

Boundary conditions for spin and charge diffusion in the presence of interfacial spin-orbit couplingJ. Borge^{1,*} and I. V. Tokatly^{1,2,3,†}¹*Nano-Bio Spectroscopy group, Departamento Física de Materiales, Universidad del País Vasco, Av. Tolosa 72, E-20018 San Sebastián, Spain*²*IKERBASQUE, Basque Foundation for Science, E48011 Bilbao, Spain*³*Donostia International Physics Center (DIPC), Manuel de Lardizabal 4, E-20018 San Sebastian, Spain*

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Breaking of the inversion symmetry at the interface between different materials may dramatically enhance spin-orbit interaction in the vicinity of the interface. We incorporate the effects of this interfacial spin-orbit coupling (ISOC) into the standard drift-diffusion theory by deriving generalized boundary conditions for diffusion equations. Our theoretical scheme is based on symmetry arguments, providing a natural classification and parametrization of all spin-charge and spin-spin conversion effects that occur due to ISOC at macroscopically isotropic interfaces between nonmagnetic materials. We illustrate our approach with specific examples of spin-charge conversion in hybrid structures. In particular, for a lateral metal-insulator structure we predict an “ISOC-gating” effect which can be used to detect spin currents in metallic films with weak bulk SOC.

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Correlations between charge and spin degrees of freedom induced by spin-orbit coupling (SOC) in crystals and nanostructures open a pathway to control spin dynamics by purely electric means, without using magnetic fields. Not surprisingly, spin-charge conversion phenomena mediated by SOC are attracting growing attention in the field of spintronics [1–4]. Among them, the most known are the spin Hall effect (SHE) [5–7], and the inverse spin-galvanic effect, also known as the Edelstein effect [8,9] (EE). The SHE universally exists in all conductors without any symmetry restriction, provided SOC is sufficiently strong. In particular, it is responsible for the spin-charge conversion in the bulk of centrosymmetric materials, such as Pt or Au [10–12]. In contrast, the EE, that is, the spin polarization induced by a charge current [6,7,13–16], occurs only in the absence of inversion symmetry or, more precisely, only in gyrotropic materials/structures [17]. Usually it is discussed for two-dimensional (2D) electron gases in semiconductor heterostructures or in surface bands at surfaces or interfaces [7,18–20] with Rashba-type SOC [21], but it is also known in bulk materials, such as Te [22–25]. SOC also leads to the spin-spin conversion via the spin swapping effect (SSE) [26–28].

The symmetry conditions for all spin-charge conversion effects are naturally met at interfaces between different materials as any interface is always locally gyrotropic. Moreover the strong inversion symmetry breaking across the interface dramatically enhances manifestations of SOC, and, depending on the nature of the materials, may produce a giant interfacial SOC (ISOC) [29–32]. This makes interfaces promising candidates for active regions in spintronics devices, where the spin-charge and spin-spin conversion occurs most efficiently. In recent years these effects have been measured using different experimental techniques for various interfaces [33–38].

First experiments on the spin-charge conversion due to ISOC were interpreted as the inverse EE (IEE) in the 2D Rashba-split interface band [20,33]. Later it has been recognized that the spin-dependent scattering of the bulk continuum states at the interface also contributes strongly to the interfacial spin-charge conversion and the spin swapping [39–43]. A closely related mechanism studied in the context of semiconductor heterostructures can be attributed to a spin-dependent tunneling through the interfacial barrier [44–50]. Currently, theoretical studies of spin transport in the presence of ISOC are limited to specific effects in specific microscopic models with simplest geometries. Apparently this is not sufficient for the description of realistic device structures, and it is highly desirable to classify all effects of ISOC and consistently incorporate them into a general theoretical scheme of device modeling.

The spin and charge transport in a typical spintronics device is usually well described by the drift-diffusion theory. Within this approach the evolution of the spin and charge densities is governed by diffusion equations [51], supplemented with proper boundary conditions (BCs) at all interfaces and boundaries. In the absence of SOC the BCs reduce to the conservation of normal to the interface components of all currents, and relations between the currents and possible discontinuities of the densities across the interface. The latter are usually formulated in terms of spin-dependent interface conductances [52–54]. The modifications of BCs by the bulk SOC in noncentrosymmetric materials have been intensively debated in the literature [55–59]. However, the role of ISOC and the ways of incorporating its effects into the BCs for the drift-diffusion theory remain largely unexplored. Recently a generalization of the magnetoelectronic circuit theory, which partly accounts for the ISOC via coupling to the in-plane electric field at the interfaces, has been proposed [60,61]. This indeed captures the interfacial generation of spin current by the in-plane charge current [38,62], but apparently it does not cover all physically expected effects of ISOC

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and the general form of the corresponding BCs still remains unknown.

The present Rapid Communication is aimed at filling this gap by deriving the full set of BCs describing all possible spin-charge and spin-spin conversion effects that may occur at the macroscopically isotropic interface separating nonmagnetic materials. We do not use any specific microscopic model, but rely solely on symmetry arguments, which is similar to the symmetry-based derivation of spin-diffusion equations in the presence of bulk SOC [51,63].

Let us consider two nonmagnetic materials labeled by the index $\alpha = 1, 2$ and separated by a flat interface characterized by unit normal vector $\hat{\mathbf{n}}$. The interface located at the surface $\hat{\mathbf{n}} \cdot \mathbf{r} = 0$ is assumed macroscopically isotropic with a symmetry group $C_{\infty v}$. In the bulk of the materials the charge and spin degrees of freedom are described, respectively, by the distribution of electrochemical potentials $\mu_\alpha(\mathbf{r})$ and the spin density $\mathbf{S}_\alpha(\mathbf{r})$. To focus on the effects of ISOC, we assume that both materials possess the inversion symmetry and the spin-charge coupling in the bulk is negligible. In this case the charge \mathbf{j}_α and spin $J_{\alpha i}^a$ currents are given by the standard diffusive formulas, $\mathbf{j}_\alpha = -\sigma_\alpha^D \nabla \mu_\alpha$, and $J_{\alpha i}^a = -D_\alpha \partial_i S_\alpha^a$, where σ_α^D and D_α are the Drude conductivity and the diffusion coefficient, respectively. In the steady state the charge and spin-diffusion equations on either side of the interface reduce to Laplace equations for $\mu_\alpha(\mathbf{r})$, and the stationary spin-diffusion equations,

$$\nabla^2 \mu_\alpha(\mathbf{r}) = 0; \quad D_\alpha \nabla^2 \mathbf{S}_\alpha(\mathbf{r}) = \frac{\mathbf{S}_\alpha(\mathbf{r})}{\tau_\alpha}, \quad (1)$$

where τ_α is the spin-relaxation time. In the absence of ISOC the BCs at the interface are well known and read

$$\sigma_\alpha^D (\hat{\mathbf{n}} \cdot \nabla) \mu_\alpha = G_0^c \Delta \mu, \quad (2)$$

$$D_\alpha (\hat{\mathbf{n}} \cdot \nabla) \mathbf{S}_\alpha = G_0^s \Delta \mathbf{S}, \quad (3)$$

where $\Delta \mu = \mu_1 - \mu_2$ and $\Delta \mathbf{S} = \mathbf{S}_1 - \mathbf{S}_2$, and $G_0^{c/s}$ is the charge/spin conductance [64]. Physically, Eqs. (2) and (3) relate the currents passing through the interface to the interfacial density/potential drops. The appearance of the differences of the densities in the BCs, and the independence of conductances on the material index α reflect the conservation of all currents in the absence of SOC.

Formally Eqs. (2) and (3) are linear relations between the densities and their first derivatives. Such relations are forbidden by the symmetry in the isotropic bulk, but they are allowed at the interface as it provides us with an additional polar vector $\hat{\mathbf{n}}$. By constructing a scalar differential operator $\hat{\mathbf{n}} \cdot \nabla$ we can compile linear relations involving the densities and their derivatives, and transforming as a scalar, Eq. (2), and a pseudovector, Eq. (3). These are the general BCs for the scalar $\mu(\mathbf{r})$ and the pseudovector $\mathbf{S}(\mathbf{r})$ densities, allowed by the interface $C_{\infty v}$ symmetry under the requirements of the charge and spin conservation in the absence of the charge-spin mixing.

In the presence of ISOC the spin-charge coupling is possible, the spin is not conserved, and therefore only the charge conservation (the gauge invariance) requirement remains. This allows for additional terms in the BCs. Let us consider first the modification of the scalar BCs in Eq. (3). The

only additional scalar invariant that is linear in the densities and their first derivatives is $(\hat{\mathbf{n}} \times \nabla) \cdot \mathbf{S}$. Therefore the most general scalar BC takes the form

$$\sigma_\alpha^D (\hat{\mathbf{n}} \cdot \nabla) \mu_\alpha = G \Delta \mu + \sum_\beta \theta_{\alpha\beta}^{sc} D_\beta (\hat{\mathbf{n}} \times \nabla) \cdot \mathbf{S}_\beta. \quad (4)$$

Because of the gauge invariance the electrochemical potentials enter only as $\Delta \mu$, and there is only one charge conductance G . The second term in Eq. (4) describes the spin-charge conversion via the interfacial inverse spin Hall effect (ISHE)—the generation of a normal charge current from in-plane spin currents at either side of the interface. This channel of the spin-charge conversion at hybrid interfaces has been discussed in Ref. [65] within a simple ballistic scattering model. Our symmetry arguments show that in general it is parametrized by four spin-charge Hall angles $\theta_{\alpha\beta}^{sc}$. The cross-interface angles θ_{12}^{sc} and θ_{21}^{sc} should vanish for nontransparent interfaces. For example, for metal-insulator interfaces there is only one spin-charge Hall angle.

Similarly we generalize the pseudovector BC of Eq. (3) by adding all symmetry-allowed pseudovectors constructed from the densities and their derivatives [66]. It is convenient to write the resulting general BC by separating the normal and the parallel to the interface spin components $\mathbf{S} = \mathbf{S}_\perp + \mathbf{S}_\parallel$, where $\mathbf{S}_\perp = \hat{\mathbf{n}}(\hat{\mathbf{n}} \cdot \mathbf{S})$ and $\mathbf{S}_\parallel = (\hat{\mathbf{n}} \times \mathbf{S}) \times \hat{\mathbf{n}}$,

$$D_\alpha (\hat{\mathbf{n}} \cdot \nabla) \mathbf{S}_{\alpha\perp} = G_\alpha^n \Delta \mathbf{S}_\perp + L_\alpha^n \bar{\mathbf{S}}_\perp + \sum_\beta \kappa_{\alpha\beta}^n D_\beta (\hat{\mathbf{n}} \times \nabla) \times \mathbf{S}_{\beta\parallel}, \quad (5)$$

$$D_\alpha (\hat{\mathbf{n}} \cdot \nabla) \mathbf{S}_{\alpha\parallel} = G_\alpha^p \Delta \mathbf{S}_\parallel + L_\alpha^p \bar{\mathbf{S}}_\parallel + \sum_\beta \kappa_{\alpha\beta}^p D_\beta (\hat{\mathbf{n}} \times \nabla) \times \mathbf{S}_{\beta\perp} + \sum_\beta \theta_{\alpha\beta}^{cs} \sigma_\beta^D (\hat{\mathbf{n}} \times \nabla) \mu_\beta, \quad (6)$$

where $\bar{\mathbf{S}} = \mathbf{S}_1 + \mathbf{S}_2$. In the presence of ISOC the spin is not conserved. Therefore the right and left values of the boundary spin can independently enter the BC. The corresponding contributions are parametrized by the spin conductances $G_\alpha^{n/p}$ and the spin loss coefficients $L_\alpha^{n/p}$, which in general depend on the material index α , and are different for the normal (n) and the parallel (p) spin components. The third term on the right-hand sides in Eqs. (5) and (6) describes the spin-spin conversion due to the interfacial SSE. Namely, the in-plane current of the parallel (normal) spin component generates the normal current of the normal (parallel) spin component. This effect of ISOC is characterized by a set of swapping coefficients $\kappa_{\alpha\beta}^{n/p}$. Finally, the last term on the right-hand side in Eq. (6) is responsible for the charge-spin coupling. It can be interpreted as an interfacial SHE—generation of the spin current across the interface by an in-plane charge current. This effect has been studied recently in Refs. [38,62] for different hybrid structures via first-principle transport calculations. The corresponding transport coefficients in Eq. (6) are the charge-spin Hall angles $\theta_{\alpha\beta}^{cs}$.

Equations (4)–(6) generalize the standard BC of Eqs. (4) and (3). However, this is not sufficient to fully describe the physics of interfaces with ISOC. The reason is that the diffusion equations and the derived BCs involve only smooth

“diffusive” parts of the densities that vary slowly on the scale of the mean free path ℓ . In addition, strongly localized (on a scale less than ℓ) interfacial charge and spin currents as well as the interfacial spin polarization in general appear near nontrivial spin-orbit active interfaces. Most obviously the localized observables can be related to the interface bands, as is commonly assumed to interpret experiments on the interfacial spin-charge conversion [19,20,33,36]. Apart from that, in the presence of ISOC the spin-dependent interference between the incident and reflected waves for bulk states also leads to the appearance of interfacial spin polarization [41] and interfacial currents [42], localized on the scale of the Fermi wavelength λ_F .

The localized contributions can be included into the drift-diffusion theory by representing the total physical observables in the following form:

$$O_{\text{tot}}(\mathbf{r}) = \Theta(-z)O_1(\mathbf{r}) + \Theta(z)O_2(\mathbf{r}) + \delta(z)O_I(\mathbf{r}_{\parallel}), \quad (7)$$

where $z = \hat{\mathbf{n}} \cdot \mathbf{r}$ is the normal to the interface coordinate, $O_{\alpha}(\mathbf{r})$ are the slow “diffusive” parts that satisfy the bulk

diffusion equations, and $O_I(\mathbf{r}_{\parallel})$ is the localized part of the observable. Within the standard linear transport theory the localized spin \mathbf{S}_I , the charge current \mathbf{j}_I , and the spin current J_{II}^a should be related linearly to the interfacial values of the diffusive observables μ_{α} and \mathbf{S}_{α} . Formally the latter act as the sources (effective driving fields) for the former. The general form of such relations for \mathbf{S}_I , \mathbf{j}_I , and J_{II}^a can be determined from the symmetry arguments by combining, respectively, all linearly independent pseudovector, vector, and pseudotensor invariants constructed out of μ_{α} , \mathbf{S}_{α} , and their first derivatives [67]. A straightforward analysis [66] leads to the following expressions for the localized parts of the spin polarization and the charge current:

$$\mathbf{S}_I = \sum_{\alpha} \sigma_{\alpha}^{cs} (\hat{\mathbf{n}} \times \nabla) \mu_{\alpha} + \sum_{\alpha} \sigma_{\alpha}^{ss} (\hat{\mathbf{n}} \times \nabla) \times \mathbf{S}_{\alpha}, \quad (8)$$

$$\mathbf{j}_I = \sum_{\alpha} \sigma_{\alpha}^{sc} (\hat{\mathbf{n}} \times \mathbf{S}_{\alpha}) + \sum_{\alpha} \theta_{I\alpha}^{sc} (\hat{\mathbf{n}} \times \nabla) (\hat{\mathbf{n}} \cdot \mathbf{S}_{\alpha}), \quad (9)$$

while the localized spin current takes the form

$$J_{II}^a = g^{cs} \epsilon_{iak} \hat{n}_k \Delta \mu + \sum_{\alpha} [g_{\alpha}^p \hat{n}_a S_{\alpha}^i + g_{\alpha}^n \delta_{ai} \mathbf{n} \cdot \mathbf{S}_{\alpha} + \theta_{I\alpha}^{cs} \hat{n}_a (\hat{\mathbf{n}} \times \nabla)_i \mu_{\alpha} + \kappa_{I\alpha} [\hat{\mathbf{n}} \times (\hat{\mathbf{n}} \times \nabla)]_a S_{\alpha}^i + \kappa'_{I\alpha} \delta_{ai} \nabla \cdot \mathbf{S}_{\alpha}]. \quad (10)$$

In the last equation the spatial index i takes only in-plane values as the interface spin current J_{II}^a flows in the interface plane [68]. For brevity we do not show the “trivial” terms proportional to \mathbf{S}_{α} , $\nabla \mu_{\alpha}$, and $\partial_i S_{\alpha}^a$, allowed in Eqs. (8), (9), and (10), respectively. These terms may describe, if necessary, the usual 2D diffusive transport in the interface bands. The contributions shown explicitly are those responsible for the spin-charge and the spin-spin conversion. The first term in Eq. (8) describes the interfacial EE—the local spin polarization induced by the in-plane charge current [41]. The second term is the interfacial spin generated by the spin current flowing along the interface, and polarized in the direction orthogonal to that of the current. The first and the second terms in Eq. (9) correspond, respectively, to the interfacial IEE and the ISHE, i.e., the charge current at the interface induced by the nonequilibrium spin polarization and the in-plane spin current. Finally, in Eq. (10) the first term can be interpreted as a cross-interface SHE (the spin current at the interface plane generated by the voltage drop across the interface), the fourth term is the 2D interfacial SHE, the last two terms describe the 2D SSE, while the second and third terms are responsible for the spin current produced directly by the nonequilibrium spin polarization.

The localized observables of Eqs. (8)–(10) were introduced on physical grounds. Now we show that the appearance of in-plane localized currents is also required by the internal consistency of the theory. Let us look at Eq. (4). The second term on the right-hand side is allowed by the symmetry and meaningful physically, but it manifestly violates conservation of the charge current. Indeed Eq. (4) states that a part of the charge current passing through the interface is lost in the presence of in-plane spin gradients. The interfacial charge current \mathbf{j}_I fixes this problem by providing a missing sink. In the presence of \mathbf{j}_I the continuity equation for the total charge

current, after the integration across the interface, reads

$$\sigma_1^D (\hat{\mathbf{n}} \cdot \nabla) \mu_1 - \sigma_2^D (\hat{\mathbf{n}} \cdot \nabla) \mu_2 = -\nabla \cdot \mathbf{j}_I. \quad (11)$$

By substituting Eqs. (4) and (9) into the left- and right-hand sides we find that the charge continuity equation is fulfilled identically if the spin-charge Hall angles $\theta_{\alpha\beta}^{sc}$ are related to the “Edelstein conductivity” σ_{α}^{sc} as follows:

$$\sigma_{\alpha}^{sc} = D_{\alpha} (\theta_{1\alpha}^{sc} - \theta_{2\alpha}^{sc}). \quad (12)$$

Therefore there is a deep connection between the inverse SHE described by Eq. (4) and the generation of the local charge current via the inverse EE in Eq. (9). Inclusion of one effect necessarily implies the presence of the other.

The BCs Eqs. (4)–(6) together with Eqs. (8)–(10) complement the standard bulk drift-diffusion equations to model spintronics devices of any experimentally relevant geometry. It is worth noting that technically the localized currents become important in non-1D geometries with interfaces of a finite size. At the edges of the interface the total currents should be conserved, and therefore the edges act as local sources and sinks, which generates nontrivial patterns of the charge and spin flows. The examples below illustrate this point and demonstrate our general phenomenological construction at work.

The first example models the spin-charge conversion at the interface [33]. We consider a conducting bilayer of a finite width W in the y direction and separated by the interface with ISOC at the $z = 0$ plane, as shown in Fig. 1. A spin current $J_z^s(z) = -D \partial_z S^x(z)$, polarized along the x axis, and injected from the left, flows in the z direction, crosses the interface, and determines via Eq. (6) the spin polarization $S^x(0)$ at the interface. The latter, in turn, generates a localized charge current in the y direction via the IEE in Eq. (9), $j_{yI} = \sigma^{sc} S^x(0)$. To determine the distribution of the potential $\mu(\mathbf{r})$

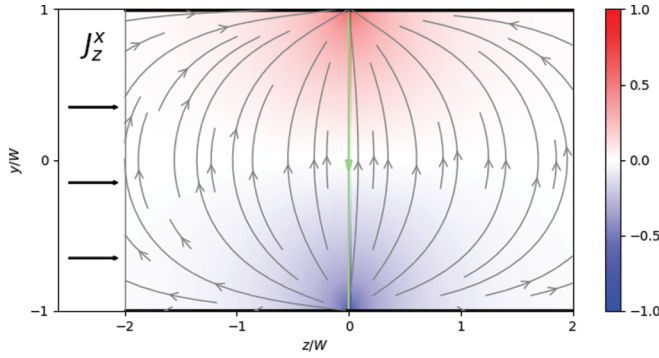


FIG. 1. Streamlines of the charge current generated by the spin current J_z^x flowing perpendicular to the interface (at $z=0$) between two conducting materials. The density plot shows the distribution of the induced electrostatic potential.

and the charge current $\mathbf{j} = -\sigma^D \nabla \mu$ in the bulk we have to solve the Laplace equation, $\nabla^2 \mu = 0$, with the condition of vanishing normal component of the *total* current at the sample boundaries at $y = \pm W/2$,

$$-\sigma^D \partial_y \mu(y, z)|_{y=\pm W/2} + j_{yI} \delta(z) = 0. \quad (13)$$

By solving this problem analytically [66] we find the spatial distribution of the charge current, and the total voltage drop across the sample

$$\Delta V = \int [\mu(W/2, z) - \mu(-W/2, z)] dz = j_{yI} \frac{W}{\sigma^D}. \quad (14)$$

The stream lines of the induced charge flow together with the density plot for the potential are shown in Fig. 1. The current in the bulk forms a counterflow that compensates the localized currents generated at the interface. Both the induced potential and the current are concentrated near the edges of the interface at a macroscopic scale of the order of the sample size W .

As a second example we consider a spin-charge conversion in a lateral hybrid structure made from a metallic film of thickness W , with a part of its upper surface covered by an insulator with large SOC, like Bi_2O_3 (see Fig. 2). In this way we create an interface with ISOC on the top boundary at $z=W$ for $x > 0$, while the rest ($x < 0$) of the top boundary as well as the bottom boundary at $z=0$ remain “trivial.” We

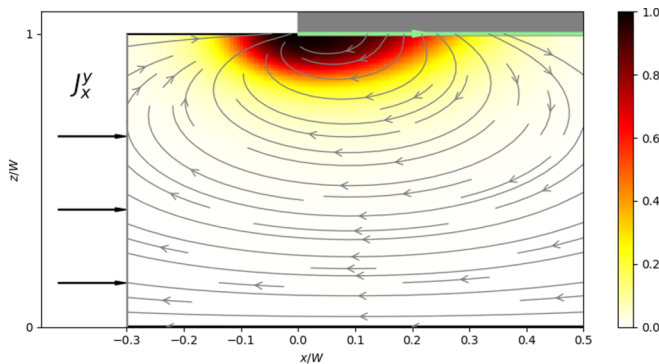


FIG. 2. Charge flow generated by the spin current $J_x^y(x)$ in the metallic film with an insulator (shown in gray) deposited on its top surface. The density plot shows the current strength.

assume a diffusive spin current polarized along y , flowing in the x direction, that is, $J_x^y(x) = -D \partial_x S^y(x)$ with $S^y(x) \sim e^{-x/l_s}$, where $l_s = \sqrt{D\tau_s}$ is the spin-diffusion length [69].

The induced potential $\mu(x, z)$ is obtained by solving the Laplace equation with two BCs. On the bottom surface the standard BC of $\sigma^D \partial_z \mu|_{z=0} = 0$ is imposed. To get the BC on the top surface we combine Eqs. (4) and (9) in the form of Eq. (11) that for the metal-insulator interface and the chosen spin density reads

$$\sigma^D \partial_z \mu|_{z=W} = -D \partial_x [\theta^{sc}(x) S^y(x)], \quad (15)$$

where $\theta^{cs}(x) = \theta^{sc} \Theta(x)$ reflects the stepwise distribution of ISOC at the top surface [70]. This problem is also solvable analytically [66]. The corresponding charge flow, shown in Fig. 2, demonstrates a typical dipolar pattern with a local sink at the edge of the interface a distributed $\sim \Theta(x) e^{-x/l_s}$ source. As the film has a finite width this dipole field generates a lateral voltage drop:

$$\Delta V = \mu(\infty, z) - \mu(-\infty, z) = \chi S^y(0) \theta^{sc} l_s / W, \quad (16)$$

where $\chi = D/\sigma^D$ is the inverse compressibility of the metal. If the top “ISOC gate” has a finite length L the voltage drop acquires an additional factor $1 - e^{-L/l_s}$. Notice that by measuring the induced lateral voltage, and using Eq. (16) we get a direct experimental access to the interfacial spin-charge Hall angle θ^{sc} .

In conclusion, we derived a full set of additional conditions that complement the standard drift-diffusion theory to model spin and charge dynamics in the presence of interfaces with strong ISOC. These conditions consist of the generalized BC describing the interfacial spin-charge and spin-spin conversion, and the expressions for the spin, the charge current, and the spin current, localized at the interface within a microscopic scale (smaller than ℓ). Our construction provides a natural classification and parametrization of all spin-charge and spin-spin conversion effects mediated by ISOC at macroscopically isotropic interfaces between nonmagnetic materials. The phenomenological coefficients entering the derived BC should be determined from comparison with experiments or first-principle calculations for specially chosen geometries. To demonstrate the working power of our theory we considered two specific examples. In particular, we predict a generation of a lateral voltage drop in a metallic film by a spin current if an insulator with a strong SOC is deposited on the top surface of the film. This ISOC gate effect can be used to detect spin currents in materials with weak bulk SOC.

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- [68] More formally this condition is expressed in terms of the interface projection $J_{il}^a \mapsto (\delta_{ik} - \hat{n}_i \hat{n}_k) J_{kl}^a$, which is implicitly assumed in Eq. (10).
- [69] For simplicity we neglect the depletion of spin density near the interface due to the interfacial spin loss described by coefficients L_α in Eqs. (5) and (6). This corresponds to considering the spin-charge conversion to the leading order in ISOC.
- [70] To arrive at this form of BC we have used the relation $\sigma^{sc} = D\theta^{sc}$ which follows from Eq. (12) for the case of a metal-insulator interface.