Theory of intrinsic electric polarization and spin Hall current in spin-orbit-coupled semiconductor heterostructures

A. V. Rodina[1,*] and A. Yu. Alekseev[2,3]
[1]*A. F. Ioffe Physico-Technical Institute, 194021, St. Petersburg, Russia*
[2]*Department of Mathematics, University of Geneva, 1211 Geneva, Switzerland*
[3]*Institute of Theoretical Physics, Uppsala University, S-75108, Uppsala, Sweden*
(Received 21 March 2008; revised manuscript received 19 June 2008; published 5 September 2008)

We present Maxwell equations with source terms for the electromagnetic field interacting with a moving electron in a spin-orbit-coupled semiconductor heterostructure. We start with the eight-band ***kp*** model and derive the electric and magnetic polarization vectors using the Gordon-type decomposition method. Next, we present the ***kp*** effective Lagrangian for the nonparabolic conduction-band electrons interacting with electromagnetic field in semiconductor heterostructures with abrupt interfaces. This Lagrangian gives rise to the Maxwell equations with source terms and boundary conditions at heterointerfaces, as well as equations for the electron envelope wave function in the external electromagnetic field, together with appropriate boundary conditions. As an example, we consider spin-orbit effects caused by the structure inversion asymmetry for the conduction-electron states. We compute the intrinsic contribution to the electric polarization of the electron gas in asymmetric quantum well in equilibrium and in the stationary spin Hall regime. We argue that this contribution, as well as the intrinsic spin Hall current, are not cancelled by the elastic-scattering processes.

DOI: 10.1103/PhysRevB.78.115304 PACS number(s): 73.21.−b, 72.25.Dc, 71.70.Ej, 77.22.Ej

I. INTRODUCTION

Spintronic is a rapidly developing and important field of condensed-matter physics. The research is mainly concentrated on effects of electron-spin transport, spin accumulation, and spin manipulation in nonsymmetric semiconductor heterostructures with strong spin-orbit coupling. The early predictions[1–3] and recent experimental observations of the spin Hall effect[4,5] have inspired a huge number of theory papers.[6–8,10–17] This research is primarily concentrated on the spin Hall current, which is a flux of carriers with opposite spins in opposite directions perpendicular to the driving electric field. This current can be generated, for example, due to the asymmetric scattering,[1–3] the diffusion of the nonequilibrium spin,[14,18] or due to the momentum dependent spin-orbit splitting in the band structure.[6,7,11] The latter effect is usually called the intrinsic effect (as it is computed with an equilibrium distribution function) and it is characterized by the universal spin Hall conductivity.[6,7,11]

Several fundamental questions concerning the spin Hall effect have inspired a wide discussion in the literature. It concerns the definition of the electron-spin current[12–16] and the issue of spin Hall current cancellation in the stationary regime.[7–10,14] A good basis for treating these issues[15–17] is the relativistic Dirac equation for an electron interacting with the electromagnetic (EM) field. This approach reveals a close relation between the spin current and the electric polarization vector. It also gives a new contribution to the spin transfer torque coming from the interaction between the intrinsic electric polarization and the external electric field.[15]

In the present paper, we describe an electron interacting with the electromagnetic field and moving in semiconductor heterostructures with strong spin-orbit coupling. We start with the eight-band ***kp*** Kane model and derive the expressions for the electric and magnetic polarization vectors, as well as the effective ***kp*** Lagrangian for the conduction-band electrons, in a semiconductor heterostructure with abrupt interfaces. Using the least-action principle, we derive Maxwell equations with source terms and boundary conditions for the electromagnetic field at the interfaces, as well as equations for the electron envelope wave function in external fields, together with appropriate boundary conditions. As an example, we consider the stationary state of the electron gas in an asymmetric quantum well. We compute the intrinsic spin-orbit contribution to the electric polarization in equilibrium and in the spin Hall regime. We argue that the intrinsic electric polarization in the spin Hall regime corresponds to an additional spin-orbit energy in the external electric field and, therefore, it cannot be cancelled by extrinsic contributions. Furthermore, the intrinsic spin Hall current does not vanish in the stationary regime, while the vanishing of the spin torque[14] is maintained by additional contributions coming from interaction between the equilibrium electric polarization and the external electric field.[15] We also predict an existence of the intrinsic-induced magnetic charge Hall current due to the inhomogeneous charge distribution in asymmetric quantum well.

The paper is organized as follows. In Sec. II we review some standard features of the Dirac equation. In Sec. III we review the properties of the eight-band ***kp*** Kane model, which includes an external electromagnetic field, and derive the expressions for the electric and magnetic polarization vectors. In Sec. IV we derive the effective ***kp*** Lagrangian for the conduction-band electron interacting with external electromagnetic field and apply the least-action principle to semiconductor heterostructures. In Sec. V we calculate the intrinsic spin-orbit contribution to the electric polarization of the electron gas in an asymmetric quantum well in equilibrium and stationary spin Hall regimes, as well as the intrinsic-induced magnetic charge Hall current. In Sec. VI we discuss the results and their relevance for the fundamental issues of the proper definition of the spin Hall current and of its noncancellation in the stationary regime.

II. ELECTROMAGNETIC POLARIZATION INDUCED BY DIRAC ELECTRON

We start with the problem of a relativistic electron interacting with the electromagnetic field in the vacuum. Maxwell equations for the electric field $\boldsymbol{E}$ and magnetic induction $\boldsymbol{B}$ can be written (in Gaussian units) as

$$\boldsymbol{\nabla}\cdot\boldsymbol{E}=4\pi\rho,\quad \boldsymbol{\nabla}\times\boldsymbol{B}=\frac{1}{c}\frac{\partial\boldsymbol{E}}{\partial t}+\frac{4\pi}{c}\boldsymbol{J}, \tag{1}$$

$$\boldsymbol{\nabla}\cdot\boldsymbol{B}=0,\quad \boldsymbol{\nabla}\times\boldsymbol{E}=-\frac{1}{c}\frac{\partial\boldsymbol{B}}{\partial t}, \tag{2}$$

where c is the velocity of light. The charge density ρ and the current density $\boldsymbol{J}$ correspond to a single moving electron and satisfy the continuity equation,

$$\frac{\partial\rho}{\partial t}+\boldsymbol{\nabla}\cdot\boldsymbol{J}=0. \tag{3}$$

For a Dirac electron, $\rho=e\Psi^*\Psi$ and $\boldsymbol{J}=ce(\Psi^*\boldsymbol{\alpha}\Psi)$, where $e=-|e|$ is the free-electron charge and Ψ is a four component (bispinor) wave function satisfying the Dirac equation,

$$\left(i\hbar\frac{\partial}{\partial t}-eV\right)\Psi=(c\boldsymbol{\alpha}\cdot\boldsymbol{\pi}+mc^2\beta)\Psi, \tag{4}$$

$$\boldsymbol{\alpha}=\begin{pmatrix}0 & \boldsymbol{\sigma}\\ \boldsymbol{\sigma} & 0\end{pmatrix},\quad \beta=\begin{pmatrix}\hat{1} & 0\\ 0 & -\hat{1}\end{pmatrix},\quad \hat{1}=\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}. \tag{5}$$

Here m is the free-electron mass, $\hat{\boldsymbol{\sigma}}=\{\hat{\sigma}_x,\hat{\sigma}_y,\hat{\sigma}_z\}$ are the Pauli matrices, $\boldsymbol{\pi}=-i\hbar\boldsymbol{\nabla}-(e/c)\boldsymbol{A}$ is the momentum operator, and V and $\boldsymbol{A}$ are scalar and vector potentials of the electromagnetic fields $\boldsymbol{E}$ and $\boldsymbol{B}$, respectively,

$$\boldsymbol{E}=-(\partial\boldsymbol{A}/\partial t)-\boldsymbol{\nabla}V,\quad \boldsymbol{B}=\boldsymbol{\nabla}\times\boldsymbol{A}. \tag{6}$$

The Gordon decomposition is a way to split ρ and $\boldsymbol{J}$ into convective and internal parts (Ref. 16) $\rho=\rho_c+\rho_i$ and $\boldsymbol{J}=\boldsymbol{J}_c+\boldsymbol{J}_i$. The convective parts are given by

$$\rho_c=\frac{i\hbar}{2mc^2}\left(\bar{\Psi}\frac{\partial\Psi}{\partial t}-\frac{\partial\bar{\Psi}}{\partial t}\Psi\right)-\frac{eV}{mc^2}\bar{\Psi}\beta\Psi, \tag{7}$$

$$\boldsymbol{J}_c=\frac{e}{2m}[\bar{\Psi}(\boldsymbol{\pi}\Psi)+(\boldsymbol{\pi}^*\bar{\Psi})\Psi], \tag{8}$$

where $\bar{\Psi}=\Psi^*\beta$. The internal parts have the form

$$\rho_i=-\boldsymbol{\nabla}\cdot\boldsymbol{\Pi},\quad \boldsymbol{J}_i=c\,\boldsymbol{\nabla}\times\boldsymbol{M}+\frac{\partial\boldsymbol{\Pi}}{\partial t}, \tag{9}$$

where electric and magnetic polarizations $\boldsymbol{\Pi}$ and $\boldsymbol{M}$ are given by

$$\boldsymbol{\Pi}=\frac{e\hbar}{2mc}\bar{\Psi}(-i\boldsymbol{\alpha})\Psi,$$

$$\boldsymbol{M}=\frac{e\hbar}{2mc}\bar{\Psi}\boldsymbol{\Sigma}\Psi,\quad \boldsymbol{\Sigma}=\begin{pmatrix}\boldsymbol{\sigma} & 0\\ 0 & \boldsymbol{\sigma}\end{pmatrix}. \tag{10}$$

The convective and internal densities are separately conserved: $\partial\rho_{c,i}/\partial t+\boldsymbol{\nabla}\cdot\boldsymbol{J}_{c,i}=0$. The internal density ρ_i and current $\boldsymbol{J}_i$ are the densities of the induced electric charge and the induced electric current of a moving electron. Starting from the Dirac Eq. (5) and its complex conjugate, we obtain the continuity equation $\partial\rho_m/\partial t+\boldsymbol{\nabla}\cdot\boldsymbol{J}_m=0$, where $\rho_m=-\boldsymbol{\nabla}\cdot\boldsymbol{M}$ is the induced magnetic charge density and

$$\boldsymbol{J}_m=\frac{\partial\boldsymbol{M}}{\partial t}-c\,\boldsymbol{\nabla}\times\boldsymbol{\Pi} \tag{11}$$

is the induced magnetic charge current. Note that the induced magnetic charge density ρ_m and the corresponding current density $\boldsymbol{J}_m$, as well as the induced electric charge density ρ_i and the current density $\boldsymbol{J}_i$, also appear in the classical electrodynamics of moving media.[19]

One can introduce an electric displacement vector $\boldsymbol{D}=\boldsymbol{E}+4\pi\boldsymbol{\Pi}$ and a magnetic-field strength $\boldsymbol{H}=\boldsymbol{B}-4\pi\boldsymbol{M}$ and rewrite the Maxwell Eqs. (1) and (2) in the symmetric form as

$$\boldsymbol{\nabla}\cdot\boldsymbol{D}=4\pi\rho_c,\quad \boldsymbol{\nabla}\times\boldsymbol{H}=\frac{1}{c}\frac{\partial\boldsymbol{D}}{\partial t}+\frac{4\pi}{c}\boldsymbol{J}_c, \tag{12}$$

$$\boldsymbol{\nabla}\cdot\boldsymbol{H}=-4\pi\rho_m,\quad \boldsymbol{\nabla}\times\boldsymbol{D}=-\frac{1}{c}\frac{\partial\boldsymbol{H}}{\partial t}-\frac{4\pi}{c}\boldsymbol{J}_m. \tag{13}$$

These equations are similar to those presented in Ref. 20 and show how the moving electron affect the electromagnetic field via the induced electric and magnetic polarizations in the media.

In the general case of dielectric and magnetic media, vectors $\boldsymbol{D}$ and $\boldsymbol{H}$ are related to vectors $\boldsymbol{E}$ and $\boldsymbol{B}$ via

$$\boldsymbol{D}=\varepsilon\boldsymbol{E}+4\pi\boldsymbol{\Pi},\quad \boldsymbol{H}=\boldsymbol{B}/\mu-4\pi\boldsymbol{M}. \tag{14}$$

Here ε and μ are electric permittivity and magnetic conductivity of the media, respectively, and vectors $\boldsymbol{\Pi}$ and $\boldsymbol{M}$ describe additional polarizations induced by a moving Dirac electron.

While the Maxwell equations are universal, the particular expressions for the source terms depend on the particular model describing the moving electron. For a Dirac electron, expressions (10) for $\boldsymbol{\Pi}$ and $\boldsymbol{M}$ are exact. Approximate expressions for $\boldsymbol{\Pi}$ and $\boldsymbol{M}$ in weakly relativistic limit were recently obtained in Ref. 15. However, the Dirac equation or its weakly relativistic limit cannot be directly applied to the case of semiconductor heterostructures with strong spin-orbit interaction.[21] In the next section, we start with the eight-band $\boldsymbol{kp}$ Kane model and we derive expressions for electric and magnetic polarizations induced by the spin-orbit coupling of conduction-band electrons.

III. KANE ELECTRON IN EXTERNAL ELECTROMAGNETIC FIELD

The energy-band structure of cubic semiconductors near the center of the first Brillouin zone can be described within

the eight-band $\boldsymbol{kp}$ model.[22,23] In homogeneous bulk semiconductor, the full wave function can be expanded as[22]

$$\Psi(\boldsymbol{r}) = \sum_{\mu=\pm 1/2} \Psi_c^{\mu}(\boldsymbol{r})|S\rangle u_{\mu} + \sum_{\mu=\pm 1/2} \sum_{\alpha=x,z,z} \Psi_{v\alpha}^{\mu}(\boldsymbol{r})|R_{\alpha}\rangle u_{\mu}, \tag{15}$$

where $u_{1/2}$ and $u_{-1/2}$ are the eigenfunctions of the spin operator $\hat{\boldsymbol{S}}=(\hbar/2)\hat{\boldsymbol{\sigma}}$. $|S\rangle$ is the Bloch function of the conduction-band edge at the Γ point of the Brillouin zone, which represents an eigenfunction of internal momentum $I=0$. $|R_x\rangle \equiv |X\rangle$, $|R_y\rangle \equiv |Y\rangle$, and $|R_z\rangle \equiv |Z\rangle$ are Bloch functions of the valence-band edge at the Γ point of the Brillouin zone. Combinations of these functions $(|R_x\rangle \pm i|R_y\rangle)/\sqrt{2}$ and $|R_z\rangle$ are eigenfunctions of the internal momentum $I=1$ with projections on the z axis equal to ± 1 and 0, respectively (see Ref. 22). Smooth functions $\Psi_c^{\pm 1/2}(\boldsymbol{r})$ are components of the conduction-band spinor envelope function

$$\Psi_c = \begin{pmatrix} \Psi_c^{1/2} \\ \Psi_c^{-1/2} \end{pmatrix}$$

and $\Psi_{vx}^{\pm 1/2}(\boldsymbol{r})$, $\Psi_{vy}^{\pm 1/2}(\boldsymbol{r})$, and $\Psi_{vz}^{\pm 1/2}(\boldsymbol{r})$ are x,y,z components of the valence-band spinor envelope vector

$$\boldsymbol{\Psi}_v = \begin{pmatrix} \boldsymbol{\Psi}_v^{1/2} \\ \boldsymbol{\Psi}_v^{-1/2} \end{pmatrix}.$$

A. Basic equations

In the bulk, the eight-component envelope function $\Psi(\boldsymbol{r}) \equiv \{\Psi_c(\boldsymbol{r}), \boldsymbol{\Psi}_v(\boldsymbol{r})\}$ is a solution of the Schrödinger equation[24–26]

$$i\hbar \frac{\partial}{\partial t} \begin{pmatrix} \Psi_c \\ \boldsymbol{\Psi}_v \end{pmatrix} = \hat{H}_{\mathrm{Kane}} \begin{pmatrix} \Psi_c \\ \boldsymbol{\Psi}_v \end{pmatrix}, \tag{16}$$

$$\hat{H}_{\mathrm{Kane}} \begin{pmatrix} \Psi_c \\ \boldsymbol{\Psi}_v \end{pmatrix} = \begin{pmatrix} \dfrac{\alpha\hbar^2}{2m}\hat{k}^2\Psi_c & iP\hbar(\hat{\boldsymbol{k}}\boldsymbol{\Psi}_v) \\ -iP\hbar\hat{\boldsymbol{k}}\Psi_c & \left(-E_g - \dfrac{\Delta}{3}\right)\boldsymbol{\Psi}_v + \dfrac{i\Delta}{3}\boldsymbol{\sigma}\times\boldsymbol{\Psi}_v \end{pmatrix}. \tag{17}$$

Here the energy of electron states is measured with respect to the bottom of the conduction band $E_c=0$, $E_g=E_c-E_v$ is the band-gap energy, Δ is the spin-orbit splitting of the valence band, $\hat{\boldsymbol{k}}=-i\boldsymbol{\nabla}$ is the wave vector, and $P=-i\hbar\langle S|\hat{p}_z|Z\rangle/m$ is the Kane matrix element describing the coupling of the conduction and valence bands. The parameter α describes the contribution to the electron effective mass m_c, which is not related to the interaction with the valence band, while the k^2 terms for the valence band are neglected. This is the so-called eight-band Kane model with dispersion for electrons only.[24–26] This model allows to describe electron states with energies in the conduction band. It takes into account spin-orbit effects induced by the interaction with the valence band in the presence of the structure inversion asymmetry.[25] Bulk inversion asymmetry terms are not included in the consideration.

We introduce an expression

$$\boldsymbol{\Psi}_l = -i\hbar\frac{\partial\boldsymbol{\Psi}_v}{\partial t} - \hbar P\,\boldsymbol{\nabla}\,\Psi_c, \tag{18}$$

and rewrite the second vector equation of (16) and (17) as $\boldsymbol{\Psi}_l=(E_g+\frac{\Delta}{3})\boldsymbol{\Psi}_v-\frac{i\Delta}{3}\boldsymbol{\sigma}\times\boldsymbol{\Psi}_v$. In this way we express the valence-band spinor vector $\boldsymbol{\Psi}_v$ and the vector product $\boldsymbol{\sigma}\times\boldsymbol{\Psi}_v$ as

$$\boldsymbol{\Psi}_v = C_1\boldsymbol{\Psi}_l + iC_2[\hat{\sigma}\times\boldsymbol{\Psi}_l], \tag{19}$$

$$\boldsymbol{\sigma}\times\boldsymbol{\Psi}_v = -2iC_2\boldsymbol{\Psi}_l + (C_1-C_2)[\hat{\sigma}\times\boldsymbol{\Psi}_l], \tag{20}$$

with the coefficients C_1 and C_2 given by

$$C_1 \equiv \frac{3E_g+2\Delta}{3E_g(E_g+\Delta)}, \quad C_2 \equiv \frac{\Delta}{3E_g(E_g+\Delta)}. \tag{21}$$

To include the interaction with the electromagnetic field, we replace $\hbar\boldsymbol{k}=-i\hbar\boldsymbol{\nabla}$ with $\boldsymbol{\pi}=-i\hbar\boldsymbol{\nabla}-e/c\boldsymbol{A}$ and $i\hbar\partial/\partial t$ with $i\hbar\partial/\partial t-eV$ in Eqs. (16)–(18) and we add the respective Zeeman Kane Hamiltonian $\hat{H}_{\mathrm{Zeeman}}$ (Ref. 25),

$$\hat{H}_{\mathrm{Zeeman}} \begin{pmatrix} \Psi_c \\ \boldsymbol{\Psi}_v \end{pmatrix} = \begin{pmatrix} \frac{1}{2}g_e\mu_B(\boldsymbol{B}\boldsymbol{\sigma})\Psi_c & 0 \\ 0 & \frac{1}{2}g_0\mu_B(\boldsymbol{B}\boldsymbol{\sigma})\boldsymbol{\Psi}_v + i\mu_B\boldsymbol{B}\times\boldsymbol{\Psi}_v \end{pmatrix}. \tag{22}$$

Here $\mu_B=|e|\hbar/2mc$ is the Bohr magneton and $g_e=g_0+g^*$, where $g_0\approx 2$ is the free-electron g factor and g^* describes the remote band contribution to the electron effective g factor g_c. In order to simplify our consideration, we assume that the only spin-orbit contributions come from the interaction between conduction-band and valence-band states. Hence, the Hamiltonian does not include any Rashba terms related to the remote band contributions.

In the presence of an additional Zeeman Hamiltonian (22), the decompositions (19) and (20) are not exact. To take into account first-order corrections coming from Eq. (22) one has to replace $\boldsymbol{\Psi}_l$ with $\boldsymbol{\Psi}_l+\boldsymbol{\Psi}_B$ in Eqs. (19) and (20). Here the correction term

$$\boldsymbol{\Psi}_B \approx \mu_B(\boldsymbol{\sigma}\boldsymbol{B})[C_1\boldsymbol{\Psi}_l + iC_2(\hat{\sigma}\times\boldsymbol{\Psi}_l)] + i\mu_B\boldsymbol{B}\times[C_1\boldsymbol{\Psi}_l + iC_2(\hat{\sigma}\times\boldsymbol{\Psi}_l)] \tag{23}$$

is by a factor of $\mu_B|B|/E_g$ smaller than $\boldsymbol{\Psi}_l$ and it can usually be neglected.

B. Electron stationary state in the stationary electromagnetic field

We would like to compute the electron stationary state with energy $\mathcal{E}$ in the stationary electromagnetic field. To this end, we replace $i\hbar\partial\Psi/\partial t$ with $(\mathcal{E}-eV)\Psi$, where V is the scalar potential $\boldsymbol{E}=-\boldsymbol{\nabla}V$. Then, the valence-band contribution takes the form

$$\Psi_v(\epsilon) = \Psi_\epsilon + \Psi_B, \tag{24}$$

$$\Psi_\epsilon = -iPC_1(\epsilon)\pi\Psi_c + PC_2(\epsilon)[\hat{\sigma}\times\pi\Psi_c], \tag{25}$$

$$\Psi_B \approx \mu_B(\sigma B)\Psi_\epsilon + i\mu_B B\times\Psi_\epsilon. \tag{26}$$

Here $\epsilon=\mathcal{E}-eV$ and the coefficients $C_1(\mathcal{E}-eV)$ and $C_2(\mathcal{E}-eV)$ coincide with coefficients C_1 and C_2 given by Eq. (21) after replacing E_g by $E_g+\mathcal{E}-eV$. The resulting nonparabolic equation for the conduction-band spinor function reads

$$\left\{\pi\frac{1}{2m_c(\epsilon)}\pi + i\pi\frac{[g_c(\epsilon)-g_e]}{4m}[\sigma\times\pi] + \frac{\mu_B}{2}g_e(\sigma B)\right\}\Psi_c + iP\pi\Psi_B = \epsilon\Psi_c, \tag{27}$$

where again $\epsilon=\mathcal{E}-eV$. The energy dependent electron effective mass $m_c(\epsilon)$ and g factor $g_c(\epsilon)$ are given by

$$\frac{m}{m_c(\epsilon)} = \alpha + E_pC_1(\epsilon), \quad g_c(\epsilon) = g_e - 2E_pC_2(\epsilon), \tag{28}$$

where $E_p=2mP^2$ is the Kane energy parameter. The contribution of Ψ_B in Eq. (26) [the last term on the left-hand side of Eq. (27)] gives corrections to the first two terms, which are proportional to a small factor $|\mu_B B|/E_g$, and usually it can be neglected.

For small energies $|\epsilon|\ll E_g$, the nonparabolic electron effective mass and electron effective g factor can be expanded near the bottom of the conduction band

$$\frac{m}{m_c(\epsilon)} = \frac{m}{m_c} - \alpha_p\epsilon, \quad g_c(E) = g_c + \alpha_{so}\epsilon, \tag{29}$$

where α_p is the mass nonparabolicity parameter and α_{so} is the g-factor nonparabolicity parameter closely related to the spin-orbit coupling constant,[21,27]

$$a_p = \frac{E_p}{3}\left[\frac{2}{E_g^2} + \frac{1}{(E_g+\Delta)^2}\right] = E_p(C_1^2+2C_2^2), \tag{30}$$

$$\alpha_{so} = \frac{2E_p}{3}\left[\frac{1}{E_g^2} - \frac{1}{(E_g+\Delta)^2}\right] = 2E_pC_2(2C_1-C_2). \tag{31}$$

Substituting the expansion of Eq. (29) into Eq. (27) and neglecting the contribution of Ψ_B in Eq. (26), we arrive at

$$\left\{\pi\frac{1}{2m_c(\epsilon)}\pi + \frac{e\hbar}{4m}\alpha_{so}E[\sigma\times\pi] + \frac{\mu_B}{2}g_c(\epsilon)(\sigma B)\right\}\Psi_c = \epsilon\Psi_c. \tag{32}$$

Note that Ψ_c in Eqs. (27) and (32) is the original conduction-band spinor and, hence, the normalization condition reads $\int(|\Psi_c|^2+(|\Psi_v|^2)d^3r=1$. Expressing Ψ_v via Ψ_c with the help of Eqs. (24)–(26) and keeping only the first-order terms in $|\epsilon|/E_g$ and $|\mu_B B|/E_g$, we obtain the approximate normalization condition for Ψ_c,

$$\int\left[|\Psi_c|^2 - \frac{\hbar^2 a_p}{4m}(\Psi_c^*\nabla^2\Psi_c + \nabla^2\Psi_c^*\Psi_c) + \frac{\alpha_{so}}{2}\mu_B\Psi_c^*(\sigma B)\Psi_c\right]d^3r = 1. \tag{33}$$

In the absence of external fields, this condition can be presented as

$$\int|\Psi_c|^2 d^3r = \frac{m_c}{m_c(\mathcal{E})}. \tag{34}$$

C. Electric and magnetic polarizations in the Kane model

The continuity [Eq. (3)] for the charge density ρ and the electric current density J in the Kane model can be obtained directly from the Schrödinger [Eqs. (16) and (17)]. A straightforward calculation leads to the following expressions:

$$\rho = e(|\Psi_c|^2 + |\Psi_v|^2), \tag{35}$$

$$J = \frac{e\alpha}{2m}[(\pi\Psi_c)^*\Psi_c + \Psi_c^*\pi\Psi_c] + ieP(\Psi_c^*\Psi_v - \Psi_v^*\Psi_c) + c\nabla\times M_0, \tag{36}$$

$$M_0 = -\frac{\mu_B g_e}{2}\Psi_c^*\sigma\Psi_c - \frac{\mu_B g_0}{2}\sum_{\gamma=x,y,z}\Psi_{v\gamma}^*\sigma\Psi_{v\gamma} - i\mu_B[\Psi_v^*\times\Psi_v]. \tag{37}$$

Using the decomposition given by Eqs. (19) and (20) one can separate convective and internal parts of ρ and J as $\rho=\rho_c+\rho_i$ and $J=J_c+J_i$, where internal parts ρ_i and J_i are related to electric and magnetic polarization vectors P and M via Eq. (9). We neglect the contribution of Ψ_B in Eq. (23) and obtain the following approximate expressions for ρ_c, J_c, Π, and M:

$$\rho_c = e|\Psi_c|^2 + \frac{e\hbar P}{2}[\Psi_c^*(\nabla\overline{\Psi}) - (\nabla\overline{\Psi}^*)\Psi_c] + \frac{ie\hbar}{2}\left(\frac{\partial\Psi_v^*}{\partial t}\overline{\Psi} - \overline{\Psi}^*\frac{\partial\Psi_v}{\partial t}\right) + \frac{e^2V}{2}(\Psi_v^*\overline{\Psi} + \overline{\Psi}^*\Psi_v), \tag{38}$$

$$\Pi = \frac{e\hbar P}{2}(\Psi_c^*\overline{\Psi} + \overline{\Psi}^*\Psi_c), \quad \overline{\Psi} = C_1\Psi_v + iC_2\sigma\times\Psi_v, \tag{39}$$

$$J_c = \frac{e}{2m_c(-eV)}[\Psi_c^*\pi\Psi_c + (\pi\Psi_c)^*\Psi_c] + \frac{\alpha_{so}e^2\hbar}{2m}\Psi_c^*(\nabla V\times\sigma)\Psi_c + \frac{eP\hbar}{2}\left(\Psi_c^*\frac{\partial\overline{\Psi}}{\partial t} + \frac{\partial\overline{\Psi}^*}{\partial t}\Psi_c - \frac{\partial\Psi_c^*}{\partial t}\overline{\Psi} - \overline{\Psi}^*\frac{\partial\Psi_c}{\partial t}\right), \tag{40}$$

$$\boldsymbol{M} = -\frac{1}{2}\mu_B g_c(-eV)\Psi_c^*\boldsymbol{\sigma}\Psi_c - \frac{\mu_B g_0}{2}\sum_{\gamma=x,y,z}\Psi_{v\gamma}^*\boldsymbol{\sigma}\Psi_{v\gamma} - i\mu_B[\boldsymbol{\Psi}_v^*\times\boldsymbol{\Psi}_v]. \quad (41)$$

It is important to note that the convective charge density ρ_c and the current $\boldsymbol{J}_c$ enter Maxwell [Eq. (12)] for vectors $\boldsymbol{D}$ and $\boldsymbol{H}$, which are related to $\boldsymbol{E}$ and $\boldsymbol{B}$ by expressions (14). Vectors $\boldsymbol{\Pi}$ and $\boldsymbol{M}$ in Eq. (14) describe contributions of a moving Kane electron into the total electric and magnetic polarizations, which are not taken into account by the material permittivity tensors ε and μ.

Finally, for an electron stationary state with energy $|\epsilon|$ in a stationary magnetic field one can apply the decomposition given by Eqs. (24)–(26) to Eqs. (35)–(37). Neglecting the contribution of Ψ_B in Eq. (26) and keeping only the first-order terms in $|\epsilon|/E_g$ and $|\mu_B B|/E_g$, we arrive at the final expressions for the source terms,

$$\rho_c = e|\Psi_c|^2 - \frac{e\hbar^2 a_p}{4m}(\Psi_c^*\nabla^2\Psi_c + \nabla^2\Psi_c^*\Psi_c) + \frac{e\alpha_{so}}{2}\mu_B\Psi_c^*(\boldsymbol{\sigma}B)\Psi_c, \quad (42)$$

$$\boldsymbol{\Pi} = -\frac{e\hbar^2 a_p}{4m}\nabla|\Psi_c|^2 - \frac{e\alpha_{so}\hbar}{8m}[\Psi^*\boldsymbol{\sigma}\times\boldsymbol{\pi}\Psi_c - (\boldsymbol{\pi}\Psi)^*\times\boldsymbol{\sigma}\Psi_c], \quad (43)$$

$$\boldsymbol{J}_c = \frac{e}{2m_c(\boldsymbol{\epsilon})}[\Psi_c^*\boldsymbol{\pi}\Psi_c + (\boldsymbol{\pi}\Psi_c)^*\Psi_c] + \frac{\alpha_{so}e^2\hbar}{2m}\Psi_c^*(\nabla V\times\boldsymbol{\sigma})\Psi_c, \quad (44)$$

$$\boldsymbol{M} = -\frac{1}{2}\mu_B g_c(\epsilon)\Psi_c^*\boldsymbol{\sigma}\Psi_c. \quad (45)$$

The obtained expressions for the source terms describe how the nonparabolic conduction-band electron influences the external electromagnetic field. They are valid when the electron energy in the external fields is much smaller than the band-gap energy.

IV. LEAST-ACTION PRINCIPLE FOR SEMICONDUCTOR HETEROSTRUCTURE IN EXTERNAL ELECTROMAGNETIC FIELD

In Sec. III C, we found the effective charge density, the electric current density, and the electric and magnetic polarization vectors associated to conduction-band electrons. The alternative approach is based on the Lagrangian formalism and on the ***kp*** analog of the least-action principle derived in Ref. 28. This approach is particularly efficient in applications to abrupt heterostructures. It has two main advantages: (i) the variation of the action provides equations of motion together with boundary conditions at heterointerfaces and (ii) incorporating of external electromagnetic field is straightforward. Here we extend the approach of Ref. 28 in order to include the electron interaction with external stationary electromagnetic field.

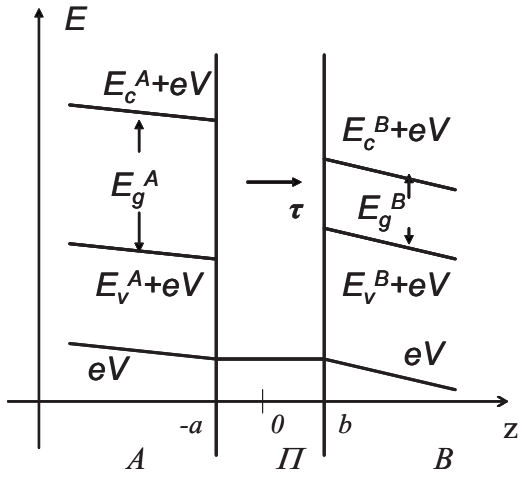

FIG. 1. Sketch of a planar heterointerface between semiconductor layers A. $E_c^{A,B}+eV$ and $E_v^{A,B}+eV$ are the conduction-band bottom and the valence-band top energies, respectively, in the regions A and B. These energies are not defined in the boundary region Π, while the scalar electromagnetic potential V is continuous everywhere.

The time-independent effective-mass Lagrangian density for Γ_6 electrons with nonparabolicity is given by[28]

$$\mathcal{L}(\mathcal{E}) = \mathcal{E}|\Psi_c|^2 - \frac{\hbar^2}{2m_c(\mathcal{E})}|\nabla\Psi_c(\boldsymbol{r})|^2 + \mathcal{L}_{SIA}(\mathcal{E}), \quad (46)$$

$$\mathcal{L}_{SIA}(\mathcal{E}) = -\frac{i\hbar^2}{4m}[g_e - g(\mathcal{E})]\nabla\Psi_c^*[\boldsymbol{\sigma}\times\nabla\Psi_c]. \quad (47)$$

In the presence of external stationary electromagnetic field, the Lagrangian density is

$$\mathcal{L}_{el-EM} = \mathcal{L}_{EM} + \mathcal{L}(\varepsilon) + \mathcal{L}_{Zeeman}. \quad (48)$$

Here the Lagrangian density $\mathcal{L}_{EM}$ of the stationary electromagnetic field takes into account material permittivity tensors ε and μ characterizing the material properties in the absence of moving electrons,

$$\mathcal{L}_{EM} = \frac{1}{8\pi}\left(\boldsymbol{E}_\alpha\varepsilon_{\alpha\beta}\boldsymbol{E}_\beta - \boldsymbol{B}_\alpha\frac{1}{\mu}_{\alpha\beta}\boldsymbol{B}_\beta\right). \quad (49)$$

The Lagrangian density $\mathcal{L}(\epsilon)$ can be obtained from Eqs. (46) and (47) by replacing $\mathcal{E}$ with $\epsilon=\mathcal{E}-eV$ and $-i\hbar\nabla$ with $\boldsymbol{\pi}=-i\hbar\nabla-e/c\boldsymbol{A}$. $\mathcal{L}_{Zeeman}$ corresponds to the conduction-band Zeeman energy

$$\mathcal{L}_{Zeeman} = -\frac{\mu_B}{2}g_e\Psi_c^*(\boldsymbol{\sigma B})\Psi_c. \quad (50)$$

We consider a planar semiconductor heterostructure consisting of two bulklike regions A and B connected by a thin boundary region Π around the abrupt heterointerface (see Fig. 1). The envelope function components Ψ_c are defined only in the bulklike regions of the heterostructure[28,29] and they obey the boundary conditions at $z=-a$ and b. The ma-

terial parameters m_c, g_c, α, g_e, E_p, and E_g may abruptly change from the region A to the region B and they are not defined in the boundary region Π. The scalar potential V and the vector potential $\boldsymbol{A}$ are continuous throughout the heterostructure and do not change inside the thin boundary region Π. The stationary fields $\boldsymbol{E}=-\boldsymbol{\nabla}V$ and $\boldsymbol{B}=\boldsymbol{\nabla}\times\boldsymbol{A}$ do not have any δ-function components and they are subject to the boundary conditions at $z=-a$ and b. For the sake of simplicity, we assume that the material permittivity tensors ε and μ are the same in A and B. Then, the Lagrangian densities in the bulklike regions A and B are given by Eqs. (46)–(50) with the material parameters of the materials A and B, respectively. Note that the energy E of the electron stationary state should be replaced with $E-E_c^{A,B}$ while $E+E_g$ should be replaced with $E-E_v^{A,B}$. Here $E_c^{A,B}$ and $E_v^{A,B}$ denote the extreme energies of the conduction and valence bands in the materials A and B, respectively.

The total action in the heterostructure is given[28] by $\mathcal{S}=\Sigma_{A,B}\int\mathcal{L}_{\text{el-EM}}\boldsymbol{d}^3\boldsymbol{r}+\mathcal{S}_\Pi$. Following the approach of Ref. 28, one can show that the contribution $\mathcal{S}_\Pi$ of the boundary region in such a model depends only on the values of Ψ_c at $z=-a$ and b. A variation of the action $\delta S=0$ with respect to Ψ_c^* (with electromagnetic potentials V and $\boldsymbol{A}$ assumed to be the constant functions of the coordinates) in a standard fashion leads to the bulk equation for the electron wave function Ψ_c [Eq. (32)] together with appropriate boundary conditions at the heterointerface. The boundary-condition parameters generally depend on the properties of the boundary region Π. For the "ideal" interface $|a+b|\to 0$ (see Ref. 28), they can be written as continuity conditions at $z=0$ of the conduction-band spinor function $\Psi_c=\text{const}$ and of the normal projection $v_\tau=(\boldsymbol{\pi v})=\text{const}$ (here $\boldsymbol{\tau}$ is the unit vector normal to the interface) of the effective velocity vector $\boldsymbol{v}$,

$$\boldsymbol{v}=\frac{1}{m_c(\epsilon)}\boldsymbol{\pi}\Psi_c+i\frac{[g_c(\epsilon)-g_e]}{2m}[\boldsymbol{\sigma}\times\boldsymbol{\pi}]\Psi_c. \tag{51}$$

For the nonideal interface, the boundary conditions can be expressed via the interface matrix that connects the components of Ψ_c and v_τ at two sides of the interface. An example of such boundary conditions for the model interface with infinite potential barrier are considered in Sec. V.

The variation of the action $\delta\mathcal{S}=0$ with respect to the electromagnetic potentials V and A_i, $(i=1,2,3)$ (with the wave function Ψ_c assumed to be the constant functions of coordinates) leads to stationary Maxwell equations for $\boldsymbol{D}=\varepsilon\boldsymbol{E}+4\pi\boldsymbol{\Pi}$ and $\boldsymbol{H}=\boldsymbol{B}/\mu-4\pi\boldsymbol{M}$,

$$\boldsymbol{\nabla}\cdot\boldsymbol{D}=4\pi\rho_c,\quad \boldsymbol{\nabla}\times\boldsymbol{H}=\frac{4\pi}{c}\boldsymbol{J}_c \tag{52}$$

together with appropriate boundary conditions at the interface,

$$(\boldsymbol{D}\boldsymbol{\tau})=\text{const},\quad (\boldsymbol{H}\times\boldsymbol{\tau})=\text{const}. \tag{53}$$

Keeping only the first-order terms in $|\epsilon|/E_g$ and $|\mu_B B|/E_g$, we obtain expressions for the source terms ρ_c and $\boldsymbol{J}_c$ and for polarization vectors $\boldsymbol{\Pi}$ and $\boldsymbol{M}$, which are exactly the same as given by Eqs. (42)–(45) of Sec. III. Thus, the two approaches, the approximation of Gordon-type decomposition of the eight-band Kane model, and the least-action principle for the nonparabolic electrons produce exactly the same results for the bulk semiconductor. In addition, the second approach gives general boundary conditions at the interface for the envelope functions in the external electromagnetic field, as well as the boundary conditions for the electromagnetic field, with account taken for the electric and magnetic polarizations induced by the moving electron.

V. INTRINSIC ELECTRIC POLARIZATION OF THE ELECTRON GAS IN A NARROW ASYMMETRIC QUANTUM WELL

In this section, we consider the spin-orbit contribution to the electric polarization, which is created by the in-plane motion of electrons in a narrow asymmetric square quantum well. In such a structure, the Rashba-type spin-orbit splitting of the electron energy levels can appear in the absence of external electromagnetic field ($\boldsymbol{E}=0$ and $\boldsymbol{A}=0$) due to the asymmetry of the interfaces at $z=\pm L$.[27,28,30] When the interfaces are modeled by infinite potential barriers (both in the conduction and in the valence bands), this asymmetry is reflected by the asymmetric boundary conditions,[28]

$$\Psi_c(\pm L)=\pm a^{\pm}\left\{\frac{m}{m_c(\mathcal{E})}\frac{\partial\Psi_c}{\partial z}+\frac{g_e-g_c(\mathcal{E})}{2}[\boldsymbol{\sigma}\times\boldsymbol{k}]_z\Psi_c\right\}\Bigg|_{z=\pm L}, \tag{54}$$

where $\boldsymbol{k}=(k_x,k_y)$ is the wave vector of the in-plane motion, $a^{\pm}=a_0/t^{\pm}$, and $a_0=\sqrt{\hbar^2/2E_p m}$; where t^+ and t^- are real numbers. Here we consider only the case of $t^{\pm}<0$, which corresponds to the electron energy levels $E_n>0$ at $\boldsymbol{k}=0$ (n is the number of the electron subband). The electron wave function can be written as

$$\Psi(\boldsymbol{r})=\sqrt{\frac{m_c}{m_c(\mathcal{E})}}f_n(z)\phi(\boldsymbol{\rho}), \tag{55}$$

where

$$f_n(z)=C^+\exp(ik_n z)+C^-\exp(-ik_n z)\quad \text{for}|z|\le L,$$

$$f_n(z)=0\quad \text{for}|z|>L \tag{56}$$

describes the electron quantization and $k_n=\sqrt{2m_c(E_n)E_n/\hbar^2}$. Constants $C^{\pm}$ are determined by the boundary conditions given by Eq. (54) together with the normalization condition $\int_{-L}^{L}|f_n|^2dz=1$. The asymmetry of the boundary conditions (54) results in the asymmetry of the electron-density distribution $|f_n(z)|^2$ inside the well, as shown schematically in Fig. 2.

The function $\phi(\boldsymbol{\rho})=\phi(x,y)$ describes the in-plane electron motion and satisfies the equation $\hat{H}_{nn}(\mathcal{E})\phi(\boldsymbol{\rho})=\mathcal{E}\phi(\boldsymbol{\rho})$ with effective nonparabolic Rashba Hamiltonian,

$$\hat{H}_{nn}(\mathcal{E})=\frac{\hbar^2(k_n^2+\boldsymbol{k}^2)}{2m_c(\mathcal{E})}+\alpha_{\text{SIA}}(\mathcal{E})[\boldsymbol{\sigma}\times\boldsymbol{k}]_z, \tag{57}$$

with the effective coupling constant approximated as[28]

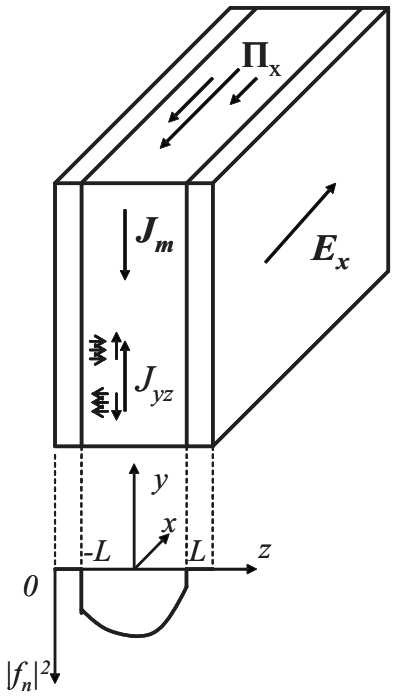

FIG. 2. Sketch of a square asymmetric quantum well with infinite potential barriers at $z=\pm L$. The asymmetric distribution of the electron density $|f_n(z)|^2$ and of the electric polarization $\Pi_x(z)$ are shown schematically. The spin Hall current J_{yz} and the induced magnetic charge Hall current $\boldsymbol{J}_m$ flow in the y direction when the electric field E_x is applied.

$$\alpha_{\mathrm{SIA}}(\mathcal{E}) = \frac{\hbar^2}{4m}\frac{m_c}{m_c(E)}[g_e - g_c(\mathcal{E})](|f_n(-L)|^2 - |f_n(+L)|^2). \tag{58}$$

The second term in the Hamiltonian $\hat{H}_{nn}(\mathcal{E})$ describes the effective intrasubband spin-orbit interaction caused by the asymmetry of the interfaces. The model allows us to include also the effective intersubband spin-orbit interaction considered recently in Ref. 31. It was found in Ref. 31 that in symmetric wells the magnitude of the intersubband spin-orbit coupling α_{12} between the first $n=1$ and the second $n=2$ subband is nonzero and is comparable to the Rashba constant. However, in the case of the asymmetric narrow well, the intersubband coupling leads to a second power in k correction to the Hamiltonian $\hat{H}_{nn}(\mathcal{E})$, which is smaller than the second term in Eq. (57) by the factor $|\alpha_{12}k|/(E_2-E_1)$. For the sake of simplicity we neglect the intrasubband spin-orbit coupling. In the presence of the external electric field $\boldsymbol{E}=(0,0,E_z)$, the effective coupling constant α_{SIA} should be replaced by $\alpha_{\mathrm{SIA}}+\alpha_R$, where $\alpha_R=(e\hbar^2/4m)\alpha_{\mathrm{so}}E_z$ is the Rashba constant. Note that in this case, functions $f_n(z)$ and the energy levels E_n should be calculated taking into account the spatial dependence of the scalar potential $V(z)=-ezE_z$. As a result, the asymmetry of $|f_n(z)|^2$ is caused by the asymmetry of the boundary conditions as well as by the effect of E_z. Although hereafter we will assume $E_z=0$, all results can be readily generalized for $E_z\neq 0$.

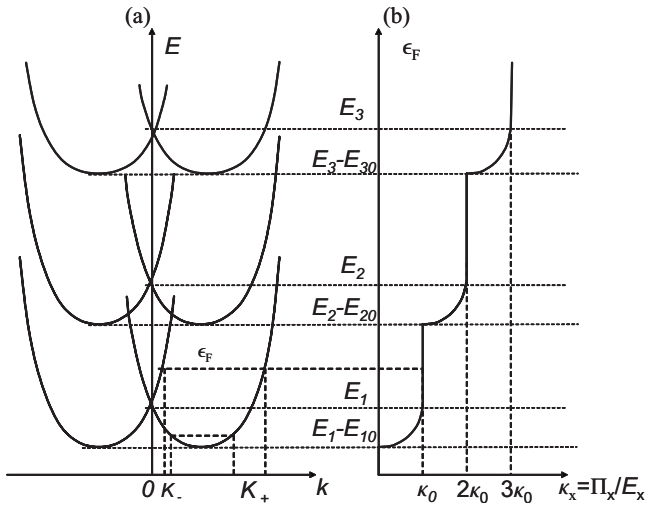

FIG. 3. Sketch of the electron energy structure in an asymmetric quantum well (a) and the dependence of the electric susceptibility $\kappa_x=\Pi_x/E_x$ on the Fermi energy ϵ_F in (b) the spin Hall regime.

The eigenfunctions $\psi_{\lambda,\boldsymbol{k}}(\boldsymbol{\rho})$ of the Hamiltonian $\hat{H}_{nn}(\mathcal{E})$ are given by

$$\phi_{\boldsymbol{k}\lambda}(\boldsymbol{\rho}) = \frac{e^{i\boldsymbol{k}\boldsymbol{\rho}}}{\sqrt{2S}}\begin{pmatrix} 1 \\ -i\lambda k_+/k \end{pmatrix}, \tag{59}$$

where $k=|\boldsymbol{k}|=\sqrt{k_x^2+k_y^2}$, $k_+=k_x+ik_y$, S is the cross section of the quantum well, and $\lambda=\pm 1$ correspond to two spin-split spectral branches. Their energies can be found from the equation

$$\epsilon_{n,\lambda,k} = E_n\frac{m_c(E_n)}{m_c(\epsilon_{n,\lambda,k})} + \frac{\hbar^2k^2}{2m_c(\epsilon_{n,\lambda,k})} + \lambda\alpha_{\mathrm{SIA}}(\epsilon_{n,\lambda,k})k. \tag{60}$$

The spin-orbit interaction shifts the energy minimum of the nth subband from E_n to (E_n-E_{n0}) [see Fig. 3(a)], where the energy shift E_{n0} can be found from the nonlinear equation

$$E_{n0} = \frac{\alpha_{\mathrm{SIA}}^2(E_n-E_{n0})m_c(E_n-E_{n0})}{2\hbar^2}. \tag{61}$$

In what follows, we neglect the nonparabolicity of the effective mass and of the coupling constant inside the nth subband and assume $m_c(\epsilon_{n,\lambda,k})\approx m_c(E_n)=m_n$ and $\alpha_{\mathrm{SIA}}(\epsilon_{n,\lambda,k})\approx\alpha_{\mathrm{SIA}}(E_n)=\alpha_n$.

Our aim is to calculate the electric polarization vector,

$$\boldsymbol{\Pi} = -\frac{e\hbar^2a_p}{4m}\boldsymbol{\nabla}|\Psi_c|^2 - \frac{e\hbar^2\alpha_{\mathrm{so}}}{8m}[\Psi_c^*\boldsymbol{\sigma}\times\boldsymbol{k}\Psi_c - (\boldsymbol{k}\Psi_c)^*\times\boldsymbol{\sigma}\Psi_c]. \tag{62}$$

In equilibrium, we have $\boldsymbol{\Pi}=(0,0,\Pi_z)$ and for the electron state characterized by the quantum numbers $n,\lambda,\boldsymbol{k}$, we obtain

$$\Pi_z^{n,\lambda,\boldsymbol{k}}(z) = -\frac{e\hbar^2 a_p}{4m}\frac{m_c}{m_n S}\frac{\partial|f_n(z)|^2}{\partial z} - \frac{e\hbar^2\alpha_{\rm so}}{4m}\frac{m_c}{m_n S}|f_n(z)|^2\lambda k. \tag{63}$$

The polarization is inhomogeneous in the z direction and it consists of two contributions. The first contribution is due to the nonparabolicity of the electron effective mass and to the asymmetry of the electron charge-density distribution in the well. It does not depend on the in-plane vector and it is the same for both spin states of the electron. In contrast, the sign of the second contribution is opposite for branches $\lambda=1$ and $\lambda=-1$. It is related to the nonparabolicity of the electron effective g factor. Regardless of this difference, both terms appear due to the interaction of the conduction-band electrons with the valence-band states.

To obtain the full polarization created in the well, one has to integrate over the equilibrium Fermi distribution corresponding to the Fermi energy ϵ_F,

$$\Pi_z^{\rm eq}(z) = \sum_{n,\lambda}\frac{S}{(2\pi)^2}\int \Pi_z^{n,\lambda,\boldsymbol{k}}(z)\boldsymbol{d}^2\boldsymbol{k} = \sum_n \Pi_z^n(z). \tag{64}$$

At zero temperature $T=0$, the integration for each occupied nth subband should be performed over $0<k\le K_\pm$, where $K_\pm$ are Fermi momenta for both spectral branches for a given n [see Fig. 3(a)]. $K_\pm$ are determined by

$$\epsilon_F = E_n + \frac{\hbar^2 K_\pm^2}{2m_n} \mp \alpha_n K_\pm. \tag{65}$$

If the Fermi level crosses only the lowest spectral branch $\lambda=-1$ of the nth subband, the integration should be carried out over $K_-<k<K_+$, where

$$K_\pm = \frac{\alpha_n m_n}{\hbar^2} \pm \sqrt{\frac{2m_n}{\hbar^2}(\epsilon_F - E_n + E_{n0})}. \tag{66}$$

For the Fermi energies $E_1<\epsilon_F\le E_2-E_{20}$, only the first electron subband is filled and both spectral branches are crossed by the Fermi level [see Fig. 3(a)]. Then, the integration over k and the sum over $\lambda=\pm 1$ give us the contribution from the $n=1$ subband as

$$\Pi_z^n(z) = -\frac{ea_p}{4\pi}\frac{m_c}{m}(\epsilon_F - E_n + 2E_{n0})\frac{\partial|f_n(z)|^2}{\partial z} + \frac{e\alpha_n\alpha_{\rm so}}{2\pi\hbar^2}\frac{m_n m_c}{m}\left(\epsilon_F - E_n + \frac{4}{3}E_{n0}\right)|f_n(z)|^2. \tag{67}$$

For the Fermi energies $E_1-E_{10}<\epsilon_F<E_1$, only the lowest spectral branch of the first electron subband is filled and crossed by the Fermi level [see Fig. 3(a)]. Then, integration over k gives us the contribution from the $n=1$ subband as

$$\Pi_z^n(z) = -\frac{ea_p\alpha_n}{4\pi}\frac{m_c}{m}\sqrt{\frac{2m_n}{\hbar^2}(\epsilon_F - E_n + E_{n0})}\frac{\partial|f_n(z)|^2}{\partial z} + \frac{e\alpha_{\rm so}}{2\pi}\frac{m_c}{m}\sqrt{\frac{2m_n}{\hbar^2}(\epsilon_F - E_n + E_{n0})}\left(\epsilon_F - E_n + \frac{5E_{n0}}{2}\right)\times|f_n(z)|^2. \tag{68}$$

When the Fermi energy is increased, more subbands give a contribution into the polarization and the final equilibrium polarization can be found as $\Pi_z^{\rm eq}(z)=\Sigma_n\Pi_z^n(z)$.

Let us now consider the effect of the dc electric field E_x in the x direction. We deal with two linear in E_x perturbations,

$$\hat{H}^{(1)} = -eE_x x, \tag{69}$$

$$\hat{H}^{(2)} = -(e\hbar^2/4m)\alpha_{\rm so}E_x\hat{\sigma}_z\hat{k}_y. \tag{70}$$

The second perturbation $\hat{H}^{(2)}$ is related to the dependence of the electron effective g factor on E_x and it describes an additional spin-orbit coupling. The perturbation related to the dependence of the electron effective mass on E_x can be neglected as far as we assume E_x to be small and the size of the sample in the x direction to be large.

The first-order correction to the in-plane wave function caused by $\hat{H}^{(1)}$ is

$$\phi_{\boldsymbol{k}\lambda}^{(1)}(\boldsymbol{\rho}) = \frac{\lambda eE_x k_y}{4\alpha_n k^3}\phi_{\boldsymbol{k}-\lambda}(\boldsymbol{\rho}). \tag{71}$$

The correction to the wave function caused by $\hat{H}^{(2)}$ is smaller by a factor of E_n/E_g and it can be neglected here. However, we shall later consider the first-order correction to the spin-orbit energy, which corresponds to $\hat{H}^{(2)}$.

We calculate the intrinsic spin-orbit contribution to the electric polarization Π_x, which is linear in the electric field E_x as

$$\boldsymbol{\Pi}_x(z) = \frac{e\hbar^2\alpha_{\rm so}}{4m}\sum_{n,\lambda}\frac{m_c}{m_n}|f_n(z)|^2\frac{S}{(2\pi)^2}\int \boldsymbol{d}^2\boldsymbol{k}[\phi_{\boldsymbol{k}\lambda}^*\hat{\sigma}_z k_y\phi_{\boldsymbol{k}\lambda}^{(1)} - (k_y\phi_{\boldsymbol{k}\lambda})^*\hat{\sigma}_z\phi_{\boldsymbol{k}\lambda}^{(1)}]. \tag{72}$$

The result is $\boldsymbol{\Pi}_x(z)=\Sigma_n\Pi_x^n(z)$, where

$$\boldsymbol{\Pi}_x^n(z) = -\frac{e^2 m_c\alpha_{\rm so}E_x}{16m\pi}|f_n(z)|^2$$

$$\text{for}\quad E_n<\epsilon_F<E_{n+1}-E_{(n+1)0}, \tag{73}$$

and

$$\boldsymbol{\Pi}_x^n(z) = -\frac{e^2 m_c\alpha_{\rm so}E_x}{16m\pi}\frac{\hbar^2}{m_n\alpha_n}\sqrt{\frac{2m_n}{\hbar^2}(\epsilon_F - E_n + E_{n0})}|f_n(z)|^2$$

$$\text{for}\quad E_n - E_{n0} < E < E_n. \tag{74}$$

Averaging over z, $\langle\Pi_x\rangle_z=\int_{-L}^{L}\Pi_x(z)dz/2L$, and introducing an electric susceptibility constant κ_x, we obtain

$$\kappa_x(\epsilon_F) = \frac{\langle \Pi_x \rangle_z}{E_x} = \sum_n \kappa_x^n(\epsilon_F). \tag{75}$$

The contribution of the nth subband is given by

$$\kappa_x^n(\epsilon_F) = \kappa_0 = -\frac{e^2 m_c \alpha_{so}}{32 m \pi L}$$

$$\text{for} \quad E_n < \epsilon_F < E_{n+1} - E_{(n+1)0}, \tag{76}$$

and

$$\kappa_x^n(\epsilon_F) = -\frac{e^2 m_c \alpha_{so}}{32 m \pi L} \frac{\hbar^2}{m_n \alpha_n} \sqrt{\frac{2m_n}{\hbar^2}(\epsilon_F - E_n + E_{n0})}$$

$$\text{for} \quad E_n - E_{n0} < \epsilon_F < E_n. \tag{77}$$

The dependence of the intrinsic electric susceptibility $\kappa_x(\epsilon_F)$ on the Fermi energy is shown in Fig. 3(b). Remarkably, the electric susceptibility keeps the constant values $\kappa_x(\epsilon_F) = n\kappa_0$ when both subbands $\lambda = 1$ and $\lambda = -1$ of the nth quantum size band E_n are crossed by the Fermi level ϵ_F and the next E_{n+1} band is empty. The value κ_0 of Eq. (76) is independent of the subband number n and of the Fermi energy ϵ_F. The physical meaning of the finite intrinsic electric polarization Π_x can be understood if one considers the spin-orbit interaction of the moving electron induced by the external field E_x. This interaction is described by the perturbation $\hat{H}^{(2)}$ and the respective spin-orbit energy can be calculated as $E_{so} = \int d^3\boldsymbol{r} \Sigma_{nk\lambda} \langle \Psi^* | \hat{H}^{(2)} | \Psi \rangle$. It is easy to see that this energy is given by

$$E_{so} = -\int d^3\boldsymbol{r} \Pi_x(z) E_x = -\kappa_x E_x^2 \, \Omega, \tag{78}$$

where $\Omega = 2LS$ is the sample volume. On the other hand, the intrinsic electric polarization Π_x can be related to the intrinsic spin Hall current $\mathcal{J}_{yz}$ corresponding to the flux in the positive (negative) y direction of the electrons with spin parallel (antiparallel) to z when the dc electric field E_x in the x direction is applied (see Fig. 2). Indeed, by comparing the definition $\hat{\mathcal{J}}_{ij} = -i\hbar^2/(4m_c)(\hat{\sigma}_j \partial_i + \partial_i \hat{\sigma}_j)$ of Ref. 15 for the spin current operator with Eq. (72) one can see that $\Pi_x(z) \propto \mathcal{J}_{yz}(z)$. For the Fermi energy $E_n < \epsilon_F < E_{n+1} - E_{(n+1)0}$, similar calculations lead to the averaged spin Hall conductivity $\sigma_{yx} = \langle \mathcal{J}_{yz}(z) \rangle_z / E_x = n|e|/8\pi$, which for $n = 1$ coincides with the universal spin Hall conductivity value $|e|/8\pi$ obtained in Refs. 6, 7, and 11.

The above derivation of the intrinsic contribution to the electric polarization $\Pi_x(z)$ in the spin Hall regime allows us to predict an appearance of the induced magnetic charge current $\boldsymbol{J}_m$ in the y direction when the dc electric field E_x in the x direction is applied (see Fig. 2). Indeed, for the stationary-state electron gas we have $d\boldsymbol{M}/dt = 0$, where $\boldsymbol{M}$ is the magnetic polarization vector, and, according to Eq. (11), the induced magnetic charge current $\boldsymbol{J}_m$ can be defined as

$$\boldsymbol{J}_m = -c \, \boldsymbol{\nabla} \times \boldsymbol{\Pi}. \tag{79}$$

Here we assume that the sample is infinite in x and y directions and we do not consider edge effects. As electric polarizations $\Pi_x(z)$ of Eqs. (73) and (74) are inhomogeneous in the z direction, the y component of the intrinsic-induced magnetic charge current is given by $J_{my}(z) = -c \, \partial \Pi_x(z)/\partial z \propto \partial |f(z)|^2/\partial z$. Averaging over z, we obtain the mean intrinsic-induced magnetic charge current,

$$\langle J_{my} \rangle_z = \int_{-L}^{L} J_{my}(z) dz / 2L = \sigma_{yx}^m E_x, \tag{80}$$

$$\sigma_{yx}^m(\epsilon_F) = \frac{\langle J_{my} \rangle_z}{E_x} = \sum_n \sigma_{yx}^{mn}(\epsilon_F). \tag{81}$$

Here $\sigma_{yx}^m(z)$ is the average magnetic Hall conductivity summarized over all electron states. The contribution of the nth subband σ_{yx}^{mn} is given by

$$\sigma_{yx}^{mn}(\epsilon_F) = -\frac{e^2 m_c \alpha_{so}}{32 m \pi L} (|f_n(-L)|^2 - |f_n(L)|^2)$$

$$\text{for} \quad E_n < \epsilon_F < E_{n+1} - E_{(n+1)0}, \tag{82}$$

and

$$\sigma_{yx}^{mn}(\epsilon_F) = -\frac{e^2 m_c \alpha_{so}}{32 m \pi L} \frac{\hbar^2}{m_n \alpha_n} \sqrt{\frac{2m_n}{\hbar^2}(\epsilon_F - E_n + E_{n0})} (|f_n(-L)|^2 - |f_n(L)|^2)$$

$$\text{for} \quad E_n - E_{n0} < \epsilon_F < E_n. \tag{83}$$

The dependence of the intrinsic magnetic Hall conductivity $\sigma_{yx}^m(\epsilon_F)$ on the Fermi energy is very similar to the dependence of the intrinsic electric susceptibility $\kappa_x(\epsilon_F)$ on the Fermi energy, which is shown in Fig. 3(b).

VI. CONCLUSION

In conclusion, we have considered the eight-band Kane model for the conduction-band electrons moving in the external electromagnetic field and showed how the Gordon-type decomposition can be adapted to this setting. This approach allowed us to derive the source terms for the Maxwell equations and the electric and magnetic polarization vectors related to a moving electron. We have also derived the effective $\boldsymbol{kp}$ Lagrangian for a nonparabolic conduction band and in the presence of the external electromagnetic field. In this way, we obtained boundary conditions for the envelope function and electromagnetic fields at the interfaces. These results give a solid basis for the analysis of the spin Hall effect and other spintronic effects in semiconductor heterostructures. As an example, we have obtained the expression for the electric polarization induced by the in-plane motion of the nonparabolic electrons in the asymmetric quantum well with infinite potential barriers and have calculated its dependence on the Fermi energy. We have predicted and calculated the intrinsic-induced magnetic charge Hall current in the spin Hall regime. This magnetic current can be detected via the electric-field induced outside the sample.[20] We are going to discuss the relevance of our results for the fundamental questions concerning the spin Hall effect.

First, we discuss the definition the spin Hall current. At present, three different definitions of the spin current operator $\hat{\mathcal{J}}_{ij}$ were suggested in the literature. They are the following: (i) the conventional definition[6,7,10,11,13,14] $\hat{\mathcal{J}}_{ij}=(\hbar/4)(\hat{\sigma}_j\hat{v}_i+\hat{v}_i\hat{\sigma}_j)$ (where $\hat{v}_i=1/\hbar(\partial\hat{H}/\partial k_i)$ is the velocity operator for the Hamiltonian $\hat{H}$); (ii) the modified definition $\hat{\mathcal{J}}_{ij}=(\hbar/2)d(\hat{r}_i\hat{\sigma}_j)/dt$ proposed in Ref. 12, and (iii) the definition $\hat{\mathcal{J}}_{ij}=-i\hbar^2/(4m_c)(\hat{\sigma}_j\partial_i+\partial_i\hat{\sigma}_j)$ obtained in Ref. 15 based on the relativistic approach. We note that the definition (iii) ensures the relation between the antisymmetric part of the current $\Lambda_\alpha=\varepsilon_{\alpha\beta\gamma}\mathcal{J}_{\beta\gamma}$ (here $\varepsilon_{\alpha\beta\gamma}$ is Levi-Civita antisymmetric tensor) and the electric polarization Π_α.[15] It is also with this definition that the universal conductance $\sigma_{yx}=|e|/8\pi$ remains unchanged when the $\hat{H}^{(2)}$ perturbation is taken into account. Finally, with this definition the intrinsic electric polarization Π_x is proportional to the intrinsic spin Hall current $\mathcal{J}_{yz}$ and the latter can be related to the spin-orbit energy $E_{\rm so}$. This fact also plays an important role in the discussion of the cancellation (or noncancellation) of the total spin Hall current in the stationary regime.

The stationary regime is possible only in the presence of scattering or disorder. In addition to the intrinsic spin Hall current, the total spin Hall current $\mathcal{J}_{yz}$ includes other contributions caused by the asymmetric scattering[1–3] and by the generated nonequilibrium spin density S_y.[14,18] It was shown[7,8] that for the standard Rashba model, when the spin-orbit coupling of the electron gas is described by the term $\hat{H}_R=\alpha_R[\boldsymbol{\sigma}\times\boldsymbol{k}]_z$, the total spin Hall current $\mathcal{J}_{yz}$ vanishes. This result was explained by the "cancellation theorem" in Ref. 10. It states that the spin torque $T_y=(i/2)[\hat{H}_R,\hat{\sigma}_y]$ is zero in the stationary regime. As, according to Ref. 10, $T_y\propto\mathcal{J}_{yz}$ for the standard Rashba model, the total spin Hall current vanishes. However, for more general model describing the spin-orbit coupling of the electron gas as $\hat{H}_R=Q_{\alpha\beta}\hat{\sigma}_\alpha\hat{k}_\beta$, where Q is a second-rank pseudotensor, one obtains[14]

$$T_y=\frac{i}{2}[\hat{H}_R,\hat{\sigma}_y]\propto\varepsilon_{y\alpha j}Q_{\alpha i}\mathcal{J}_{ij}. \tag{84}$$

It follows from Eq. (84) that if the perturbation $\hat{H}^{(2)}$ of Eq. (70) is included into $\hat{H}_R$, then an additional contribution to the spin torque T_y arises and, hence, $\mathcal{J}_{yz}$ does not vanish. This additional contribution $1/2E_x\Pi_z^{\rm eq}$ to the torque T_y was also obtained in Ref. 15 on the basis of the relativistic approach. We note that the perturbation $\hat{H}^{(2)}$ of Eq. (70) comes from the nonparabolicity of the electron effective g factor caused by the interaction with the valence-band states.

The direct relation between $\mathcal{J}_{yz}$ and Π_x allows us to relate the intrinsic spin Hall current with the additional spin-orbit energy $E_{\rm so}$ of the electron in the external electric field E_x. If we assume that this energy is determined by the intrinsic properties of the system and that it is not affected by the elastic scattering, we conclude that it is exactly the intrinsic parts of the spin Hall current of the electric polarization Π_x, which does not vanish in the stationary regime. The extrinsic current is cancelled in the way discussed in Ref. 14 and it does not contribute to the total electric polarization Π_x.

ACKNOWLEDGMENTS

We are grateful to I. A. Merkulov for the discussion of the Kane model and to V. L. Korenev for the discussion of the spin Hall current "cancellation theorem." A.V.R. acknowledges the support from the Swiss National Science Foundation. This work was partly conducted within the project of CRDF with Project No. RUP1-2890-ST-07.

*anna.rodina@mail.ioffe.ru

[1] M. I. Dyakonov and V. I. Perel, Zh. Eksp. Teor. Fiz. Pis'ma Red. **13**, 657 (1971) [JETP Lett. **13**, 467 (1971)].
[2] M. I. Dyakonov and V. I. Perel, Phys. Lett. **35A**, 459 (1971).
[3] J. E. Hirsch, Phys. Rev. Lett. **83**, 1834 (1999).
[4] Y. K. Kato, R. C. Myers, A. C. Gossard, and D. D. Awschalom, Science **306**, 1910 (2004).
[5] J. Wunderlich, B. Kaestner, J. Sinova, and T. Jungwirth, Phys. Rev. Lett. **94**, 047204 (2005).
[6] J. Sinova, D. Culcer, Q. Niu, N. A. Sinitsyn, T. Jungwirth, and A. H. MacDonald, Phys. Rev. Lett. **92**, 126603 (2004).
[7] E. I. Rashba, Phys. Rev. B **70**, 161201(R) (2004).
[8] J. I. Inoue, G. E. W. Bauer, and L. W. Molenkamp, Phys. Rev. B **70**, 041303(R) (2004).
[9] O. Chalaev and D. Loss, Phys. Rev. B **71**, 245318 (2005).
[10] O. V. Dimitrova, Phys. Rev. B **71**, 245327 (2005).
[11] S. Zhang and Z. Yang, Phys. Rev. Lett. **94**, 066602 (2005).
[12] Sun Qing-Feng and X. C. Xie, Phys. Rev. B **72**, 245305 (2005).
[13] Junren Shi, Ping Zhang, Di Xiao, and Qian Niu, Phys. Rev. Lett. **96**, 076604 (2006).
[14] V. L. Korenev, Phys. Rev. B **74**, 041308(R) (2006).
[15] Y. Wang, K. Xia, Z.-B. Su, and Z. Ma, Phys. Rev. Lett. **96**, 066601 (2006).
[16] R. Shen, Y. Chen, Z. D. Wang, and D. Y. Xing, Phys. Rev. B **74**, 125313 (2006).
[17] A. Vernes, B. L. Györffy, and P. Weinberger, Phys. Rev. B **76**, 012408 (2007).
[18] V. K. Kalevich, V. L. Korenev, and I. A. Merkulov, Solid State Commun. **91**, 559 (1994).
[19] J. Carstoiu, Proc. Natl. Acad. Sci. U.S.A. **57**, 1536 (1967).
[20] Q. F. Sun, H. Guo, and J. Wang, Phys. Rev. B **69**, 054409 (2004).
[21] R. Winkler, Physica E (Amsterdam) **22**, 450 (2004).
[22] E. I. Ivchenko and G. E. Pikus, *Superlattices and Other Heterostucture* (Springer, Berlin, 1995).
[23] E. L. Ivchenko, *Optical Spectroscopy of Semiconductor Nanostructures* (Alpha Science, Harrow, UK, 2005).
[24] A. S. Polkovnikov and G. G. Zegrya, Phys. Rev. B **58**, 4039 (1998).
[25] A. V. Rodina, Al. L. Efros, and A. Yu. Alekseev, Phys. Rev. B **67**, 155312 (2003).
[26] I. A. Merkulov and A. V. Rodina, in *Introduction to Physics of*

Diluted Magnetic Semiconductors, edited by J. Kossut and J. Gaj (Springer, Berlin, in press).

[27] E. A. de Andrada e Silva, G. C. La Rocca, and F. Bassani, Phys. Rev. B **55**, 16293 (1997).

[28] A. V. Rodina and A. Yu. Alekseev, Phys. Rev. B **73**, 115312 (2006).

[29] A. V. Rodina, A. Yu. Alekseev, Al. L. Efros, M. Rosen, and B. K. Meyer, Phys. Rev. B **65**, 125302 (2002).

[30] F. T. Vasko, Pis'ma Zh. Eksp. Teor. Fiz. **30**, 574 (1979) [JETP Lett. **30**, 541 (1979)].

[31] E. Bernardes, J. Schliemann, M. Lee, J. C. Egues, and D. Loss, Phys. Rev. Lett. **99**, 076603 (2007).