2m_0$ is conserved: $\boldsymbol{\nabla}\boldsymbol{j} = 0$, the microscopic wave function $\Phi$ is continuous everywhere in the heterostructure.

It is our aim to pass from the description in terms of the microscopic wave function $\Phi$ to the envelope function approximation. To this end, we use expansions $\Phi(\boldsymbol{r}) = \Sigma\Psi_n^{A,B}(\boldsymbol{r})u_n^{A,B}$ within two bulklike regions $A$ and $B$, respectively. Here the Bloch functions at extremum points of the bulk energy band structure $u_n^{A,B}$ represent the complete basis in $A$ and $B$, respectively, and the envelope functions $\Psi_n^{A,B}(\boldsymbol{r})$ are smooth in the $A$ and $B$ regions. We do not define any basis functions and do not use any expansion for $\Phi$ in the boundary region $\Pi$. We restrict the $\boldsymbol{k}\cdot\boldsymbol{p}$ approximation by direct consideration of $N_A$ ($N_B$) components of the envelope function, which satisfy matrix Schrödinger equations

$$\hat{H}^{A,B}(\hat{\boldsymbol{k}})\Psi^{A,B}(r) = E\Psi^{A,B}(\boldsymbol{r}) \tag{3}$$

in $A$ ($B$) regions. Here $\hat{H}^{A,B} = \hat{C} + \hbar\hat{B}^{\mu}\hat{k}_{\mu} + \hbar^2\hat{D}^{\mu\nu}\hat{k}_{\mu}\hat{k}_{\nu}$ are the standard $\boldsymbol{k}\cdot\boldsymbol{p}$ Hamiltonians including the terms up to the second order in the wave vector operator $\hat{\boldsymbol{k}} = -i\boldsymbol{\nabla}$. The matrices $\hat{C}$, $\hat{B}^{\mu}$, and $\hat{D}^{\mu\nu}$ ($\mu,\nu = x,y,z$) are Hermitian $N_{A,B}\times N_{A,B}$ tensors of rank 0, 1, and 2, respectively. The Hamiltonians $\hat{H}^{A,B}$ give a direct description of the $N_{A,B}$ basic bands as well as the contributions of other remote bands in the second order of perturbation theory.[11] We assume that the $N_A$ ($N_B$) solutions of Eq. (3) give a satisfactory description of the bulk energy structure of $A$ ($B$) material in the range of energies $E$ that is of interest to our heterostructure problem. Note that symmetry of the materials and the number of basic bands $N_A$, $N_B$ in the $\boldsymbol{k}\cdot\boldsymbol{p}$ approximation can be different on two sides of the interface. Moreover, parameters of bulk Hamiltonians $\hat{H}^{A,B}$ can vary significantly across the interface which cannot be treated as a weak perturbation of the bulk problem.

In order to derive the $\boldsymbol{k}\cdot\boldsymbol{p}$ version of Lagrangian variational principle, we represent the variation of the action $\delta\mathcal{S}[\delta\Phi^*]$ as $\delta\mathcal{S} = \delta\mathcal{S}_A + \delta\mathcal{S}_B + \delta\mathcal{S}_{\Pi}$, where $\delta\mathcal{S}_{A,B} = \delta\int_{A,B}\boldsymbol{d}^3\boldsymbol{r}\mathcal{L}(\Phi^*,\Phi) = \delta\int_{A,B}d^3\boldsymbol{r}\mathcal{L}_{A,B}(\Psi^*,\Psi)$ and $\delta\mathcal{S}_{\Pi} = \delta\int_{\Pi}\boldsymbol{d}^3\boldsymbol{r}\mathcal{L}(\Phi^*,\Phi)$. The bulk multiband Lagrangian densities $\mathcal{L}_{A,B}(\Psi^*,\Psi)$ are obtained from the microscopic Lagrangian by averaging over the unit cells in $A$ and $B$, respectively, with taking into account the direct interaction of the $N_{A,B}$ basic bands and the contributions of other remote bands in the second order of perturbation theory. They have the form:

$$\begin{aligned}\mathcal{L}(\Psi^*,\Psi) = E|\Psi|^2 - \Psi^*\hat{C}\Psi - \frac{\hbar^2}{2}\nabla_{\mu}\Psi^*\hat{A}^{\mu\nu}\nabla_{\nu}\Psi \\ - \frac{i\hbar}{2}(\boldsymbol{\nabla}\Psi^*\hat{B}\Psi - \Psi^*\hat{B}\boldsymbol{\nabla}\Psi) \\ + \frac{\hbar^2}{2}\boldsymbol{\nabla}\Psi^*\cdot[\hat{\boldsymbol{K}}\times\boldsymbol{\nabla}\Psi].\end{aligned} \tag{4}$$

Here $\hat{A}^{\mu\nu} = \hat{D}^{\mu\nu} + \hat{D}^{\nu\mu}$, $\hat{K}^{\eta} = \varepsilon_{\eta\mu\nu}\hat{D}^{\mu\nu}$, $\eta,\mu,\nu = x,y,z$ and $\varepsilon_{xyz}$ is Levi-Civita anti-symmetric tensor.

Let us first focus on the contribution of the boundary region $\Pi$. Integrating by parts $\delta\mathcal{S}_{\Pi}$ we arrive at

$$\delta\mathcal{S}_{\Pi}[\delta\Phi^*] = -\int_{\Pi}\boldsymbol{d}^3\boldsymbol{r}[\delta\Phi^*(\hat{H}_{\text{micro}} - E)\Phi] + \delta\mathcal{S}_{\text{sur}}(\Pi), \tag{5}$$

$$\mathcal{S}_{\text{sur}} = \frac{\hbar^2}{2m_0}\int d^2\boldsymbol{\rho}[\Phi^*(A)\Phi'(A) - \Phi^*(B)\Phi'(B)]. \tag{6}$$

Here $\boldsymbol{\rho} = (y,z)$, $\Phi' = \boldsymbol{\tau}\cdot\boldsymbol{\nabla}\Phi$, where $\boldsymbol{\tau}$ is the normal vector to the interface, and $\Phi(B) = \Phi(b,\boldsymbol{\rho})$ and $\Phi(A) = \Phi(-a,\boldsymbol{\rho})$ are the values of $\Phi$ at the edges $x = b$ and $x = -a$, respectively, of the boundary region $\Pi$ (see Fig. 1). As the microscopic function $\Phi$ is an exact solution of the microscopic Schrödinger equation in $\Pi$ we have $\delta\mathcal{S}_{\Pi} = \delta\mathcal{S}_{\text{sur}}$. Using a microscopic transfer matrix model[12] one can express $\mathcal{S}_{\text{sur}}$ as $\mathcal{S}_{\text{sur}}(\Pi) = \Phi^*(A)\times(\Pi_a\Phi(A) + \Pi_{ab}\Phi(B)) + \Phi^*(B)(\Pi_{ab}^*\Phi(A) + \Pi_b\Phi(B))$, where the microscopic interface matrix

$$\hat{T}_{\text{sur}}^{\text{micro}} = \begin{pmatrix}\Pi_a & \Pi_{ab}\\ \Pi_{ab}^* & \Pi_b\end{pmatrix} \tag{7}$$

is Hermitian. The same result can be expressed via a quadratic form of envelopes $\mathcal{S}_{\text{sur}}(\Pi) = \Psi_n^{a*}(\hat{T}_{n\mu}^{A}\Psi_{\mu}^{a} + \hat{T}_{nm}\Psi_m^b) + \Psi_m^{b*}(\hat{T}_{m\mu}^{*}\Psi_{\mu}^{a} + \hat{T}_{m\nu}^{B}\Psi_{\nu}^{b})$, where $\Psi^a = \Psi^A(-a,\boldsymbol{\rho})$ and $\Psi^b = \Psi^B(b,\boldsymbol{\rho})$, $n,\mu = 1,2\ldots N_A$, $m,\nu = 1,2\ldots N_M$, and

$$\hat{T}_{\text{sur}} = \begin{pmatrix}\hat{T}^A & \hat{T}\\ \hat{T}^* & \hat{T}^B\end{pmatrix} = \frac{\hbar^2}{2m_0}\begin{pmatrix}\hat{t}^A/a & \hat{t}/d\\ \hat{t}^*/d & \hat{t}^B/b\end{pmatrix} \tag{8}$$

is a Hermitian $(N_A + N_B)\times(N_A + N_B)$ interface matrix. In general, parameters of $\hat{T}_{\text{sur}}^{\text{micro}}$ may depend on the electron energy. However, the key condition for the validity of the $\boldsymbol{k}\cdot\boldsymbol{p}$ modeling of the heterosctucture is the possibility to neglect the

contribution of the boundary region $\Pi$ in the charge conservation law[2] by taking $d/dt\int_\Pi \boldsymbol{d}^3\boldsymbol{r}|\Phi|^2 \approx 0$. In turn, the charge conservation in $\Pi$ for arbitrarily state of the system is equivalent to the condition $\int_\Pi \boldsymbol{d}\boldsymbol{\pi}\boldsymbol{j} \approx 0$, where $\boldsymbol{\pi}$ is the inner surface of the boundary region $\Pi$. As a consequence, the energy dependence of the microscopic interface matrix $\hat{T}_{\rm sur}^{\rm micro}$ is to be negligible in the range of energies where the $\boldsymbol{k}\cdot\boldsymbol{p}$ modeling of the heterosctucture is valid. Under this condition, the resulting $\boldsymbol{k}\cdot\boldsymbol{p}$ interface matrix $\hat{T}_{\rm sur}$ is energy independent. The structure of $\hat{T}_{\rm sur}$ depends on the symmetry of both bulk materials and of the interface. It can be constructed by using the method of invariants[7,11] or calculated directly via the microscopic modeling of the potential $U(r)$ in the interface region $\Pi$.

The $\boldsymbol{k}\cdot\boldsymbol{p}$ version of Lagrangian variational principle has the form $\delta\mathcal{S}_{\mathbf{kp}}=\delta\mathcal{S}_A+\delta\mathcal{S}_B+\delta\mathcal{S}_{\rm sur}=0$, and it contains $\tilde{N}=N_A+N_B$ independent variations of the envelope wave functions $\delta\Psi_n^A, \delta\Psi_n^B$. We rewrite the surface contribution to the variation of action as $\delta\mathcal{S}_{\rm sur}=\delta\Psi_n^{a*}(\hat{T}_{n\mu}^A\Psi_\mu^a+\hat{T}_{nm}\Psi_m^b)+\delta\Psi_m^{b*}(\hat{T}_{m\mu}^*\Psi_\mu^a+\hat{T}_{m\nu}^B\Psi_\nu^b)=\delta\int_\Pi \boldsymbol{d}^3\boldsymbol{r}\,\delta(x)\mathcal{L}_{\rm sur}$, where $\delta(x)$ is the Dirac delta-function. The surface Lagrangian is nonlocal and it is written as

$$\mathcal{L}_{\rm sur}=\tilde{\Psi}^*\hat{T}_{\rm sur}\tilde{\Psi},\quad \tilde{\Psi}=\begin{pmatrix}\Psi^A(x-a,\boldsymbol{\rho})\\ \Psi^B(x+b,\boldsymbol{\rho})\end{pmatrix}. \tag{9}$$

The effective Lagrangians $\mathcal{L}_{A,B}$ together with $\mathcal{L}_{\rm sur}$ contain all the relevant information about the bulk and interface properties of the heterostructure. Application of the least action principle $\delta\mathcal{S}_{\mathbf{kp}}=0$ generates the Schrödinger equation $\hat{H}_{AB}\tilde{\Psi}=E\tilde{\Psi}$ with the complete heterostructure $\boldsymbol{k}\cdot\boldsymbol{p}$ Hamiltonian $\hat{H}_{AB}$ and with the general boundary conditions (GBC) to be imposed on $\Psi^a=\Psi^A(-a,\boldsymbol{\rho})$ and $\Psi^b=\Psi^B(b,\boldsymbol{\rho})$. For example, integration by parts of $\delta\mathcal{S}_A$ leads to

$$\delta\mathcal{S}_A[\delta\Psi_n^{A*}]=-\int_A \boldsymbol{d}^3\boldsymbol{r}[\delta\Psi_n^{A*}(\hat{H}_{nm}^A-E)\Psi_n^A]+\int d^2\boldsymbol{\rho}\,\delta\Psi_n^{a*}\left(\boldsymbol{\tau}\cdot\frac{\partial\mathcal{L}_A}{\partial\boldsymbol{\nabla}\Psi_n^{a*}}\right). \tag{10}$$

The GBC can be written as

$$\begin{pmatrix} i\hat{V}_\tau\Psi^a\\ -i\hat{V}_\tau\Psi^b\end{pmatrix}=\frac{2\hat{T}_{\rm sur}}{\hbar}\begin{pmatrix}\Psi^a\\ \Psi^b\end{pmatrix}, \tag{11}$$

or, alternatively, in the form of Ref. 2 as

$$\begin{pmatrix}\Psi^a\\ i\hat{V}_\tau\Psi^a\end{pmatrix}=\hat{T}_{\rm tr}\begin{pmatrix}\Psi^b\\ i\hat{V}_\tau\Psi^b\end{pmatrix}. \tag{12}$$

Here the components of the $2N_A\times 2N_B$ transfer matrix $\hat{T}_{\rm tr}$ (see Refs. 2 and 3) can be readily expressed via the components of the surface matrix $\hat{T}_{\rm sur}$ (see also Ref. 13), $\hat{V}_\tau=\boldsymbol{\tau}\cdot\hat{\boldsymbol{V}}$, and the envelope velocity operator $\hat{\boldsymbol{V}}_{nm}\Psi_m=2i/\hbar(\partial\mathcal{L}/\partial\boldsymbol{\nabla}\Psi_n^*)$ can be explicitly written as

$$\hat{\boldsymbol{V}}=\hat{\boldsymbol{B}}+\hbar\frac{\partial\hat{A}^{\mu\nu}\{\hat{k}_\mu\hat{k}_\nu\}}{\partial\boldsymbol{k}}-\hbar[\hat{\boldsymbol{K}}\times\hat{\boldsymbol{k}}]. \tag{13}$$

The last term is new in comparison to Ref. 2. The corresponding extra term in the envelope flux density $\boldsymbol{J}(\boldsymbol{r})=\frac{1}{2}(\Psi_n^*\hat{\boldsymbol{V}}_{nm}\Psi_m+\Psi_n(\hat{\boldsymbol{V}}_{nm}\Psi_m)^*)$ is proportional to $\boldsymbol{\nabla}(\Psi^*\hat{\boldsymbol{K}}\Psi)$ and does not alter the continuity property $\boldsymbol{\nabla}\cdot\boldsymbol{J}=0$. It is straightforward to verify that $J_\tau^{\alpha\beta}=\boldsymbol{\tau}\cdot\boldsymbol{J}^{\alpha\beta}(\boldsymbol{r})=\frac{1}{2}(\Psi_n^{\alpha*}\hat{\boldsymbol{V}}_{nm}\Psi_m^\beta+\Psi_n^\beta(\hat{\boldsymbol{V}}_{nm}\Psi_m^\alpha)^*)=\text{const}$, where $\alpha$ and $\beta$ label two functions $\Psi_\alpha$ and $\Psi_\beta$ satisfying the same GBC (see Ref. 2). This ensures that the heterostructure $\boldsymbol{k}\cdot\boldsymbol{p}$ Hamiltonian $\hat{H}_{AB}$ acting on $\tilde{\Psi}$ is self-adjoint. It has the form:

$$\hat{H}_{AB}=\begin{pmatrix}\hat{H}_h^A+\delta(x)\hat{H}_{\rm sri}^A & \delta(x)\hat{H}_{\rm sri}^{AB}\\ \delta(x)\hat{H}_{\rm sri}^{BA} & \hat{H}_h^B+\delta(x)\hat{H}_{\rm sri}^B\end{pmatrix}, \tag{14}$$

where $\hat{H}_h^A=\Theta(-x)\hat{H}^A(\boldsymbol{\rho},x-a)$, $\hat{H}_h^B=\Theta(x)\hat{H}^A(\boldsymbol{\rho},x+b)$, $\Theta(x)$ is the Heaviside step function and

$$\hat{H}_{\rm sri}^A=\frac{\hbar}{2}\left(i\hat{V}_\tau^A-\frac{\hbar}{m_0a}\hat{t}_a\right),\quad H_{\rm sri}^{AB}=-\frac{\hbar^2}{2m_0d}\hat{t},$$

$$\hat{H}_{\rm sri}^B=\frac{\hbar}{2}\left(-i\hat{V}_\tau^B-\frac{\hbar}{m_0b}\hat{t}_b\right),\quad H_{\rm sri}^{BA}=-\frac{\hbar^2}{2m_0d}\hat{t}^*. \tag{15}$$

We see that there are two physically distinct contributions to the short-range interface (SRI) terms of the Hamiltonian $\hat{H}_{AB}$. The first one arises from the nonlocal surface Lagrangian $\mathcal{L}_{\rm sur}$ and it depends on the properties of the interface via the energy independent parameters of the GBC. The other contribution comes from the velocity operator $\hat{V}_\tau$. It is entirely determined by the bulk parameters and it arises from the nonvanishing variation of the bulk Lagrangians $\mathcal{L}_{A,B}$ at the interface. The important feature of this contribution is the presence of the asymmetric $\hat{\boldsymbol{K}}$ term. In homogeneous semiconductors the asymmetric $\hat{\boldsymbol{K}}$ term does not contribute to $\hat{H}$ in the absence of external fields.[7,14] Examples below demonstrate that the $\hat{\boldsymbol{K}}$ terms in the Lagrangian of Eq. (4) and in the velocity operator of Eq. (13) become important if the symmetry is broken due to the presence of external fields or asymmetric interfaces.

## III. APPLICATIONS OF THE $k\cdot p$ VARIATIONAL METHOD

### A. $\Gamma_6$ conduction band

We consider the effective mass Hamiltonian $\hat{H}(\Gamma_6)=E_c+\hbar^2\hat{k}^2/2m$ for the spinor envelope function $\Psi_\alpha$ ($\alpha=\pm 1/2$), where $E_c$ is the bottom of the conduction band and $m$ is the effective mass. Following our method we introduce the effective mass Lagrangian density

$$\mathcal{L}=(E-E_c)|\Psi|^2-\frac{\hbar^2}{2m}|\nabla\Psi(\boldsymbol{r})|^2+\mathcal{L}_{\rm SIA}, \tag{16}$$

which contains the asymmetric term

$$\mathcal{L}_{\mathrm{SIA}}(\Gamma_6) = -\frac{i\hbar^2}{4m_0}\tilde{g}\,\boldsymbol{\nabla}\Psi^*[\boldsymbol{\sigma}\times\boldsymbol{\nabla}\Psi] \tag{17}$$

obtained with $\boldsymbol{K}(\Gamma_6)=-(i\tilde{g}/2m_0)\boldsymbol{\sigma}$, where $\sigma_x$, $\sigma_y$, $\sigma_z$ are Pauli matrices, and $\tilde{g}=g_0-g$ is the difference between the free electron and the effective electron $g$-factors. Note that $\tilde{g}\neq 0$ only if the spin-orbit splitting $\Delta$ of the valence band or $\Delta^c$ of the remote conduction band is taken into account. For $\tilde{g}\neq 0$, the asymmetric term $L_{\mathrm{SIA}}(\Gamma_6)$ produces the magnetic energy term $-\frac{1}{2}\mu_B\tilde{g}(\boldsymbol{\sigma H})$ additional to the free electron magnetic energy $\frac{1}{2}\mu_B g_0(\boldsymbol{\sigma H})$ in the bulk Hamiltonian in external magnetic field $\boldsymbol{H}$. Here $\mu_B$ is the Bohr magneton. To focus on the role of the $L_{\mathrm{SIA}}$ term we neglect in this and other examples the effects of bulk inversion asymmetry.

This is the asymmetric term $L_{\mathrm{SIA}}(\Gamma_6)$ (missing in Refs. 5 and 15) which induces the spin dependence of the velocity operator $\hat{\boldsymbol{V}}=(\hbar/m)\hat{\boldsymbol{k}}-(i\hbar\tilde{g}/2m_0)[\boldsymbol{\sigma}\times\hat{\boldsymbol{k}}]$ and thus the spin dependence of the standard boundary conditions $\Psi^a=\Psi^b$, $\hat{V}_\tau\Psi^a=\hat{V}_\tau\Psi^b$ at the interface. Such spin-dependent boundary conditions were used and discussed, for example, in Refs. 4, 16, and 17. The short-range interface SIA term in the heterostructure Hamiltonian $\hat{H}_{AB}$ of Eq. (14) also results from $L_{\mathrm{SIA}}(\Gamma_6)$.

Moreover, exactly this term $L_{\mathrm{SIA}}(\Gamma_6)$ generates the macroscopic SIA term $\hat{H}^{\mathrm{so}}=\alpha_R[\boldsymbol{\sigma}\times\hat{\boldsymbol{k}}]\boldsymbol{\tau}$, postulated by Rashba[18] for the asymmetric 2D structure. To demonstrate this, we take into consideration the dependence of $g$ on the potential $V=-|e|\mathcal{E}x$, where the average electric field $\boldsymbol{E}=\mathcal{E}\boldsymbol{\tau}$ characterizes the macroscopic asymmetry. In the eight band model for cubic semiconductors $g=g_0-g_r-2E_p\Delta/3(E_g-V)(E_g-V+\Delta)$, where $E_p$ is Kane energy, $E_g$ is the band gap and $g_r$ is the correction from remote bands, and the effective Rashba constant is $\alpha_R\propto \partial g/\partial x|_{x=0}\propto\Delta$. Using the expression for $g$ in the 14 band model one finds that the correction to $\alpha_R$ is proportional to $\Delta^c$.

Let us now discuss the role of $\hat{T}_{\mathrm{sur}}$ for $\Gamma_6$ electrons. The widely used standard boundary conditions $\Psi^a=\Psi^b$, $\hat{V}_\tau\Psi^a=\hat{V}_\tau\Psi^b$ correspond to the limit case of the "ideal" interface described by the surface matrix

$$\hat{T}_{\mathrm{sur}}=\frac{\hbar^2}{2m_0}\begin{pmatrix}\hat{I}_2 t_a/a & \hat{I}_2 t/d\\ \hat{I}_2 t^*/d & \hat{I}_2 t_b/b\end{pmatrix}, \tag{18}$$

where $\hat{I}_2$ is $2\times 2$ unit matrix, $t_a=t_b=-t/2$ are real numbers, and $a=b\to 0$. However, the effect of the different electron effective masses in $A$ and $B$ is of the same order of magnitude as the effect of the band nonparabolicity.[9] The nonparabolicity is caused by the interband interaction and can be taken into account by assuming the energy dependent electron effective mass $m(E)$ and energy dependent electron $g$ factor $g(E)$. The parameters of the interface matrix $t_a$, $t_b$, and $t$ remain energy independent real numbers.[2,19] However, the model of the ideal interface with $a=b\to 0$ and thus the standard boundary conditions can not be used if the interband interaction is taken into account. The width of the interface-induced interband coupling region is estimated as $|a/t_a|=\sqrt{\hbar^2/2E_p^A m_0}$ and $|b/t_b|=\sqrt{\hbar^2/2E_p^B m_0}$ (see Ref. 2). The discontinuity of the envelope function $\Psi^A\neq\Psi^B$ at the interface produces an additional short-range SIA contribution to the spin splitting of 2D electron states.[20,21] Below we discuss this effect in more details for the case of asymmetric square quantum well with infinite potential barriers.

### B. $\Gamma_{15}$ and $\Gamma_8$ valence band

Another useful example is provided by the degenerate valence band at the $\Gamma$ point described by the envelope Hamiltonians obtained in Ref. 14. We consider the cases of $\Delta=0$ and $\Delta\to\infty$. The remarkable property of the respective envelope Lagrangians obtained according to Eq. (4) is the presence of the asymmetric term with $\boldsymbol{K}(\Gamma_{15})=-i(1+3\kappa)/m_0\boldsymbol{I}$ even in the case $\Delta=0$:

$$\mathcal{L}_{\mathrm{SIA}}(\Gamma_{15}) = -\frac{i\hbar^2}{2m_0}(1+3\kappa)\,\boldsymbol{\nabla}\Psi_\alpha^*[\boldsymbol{I}\times\boldsymbol{\nabla}\Psi_\alpha]. \tag{19}$$

Here $\kappa$ is the magnetic Luttinger constant, $\hat{\boldsymbol{I}}$ is the internal angular momentum operator ($I=1$) and $\Psi_\alpha$, $\alpha=0,\pm1$, is the 3 component envelope function. The SIA component of the velocity operator $\hat{\boldsymbol{V}}_{\mathrm{so}}=i\hbar(1+3\kappa)/m_0[\boldsymbol{I}\times\boldsymbol{k}]$ induces a new short range SIA term in the heterostructure Hamiltonian for the $\Gamma_{15}$ holes as well as the $\boldsymbol{I}$-dependent boundary conditions. This leads to the splitting of the heavy hole subband in asymmetric structures mediated by the interaction with light hole states. Note that it is this asymmetric term $L_{\mathrm{SIA}}(\Gamma_{15})$ which is responsible for the magnetic energy term $\propto\mu_B(1+3\kappa)(\boldsymbol{IH})$ in the bulk Hamiltonian of Ref. 14.

In the case of $\Delta\to\infty$, the top of valence band is fourfold degenerate corresponding to the $J=3/2$ subspace of the total internal momentum $\boldsymbol{J}=\boldsymbol{I}+1/2\boldsymbol{\sigma}$. We obtain the asymmetric term in the envelope Lagrangian with $\boldsymbol{K}(\Gamma_8)=-i(2/3+2\kappa)/m_0\boldsymbol{J}-iq/m_0\boldsymbol{F}$, where $q$ is the cubically anisotropic magnetic Luttinger constant and $\boldsymbol{F}=(F_x,F_y,F_z)\equiv(J_x^3,J_y^3,J_z^3)$:

$$\mathcal{L}_{\mathrm{SIA}}(\Gamma_8) = \frac{\hbar^2}{2}\,\boldsymbol{\nabla}\Psi_\alpha^*[\boldsymbol{K}(\Gamma_8)\times\boldsymbol{\nabla}\Psi_\alpha]. \tag{20}$$

Here $\Psi_\alpha$, $\alpha=\pm3/2,\pm1/2$, is the four component envelope wave function. The SIA component of the velocity operator $\hat{\boldsymbol{V}}_{\mathrm{so}}=i\hbar/m_0\left(\left(\frac{2}{3}+2\kappa\right)[\boldsymbol{J}\times\boldsymbol{k}]+q[\boldsymbol{F}\times\boldsymbol{k}]\right)$ produces a new short range SIA term in the heterostructure Hamiltonian as well as the asymmetric contribution to the boundary conditions for the $\Gamma_8$ holes (see Refs. 16 and 22). The very same asymmetric term $L_{\mathrm{SIA}}(\Gamma_8)$ induces the magnetic energy terms $\propto(\boldsymbol{JH})$ and $\propto q(\boldsymbol{FH})$ in the bulk Hamiltonian of Ref. 14, as well as the macroscopic SIA term $H_{8v}^{\mathrm{so}}=\beta_1[\boldsymbol{J}\times\boldsymbol{k}]\boldsymbol{E}+\beta_2[\boldsymbol{F}\times\boldsymbol{k}]\boldsymbol{E}$ postulated recently in Ref. 23. The cubically anisotropic constant $q$ and, consequently, $\beta_2$ are proportional to $\Delta^c$ and usually small. Considering the dependence of $\kappa=\kappa_r+E_p/6(E_g+V)$ on $V=-|e|\mathcal{E}x$, where $\kappa_r$ is the contribution from remote bands, we derive for the first time the effective SIA constant $\beta_1\propto\partial\kappa/\partial x|_{x=0}$ for the $\Gamma_8$ valence band:

$$\beta_1 = \frac{|e|\hbar^2}{6m_0}\frac{E_p}{E_g^2}. \quad (21)$$

We find that in contrast to the Rashba constant, $\beta_1$ is not proportional to the spin-orbit splittings $\Delta$ or $\Delta_c$. For instance, for GaAs we obtain $\beta_1/|e|=15.9$ Å$^2$ while the calculated value of the electron Rasba constant (Ref. 16) in the eight band model is $\alpha_R/(|e|\mathcal{E})=4.4$ Å$^2$.

### C. Asymmetric square quantum well with infinite potential barriers for $\Gamma_6$ electrons

We consider the square quantum well with two interfaces at $x=-L$ and $x=L$ modeled by infinite potential barriers. We assume, however, that these interfaces are microscopically asymmetric. This may occur even when two opposite interfaces are formed by contacts with the same materials (see Refs. 24 and 25). The standard boundary conditions for the infinite potential barrier read $\Psi(\pm L)=0$ and do not allow to take into account the asymmetry of two interfaces. Moreover, the standard boundary conditions fail if the nonparabolicity of electron spectra is taken into account.[2,19]

The Hamiltonian for the $\Gamma_6$ electrons that includes the band nonparabolicity and the short-range interface terms has the form:

$$\hat{H}_{\rm well} = \hat{H}(\Gamma_6) + \frac{i\hbar^2}{2m(E)}[\delta(x-L)-\delta(x+L)]\hat{k}_x - \frac{\hbar^2}{2m_0 a^+}\delta(x-L) - \frac{\hbar^2}{2m_0 a^-}\delta(x+L) + \frac{\hbar^2}{4m_0}[g_0-g(E)] \times [\delta(x-L)-\delta(x+L)][\boldsymbol{\sigma}\times\boldsymbol{k}]_x, \quad (22)$$

where $a^+=a^*/t^+$ and $a^-=a^*/t^-$, $a^*=\sqrt{\hbar^2/2E_p m_0}$ and $t^+$ and $t^-$ are real numbers. We use the expressions for the energy-dependent electron effective mass $m(E)$ and effective $g$-factor $g(E)$ obtained in the eight-band model (see, for example, Ref. 19):

$$\frac{1}{m(E)} = \frac{1}{m_0}\left(\alpha + \frac{E_p}{3}\left[\frac{2}{E_g+E} + \frac{1}{E_g+E+\Delta}\right]\right), \quad (23)$$

$$g(E) = g_0 - g_r - \frac{2E_p}{3}\frac{\Delta}{(E_g+E)(E_g+\Delta+E)}. \quad (24)$$

Here $E$ is calculated from the bottom of the conduction band, $(\alpha-1)$ and $g_r$ are the contributions from the remote bands. The Hamiltonian of Eq. (22) corresponds to the spin-dependent boundary conditions in the form

$$\Psi(\pm L) = \pm a^{\pm}\left(\frac{m_0}{m(E)}\Psi'(\pm L) + \frac{g_0-g(E)}{2}[\boldsymbol{\sigma}\times\boldsymbol{k}]_x\Psi(\pm L)\right). \quad (25)$$

We direct the in-plain wave vector along $y$. Then the solutions of the Hamiltonian Eq. (23) can be written as $\Psi_{\pm 1/2} = \exp(ik_y y)(C^+\exp(ik_n x)+C^-\exp(-ik_n x))v_{\pm 1/2}$, where $v_{\pm 1/2}$ are the eigenspinors of the Pauli matrix $\sigma_z$, and the constants $C^{\pm}$ are to be determined from Eq. (25) and the normalization condition. Neglecting first the spin-orbit term $\propto k_y\sigma_z$ in the boundary conditions of Eq. (25), we find the energy spectrum from the equation

$$\sin(2k_nL)\left[1+\left(\frac{m_0}{m(E)}k_nb\right)^2-\left(\frac{m_0}{m(E)}k_na\right)^2\right] - \left(2\frac{m_0}{m(E)}k_na\right)\cos(2k_nL)=0, \quad (26)$$

where $a=(a^++a^-)/2$, $b=(a^+-a^-)/2$, and $k_n$ is related to the energy $E$ by

$$E = E_n + \frac{\hbar^2k_y^2}{2m(E)}, \quad E_n = \frac{\hbar^2k_n^2}{2m(E)}. \quad (27)$$

In the asymmetric well with $b\neq 0$, the spin-dependent term $\propto k_y\sigma_z$ leads to the spin splitting of the electron states at finite values of the wave vector $k_y\neq 0$. The energies $E^+$ and $E^-$ of the spin-up and spin-down states, respectively, can be found from Eqs. (26) and (27) by replacements $a^{\pm}\to a^{\pm}/(1\pm(g_0-g(E))a^{\pm}k_y/2)$ for $E^+$ and $a^{\pm}\to a^{\pm}/(1\mp(g_0-g(E))a^{\pm}k_y/2)$ for $E^-$, respectively. The splitting $\Delta_{\rm SIA}=E^+-E^-$ between the energies of the spin-up and spin-down states can be described by the effective SIA Hamiltonian

$$\hat{H}_{\rm SIA}^{\rm eff} = \alpha_{\rm SIA}(E)\sigma_z k_y, \quad (28)$$

where $\Delta_{\rm SIA}=2\alpha_{\rm SIA}k_y$. For the small values of $k_y$, the short-range SIA constant is derived by using the perturbation theory as

$$\alpha_{\rm SIA} = \frac{\hbar^2}{4m_0}(g_0-g(E))(|\Psi(-L)|^2-|\Psi(+L)|^2). \quad (29)$$

Using the approximate[19] normalization condition $\int_{-L}^{L}|\Psi|^2dx=1$ we obtain

$$|\Psi(\pm L)|^2 = \frac{4(m_0k_na^{\pm}/m(E))^2}{1+(m_0k_na^{\pm}/m(E))^2}\left[4L - \frac{m_0a^+/m(E)}{1+(m_0k_na^+/m(E))^2} + \frac{m_0a^-/m(E)}{1+(m_0k_na^-/m(E))^2}\right]^{-1}. \quad (30)$$

In Fig. 2 we show the calculated spin splitting energy of the first bound electron state in GaAs quantum well as the function of the well width $2L$. The interface parameter is $a=-a^*=-0.36$ Å, and the asymmetry parameter $t=-b/a=0.25$ for set 1 and $t=0.5$ for set 2. The solid curves calculated for the in-plane wave vector $k_y=0.02$ Å$^{-1}$ and dashed curves for $k_y=0.04$ Å$^{-1}$. One can see, that in the asymmetric quantum well with infinite potential barriers and $|b/a|=0.5$, the spin splitting is of the same order of magnitude as the splitting presented in Ref. 16 for AlAs/GaAs/$Al_{0.15}Ga_{0.85}As$ asymmetric quantum well.

For positive values of the interface parameters $a^{\pm}>0$, the formation of the interface localized Tamm states with $E_n<0$ is possible.[2,20] Recently, the interface localized Tamm states were observed experimentally in the periodic ZnSe/BeTe 2D heterostructures (Ref. 25). The interfaces of the ZnSe quantum well with BeTe barriers are known to be nonequivalent.[25] Therefore, it is instructive to look at the SIA induced splitting of the interface localized states in asymmetric ZnSe quantum well. In Fig. 3 we show the calculated

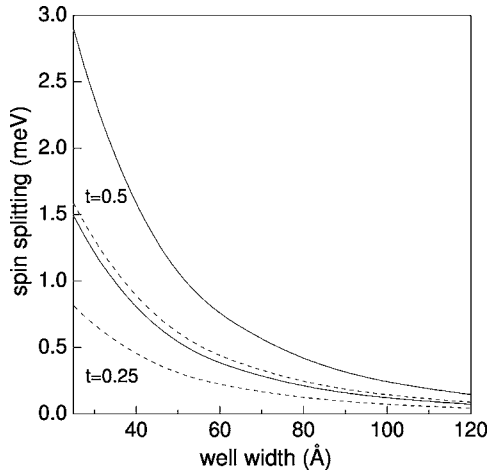


FIG. 2. Structure inversion asymmetry spin splitting energy of the first bound electron state in GaAs asymmetric square well with infinite potential barriers. The interface parameter is $a=-a^*=-0.36$ Å. The asymmetry parameter is $t=-b/a=0.25$ for two lower curves and $t=0.50$ for two upper curves. The solid curves are calculated for the in-plane wave vector $k_y=0.02$ Å$^{-1}$ and dashed curves for $k_y=0.04$ Å$^{-1}$.

energies of the Tamm states at $k_y=0.04$ Å$^{-1}$ in asymmetric ZnSe square well with infinite potential barriers as the function of the asymmetry parameter $t=-b/a$. The well width is $2L=40$ Å and the interface parameter is $a=a^*=0.41$ Å. The spin up states are shown by the solid curves and the spin down states are shown by the dashed curves. The energies of the Tamm states weakly depend on the well width and are close to the asymptotic values, that can be found analytically from Eq. (26) in a wide well which corresponds to $L/a \gg E_p/E_g$.

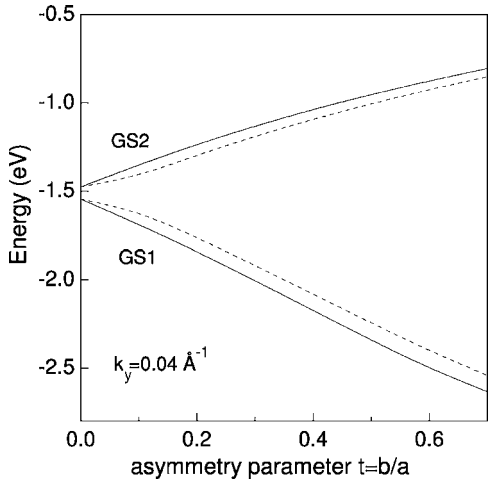


FIG. 3. Energy position of the interface localized Tamm states in ZnSe square well of the width $2L=40$ Å with infinite potential barriers as the function of the asymmetry parameter $t=-b/a$. The interface parameter is $a=a^*=0.41$ Å and the in-plain wave vector is $k_y=0.04$ Å$^{-1}$. The energy is calculated from the bottom of the conduction band. The top of the valence band is at $-E_g=-2.79$ eV. The solid curves are for the spin up states and dashed curves for spin down states.

In the symmetric case $b=0$, the energies of two Tamm states $GS1$ and $GS2$ at $k_y=0$ are very close and described by[2]

$$E_{GS}=-\frac{\hbar^2}{2m_0a^2}\frac{m(E)}{m_0}. \tag{31}$$

For $a=a^*$, the position of $E_{GS}$ is close to the middle of the forbidden gap. When the asymmetry $b\neq 0$ is present, the energies of $GS1$ and $GS2$ become different and their asymptotic values at $k_y=0$ in a wide well are determined from Eq. (26) as

$$E_{GS1}=-\frac{\hbar^2}{2m_0a^{+2}}\frac{m(E)}{m_0}, \quad E_{GS2}=-\frac{\hbar^2}{2m_0a^{-2}}\frac{m(E)}{m_0}. \tag{32}$$

At finite value of $k_y$, the energies of the spin up ($E^+_{GS1}$, $E^+_{GS2}$) and spin down ($E^-_{GS1}$, $E^-_{GS2}$) states become

$$E^{\pm}_{GS1}=-\frac{\hbar^2}{2m_0a^{+2}}\frac{m(E)}{m_0}\left(1\pm\frac{g_0-g(E)}{2}a^+k_y\right)^2+\frac{\hbar^2k_y^2}{2m(E)}, \tag{33}$$

$$E^{\pm}_{GS2}=-\frac{\hbar^2}{2m_0a^{-2}}\frac{m(E)}{m_0}\left(1\mp\frac{g_0-g(E)}{2}a^-k_y\right)^2+\frac{\hbar^2k_y^2}{2m(E)}. \tag{34}$$

One can see, that in the symmetric well with $b=0$, the finite value of $k_y\neq 0$ induces the interaction between $GS1$ and $GS1$ states which also leads to their splitting (see Fig. 3). The asymmetry $b=(a^+-a^-)/2\neq 0$ splits the energies of $E_{GS1}$ and $E_{GS2}$ states at $k_y=0$ and induces the spin splitting of both states $\Delta_{\mathrm{SIA}}(GS1)=E^+_{GS1}-E^-_{GS1}$ and $\Delta_{\mathrm{SIA}}(GS2)=E^+_{GS2}-E^-_{GS2}$ at finite values of $k_y$, so that four Tamm states appear. Since the respective wave functions are localized near the interfaces, the spin splitting is very large, and the perturbation theory cannot be used for evaluation of $\alpha_{\mathrm{SIA}}$. It follows from Eqs. (33) and (34) that the spin splitting of the Tamm states in the wide well is given by $\Delta_{\mathrm{SIA}}(GS1)=2\alpha^+_{\mathrm{SIA}}k_y$ and $\Delta_{\mathrm{SIA}}(GS2)=2\alpha^-_{\mathrm{SIA}}k_y$, where

$$\alpha^{\pm}_{\mathrm{SIA}}=\mp\frac{\hbar^2}{2m_0a^{\pm 2}}\frac{m(E)}{m_0}(g_0-g(E)). \tag{35}$$

We predict the spin-splitting of the interface localized Tamm states in ZnSe/BeTe heterostructures to be about 10–50 times larger than the respective splitting of the bound states in the conduction band.

In the case of the single parabolic band effective mass approximation with $m(E)=m(0)=m$, $g(E)=g(0)=g$, the boundary conditions given by Eq. (25) and the corresponding energy spectra can be directly compared with those presented in Ref. 20. In more details, in Ref. 20 one introduces characteristic momenta $p^{\pm}$ of the surfaces related to the surface parameters $a^{\pm}$ of our model via $p^{\pm}a^{\pm}=-\hbar m/m_0$. In the parabolic case, both $p^{\pm}$ and $a^{\pm}$ do not depend on $E$. The surface parameters $a^{\pm}$ remain energy independent when the nonparabolicity coming from multiband approximation is included [because the Hamiltonian of Eq. (22) is self-adjoint], whereas momenta $p^{\pm}=-\hbar m(E)/m_0a^{\pm}$ become energy dependent. Note that the multiband consideration is crucial for

proper treatment of the spin splitting of both conduction band states (see, for example, Ref. 16) and interface localized Tamm states. The single band model only describes shallow Tamm states with energies close to the conduction band edge,[20] whereas our multiband model successfully describes the Tamm states with energies in the middle of the forbidden gap formed by the conduction band electrons and light holes as well as the large SIA splitting of the Tamm states in the asymmetric wells (see Fig. 3).

## IV. INTERFACE CONTRIBUTION TO THE MAGNETIC ENERGY

The variational principle approach allows a straightforward incorporation of the external magnetic field $\boldsymbol{H}$ into the model. It is included into the bulk Lagrangian of Eq. (4) by adding the magnetic energy term $g_0\mu_B(\boldsymbol{\sigma H})$ in the matrix $\hat{C}$ and by replacing $\boldsymbol{\nabla}\rightarrow\boldsymbol{\nabla}+(i|e|/2\hbar c)[\boldsymbol{H}\times\boldsymbol{r}]$. This procedure produces well-known magnetic energy terms $g_0\mu_B(\boldsymbol{\sigma H})+\mu_B(\hat{\mathbf{K}}\boldsymbol{H})$ in the bulk Hamiltonians. In addition, the developed approach reveals a new short-range magnetic energy term in the heterostructure Hamiltonian $\hat{H}_{AB}$. For example, in the presence of the in-plane external magnetic field $\boldsymbol{H}\|z$ we obtain the new term in the velocity operators $V_\tau\Psi$ which is proportional to $Hx(\hat{K}_z\Psi)$. In small fields this term can be treated perturbatively and the parameters of the interface matrix $\hat{T}_{\mathrm{sur}}$ remain field independent. The short-range contribution to the Zeeman energy is proportional to the sum of discontinuities of $(\Psi^*\hat{K}_z\Psi)$ at the interfaces. Unlike the zero field splitting, this interface magnetic energy contribution is present even in completely symmetric 2D structures as well as in spherical dots (see Ref. 19). For the quantum well considered above in Sec. III C, the interface contribution to the magnetic energy is given by

$$\hat{H}_{\mathrm{sur}}(H)=\tfrac{1}{2}g_{\mathrm{sur}}\sigma_z(\mu_B H), \tag{36}$$

$$g_{\mathrm{sur}}=-(g_0-g(E))(|\Psi(-L)|^2+|\Psi(+L)|^2)L, \tag{37}$$

where the values of $|\Psi(\pm L)|^2$ are determined by Eq. (30). One can see, that even in the symmetric case $a^+=a^-$ there is a nonvanishing surface contribution to the electron $g$ factor

$$g_{\mathrm{sur}}=-(g_0-g(E))\frac{2(m_0k_na/m(E))^2}{1+(m_0k_na/m(E))^2}. \tag{38}$$

Figure 4 shows the dependence of $g_{\mathrm{sur}}$ on the well width $2L$ for the first bound electron state in GaAs quantum well. For the interface localized Tamm states discussed above in Sec. III C the surface contribution to the electron effective $g$-factor is large and cannot be described by Eq. (37). Instead, the modification of the interface parameters $a^+$ and $a^-$ in the magnetic field shall be considered. This consideration will be reported elsewhere.

In large magnetic fields, the magnetic energy term should be directly included into the boundary conditions. This leads to the surface renormalization of the effective $g$ factor for electrons in Landau levels similar to the renormalization suggested previously in Ref. 21 in the framework of the single band effective mass approximation. However, in the multiband approximation the energy dependence of the $g$ factor causes more complicated dependence of the $g$ factor on the surface parameters.[19]

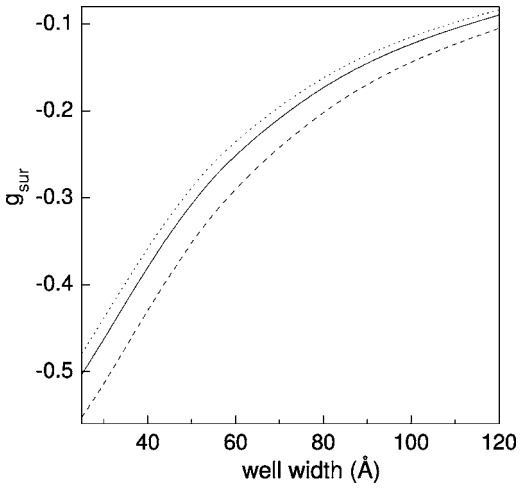


FIG. 4. Surface contribution to the electron $g$-factor in the first bound electron state in GaAs asymmetric square well with infinite potential barriers. The interface parameters are $a=-a^*=-0.36$ Å, $b=0$ for dotted line, $t=-b/a=0.25$ for solid line and $t=0.50$ for dashed line.

## V. DISCUSSION AND CONCLUSION

In conclusion, the variational least action principle allows to consistently extend the envelope function approach to heterostructures with abrupt interfaces. The short-range interface terms in the heterostructure Hamiltonian $\hat{H}_{AB}$ and the general boundary conditions are equally valid representation of the interface properties and can be written for any interface between dissimilar materials including the case $N_A\neq N_B$. For lattice-matched heterostructures ($N_A=N_B=N$) the obtained $\hat{H}_{AB}$ allows direct comparison with previously derived Hamiltonians.[7–9] The discretization of $\hat{H}_{AB}$ for numerical calculations is straightforward and requires no additional symmetrization.

The least action principle approach reveals the origin of two physically distinct contributions to the short-range interface terms of the heterostructure $\boldsymbol{k}\cdot\boldsymbol{p}$ Hamiltonian $\hat{H}_{AB}$. They arise from the nonvanishing variation of the Lagrangian in the boundary region and in the bulklike regions, respectively. The contribution from the boundary region is the only one that depends on the properties of the interface and contains new parameters. These parameters of the interface matrix $\hat{T}_{\mathrm{sur}}$ can be considered as phenomenological parameters of the $\boldsymbol{k}\cdot\boldsymbol{p}$ model additional to the bulk parameters. For instance, the surface parameter for the CdSe spherical nanocrystals was determined from the comparison with experimental data for the electron $g$-factor in Refs. 19 and 26.

Our approach reveals that all macroscopic and short-range interface SIA terms as well as the magnetic energy terms in

$\hat{H}_{AB}$ originate from the asymmetric term $\mathcal{L}_{\mathrm{SIA}}$ in the bulk envelope Lagrangian. This implies, for example, that the short-range SIA terms do not contain any new unknown parameters in contrast to the assumption of Ref. 7. We find that all short-range SIA parameters are directly related to the magnetic parameters (such as effective electron $g$-factor and magnetic Luttinger parameters $\kappa$, $q$) that are known from bulk magneto-optical experiments. The expressions for the macroscopic Rashba parameters, in turn, can be analytically derived from the energy dependent expressions for the short-range SIA parameters. Using this approach, we have derived for the first time the effective Rashba constant for the $\Gamma_8$ holes. Insight into the common origin of all SIA terms and magnetic energy terms explains the well-known analogy between the description of the macroscopic spin-orbit effects and magnetic field effects. The same analogy can be used for the description of the short-range spin-orbit and magnetic field effects. The short-range SIA terms in the heterostructure Hamiltonian are responsible for the interface and surface contributions to the SIA splitting of electron and hole energy levels in asymmetric structures[4,16,17,20] while the short-range magnetic energy terms are responsible for the interface and surface contributions to the electron effective $g$ factor in both symmetric and asymmetric structures.[19,21,27]

The short-range SIA contribution to the zero field splitting becomes more pronounced in the case of the interface between very dissimilar materials. The general Hamiltonian $\hat{H}_{AB}$ given by Eqs. (14)–(16) enables one to describe, for example, an interface-induced $\Gamma/X$ intervalley coupling or interface coupling between $\Gamma_6$ electrons and $\Gamma_8$ holes. It allows to describe SIA effects in types II and III quantum wells and to take into consideration the microscopic asymmetry caused by the nonequivalence of two opposite interfaces. An ultimate case of the interface between two very dissimilar material is given by the semiconductor/dielectric interface modeled by the infinite potential barrier for the electrons. It was suggested in Ref. 17 that the infinite barrier model does not describe the spin splitting of the electrons properly because it neglects the interface contribution to the splitting.[17] In contrast, we have demonstrated that the nonvanishing interface contribution to the spin splitting can be described even in the model of infinite potential barrier. Moreover, using the infinite barrier model we predict an unusually large spin splitting of the interface localized Tamm states which is determined by the interface contribution.

The least action principle approach can also be extended to the case when the microscopic potential $U(\boldsymbol{r})$ contains the long-range contribution that is caused by the presence of the interface but is not localized in the boundary region $\Pi$ of the width $d \ll L$. Such long-range potential can be, for example, the multipole Coulomb potentials or strain. The multipole potentials were considered in Ref. 7 and shown to have no qualitative effect in two-dimensional systems. The strain potentials can be directly incorporated into the bulklike Lagrangians in $A$ and $B$ by using the method of invariants.

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[1] B. A. Foreman, Phys. Rev. Lett. **80**, 3823 (1998).
[2] A. V. Rodina, A. Yu. Alekseev, A. L. Efros, M. Rosen, and B. K. Meyer, Phys. Rev. B **65**, 125302 (2002).
[3] I. V. Tokatly, A. G. Tsibizov, and A. A. Gorbatsevich, Phys. Rev. B **65**, 165328 (2002); M. V. Kisin, B. L. Gelmont, and S. Luryi, *ibid.* **58**, 4605 (1998); C. Aversa and J. E. Sipe, *ibid.* **49**, 14542 (1994).
[4] F. T. Vasko and A. V. Kuznetsov, *Electronic states and optical transitions in semiconductor heterostructures* (Springer, New York, 1999).
[5] Smadar de-Leon, B. Laikhtman, and L. D. Shvartsman, J. Phys.: Condens. Matter **10**, 8715 (1998).
[6] E. L. Ivchenko, A. Yu. Kaminski, and U. Rössler, Phys. Rev. B **54**, 5852 (1996).
[7] B. A. Foreman, Phys. Rev. B **72**, 165345 (2005).
[8] M. G. Burt, J. Phys.: Condens. Matter **4**, 6651 (1992); B. A. Foreman, Phys. Rev. B **54**, 1909 (1996); B. A. Foreman, Phys. Rev. Lett. **81**, 425 (1998).
[9] E. E. Takhtamirov and V. A. Volkov, Semicond. Sci. Technol. **12**, 77 (1997); E. E. Takhtamirov and V. A. Volkov, Zh. Eksp. Teor. Fiz. **116**, 1843 (1999) [JETP **89**, 1000 (1999)].
[10] L. P. Rokhinson, V. Larkina, Y. B. Lyanda-Geller, L. N. Pfeiffer, and K. W. West, Phys. Rev. Lett. **93**, 146601 (2004); M. Khodas, A. Shekhter, and A. Finkel'stein, *ibid.* **92**, 086602 (2004); E. I. Rashba and Al. L. Efros, *ibid.* **91**, 126405 (2003).
[11] E. I. Ivchenko and G. E. Pikus, *Superlattices and Other Heterostucture* (Springer, Berlin, 1995).
[12] W. Trzeciakowski, Phys. Rev. B **38**, 12493 (1988); **38**, 4322 (1988).
[13] R. Balian, D. Bessis, and G. A. Mezincescu, Phys. Rev. B **51**, 17624 (1995).
[14] J. M. Luttinger, Phys. Rev. **102**, 1030 (1956).
[15] F. S. A. Cavalcante, R. N. Costa Filho, J. Ribeiro Filho, C. A. S. de Almeida, and V. N. Freire, Phys. Rev. B **55**, 1326 (1997); H. C. Liu, Superlattices Microstruct. **3**, 413 (1987).
[16] E. A. de Andrada e Silva, G. C. La Rocca, and F. Bassani, Phys. Rev. B **55**, 16293 (1997).
[17] W. Zawadszki and P. Pfeffer, Semicond. Sci. Technol. **19**, R1 (2004); P. Pfeffer and W. Zawadzki, Phys. Rev. B **59**, R5312 (1999).
[18] Yu. A. Bychkov and E. I. Rashba, Pis'ma Zh. Eksp. Teor. Fiz. **39**, 66 (1984) [JETP Lett. **39**, 78 (1984)].
[19] A. V. Rodina, Al. L. Efros, A. Yu. Alekseev, Phys. Rev. B **67**, 155312 (2003).
[20] F. T. Vasko, Pis'ma Zh. Eksp. Teor. Fiz. **30**, 574 (1979) [JETP Lett. **30**, 541 (1979)].
[21] F. T. Vasko and N. A. Prima, Fiz. Tverd. Tela (Leningrad) **23**, 2042 (1981) [Sov. Phys. Solid State **23**, 1192 (1981)].

[22] B. W. A. Foreman, Phys. Rev. B **48**, R4964 (1993); G. F. Glinskii and K. O. Kravchenko, Fiz. Tverd. Tela (S.-Peterburg) **40**, 872 (1998) [Phys. Solid State **40**, 803 (1998)].

[23] R. Winkler, Phys. Rev. B **62**, 4245 (2000).

[24] T. Reker, H. Im, L. E. Bremme, H. Choi, Y. Chung, P. C. Klipstein, and H. Shtrikman, Phys. Rev. Lett. **88**, 056403 (2002); A. V. Platonov, V. P. Kochereshko, E. L. Ivchenko, G. V. Mikhailov, D. R. Yakovlev, M. Keim, W. Ossau, A. Waag, and G. Landwehr, *ibid.* **83**, 3546 (1999); J. A. Majewski, P. Vogl, and P. Lugli, in *Proceedings of the 25th International Conference on Physics of Semiconductors, Osaka, 2000* (Springer, Berlin, 2001), p. 791.

[25] A. S. Gurevich, V. P. Kochereshko, A. V. Platonov, B. A. Zakin, A. Waag, and G. Landwer, Fiz. Tverd. Tela (S.-Peterburg) **47**, 1886 (2005) [Phys. Solid State **47**, 1964 (2005)].

[26] J. A. Gupta, D. D. Awschalom, Al. L. Efros, and A. V. Rodina, Phys. Rev. B **66**, 125307 (2002).

[27] A. A. Kiselev, E. L. Ivchenko and U. Rössler, Phys. Rev. B **58**, 16353 (1998); E. L. Ivchenko and A. A. Kiselev, Pis'ma Zh. Eksp. Teor. Fiz. **67**, 41 (1998) [JETP Lett. **67**, 43 (1998)].