

# Long-range scattering effects on spin Hall current in *p*-type bulk semiconductors

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Employing a nonequilibrium Green's-function approach, we examine the effects of long-range hole-impurity scattering on spin-Hall current in *p*-type bulk semiconductors within the framework of the self-consistent Born approximation. We find that, contrary to the null effect of short-range scattering on spin-Hall current, long-range collisions do produce a nonvanishing contribution to the spin-Hall current, which is independent of impurity density in the diffusive regime and relates only to hole states near the Fermi surface. The sign of this contribution is opposite to that of the previously predicted disorder-independent spin-Hall current, leading to a sign change of the total spin-Hall current as hole density varies. Furthermore, we also make clear that the disorder-independent spin-Hall effect is a result of an interband polarization directly induced by the dc electric field with contributions from all hole states in the Fermi sea.

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## I. INTRODUCTION

Recently, there have been extensive studies of the physics of the spin-orbit (SO) interaction in condensed matter. The most intriguing phenomenon induced by SO coupling is the spin-Hall effect (SHE): when a dc electric field is applied, the SO interaction may result in a net nonvanishing spin current flow along the transverse direction. The SHE is classified into two types according to its origin, an *extrinsic* spin-orbit Hamiltonian term induced by carrier-impurity scattering potentials<sup>1,2</sup> and an *intrinsic* spin-orbit Hamiltonian term arising from free carrier kinetics.<sup>3,4</sup> The intrinsic spin-Hall effect was originally thought to be independent of carrier-impurity scattering. Experimentally, the SHE was observed in a *n*-type bulk semiconductor<sup>5</sup> and in a two-dimensional (2D) heavy-hole system.<sup>6</sup>

However, further studies have indicated that the spin-Hall effect associated with the intrinsic mechanism can be strongly affected by carrier-impurity scattering (disorder).<sup>7-22</sup> (To avoid confusion, we use the term "intrinsic SHE" to refer to the total spin-Hall effect arising from the SO coupling terms of the Hamiltonian that do not explicitly involve scattering; ultimately, this is corrected by scattering, but the part that is unaffected by scattering will be termed the intrinsic "disorder-independent" SHE.) In diffusive 2D semiconductors, there always exists a contribution to the intrinsic spin-Hall current which arises from spin-conserving electron-impurity scattering, but it is independent of impurity density within the diffusive regime. For 2D *electron* systems with Rashba SO coupling, this disorder-related spin-Hall current leads to the vanishing of the total intrinsic spin-Hall current, irrespective of the specific form of the scattering potential, of the collisional broadening, and of temperature.<sup>17</sup> In 2D Rashba *heavy-hole* systems, disorder affects the intrinsic SHE in a different fashion: contributions from short-range collisions to the SHE vanish,<sup>18</sup> while long-range electron-impurity scattering produces a nonvanishing disorder-related spin-Hall current, whose sign changes with variation of the hole density.<sup>19,20</sup>

To date, the effect of disorder on the intrinsic spin-Hall current in *p*-type bulk semiconductors has been studied rela-

tively little. Employing a Kubo formula, Murakami found a null disorder effect on the intrinsic SHE for short-range hole-impurity collisions.<sup>21</sup> The crossover of the SHE from the diffusive to the hopping regime has been investigated by modeling finite-size samples (with a maximum of  $50 \times 50 \times 50$  lattice sites) by Chen *et al.*<sup>22</sup> In this paper, we employ a nonequilibrium Green's function approach to study the effect of more realistic *long-range* hole-impurity scattering on the intrinsic spin-Hall current in a diffusive *p*-type bulk semiconductor. We find that, in such a system, the contribution of hole-impurity collisions to the intrinsic spin-Hall current is finite and it is independent of impurity density within the diffusive regime. Moreover, this disorder contribution has its sign opposite to that of the disorder-independent one, leading to a sign change of the total spin-Hall current as the hole density varies. Furthermore, we make clear that the disorder-independent spin-Hall effect arises from an interband polarization process directly induced by the dc electric field and it involves all hole states below the Fermi surface. In contrast to this, the disorder contribution to the intrinsic SHE originates from a disorder-mediated polarization between two hole bands and is associated only with hole states in the vicinity of the Fermi surface. Also, we numerically examine the hole-density dependencies of the spin-Hall conductivity and mobility.

This paper is organized as follows. In Sec. II, we derive the kinetic equation for the nonequilibrium distribution function and discuss the origins of the disorder-independent and disorder-related spin-Hall currents. In Sec. III, we perform a numerical calculation to investigate the effect of long-range hole-impurity scattering on the spin-Hall current. Finally, we review our results in Sec. IV.

## II. FORMALISM

### A. Kinetic equation

It is well known that for semiconductors with diamond structure (e.g., Si, Ge) or zinc-blende structure (e.g., GaAs), the tops of the valence bands usually are split into fourfold

degenerate  $S=3/2$  and twofold degenerate  $S=1/2$  states due to the spin-orbit interaction ( $S$  denotes the total angular momentum of the atomic orbital). Near the top of the  $S=3/2$  valence bands, the electronic structure can be described by a simplified Luttinger Hamiltonian,<sup>23</sup>

$$\check{h}_0(\mathbf{p}) = \frac{1}{2m} \left[ \left( \gamma_1 + \frac{5}{2} \gamma_2 \right) p^2 - 2 \gamma_2 (\mathbf{p} \cdot \mathbf{S})^2 \right], \quad (1)$$

where  $\mathbf{p} \equiv (p_x, p_y, p_z) \equiv (p \sin \theta_p \cos \phi_p, p \sin \theta_p \sin \phi_p, p \cos \theta_p)$  is the three-dimensional (3D) hole momentum,  $m$  is the free electron mass,  $\mathbf{S} \equiv (S_x, S_y, S_z)$  are the spin-3/2 matrices, and  $\gamma_1$  and  $\gamma_2$  are the material constants. (As in previous studies,<sup>3,21,22,24</sup> we simplified by setting  $\gamma_3 = \gamma_2$  in the original Luttinger Hamiltonian presented in Ref. 23).

By a local unitary spinor transformation,  $U_{\mathbf{p}} = \exp(-iS_x \phi_p) \exp(-iS_y \theta_p)$ , Hamiltonian (1) can be diagonalized as  $\hat{h}_0(\mathbf{p}) = U_{\mathbf{p}}^\dagger \check{h}_0(\mathbf{p}) U_{\mathbf{p}} = \text{diag}[\varepsilon_H(p), \varepsilon_L(p), \varepsilon_L(p), \varepsilon_H(p)]$ . Here,  $\varepsilon_H(p) = \frac{\gamma_1 - 2\gamma_2}{2m} p^2$  and  $\varepsilon_L(p) = \frac{\gamma_1 + 2\gamma_2}{2m} p^2$  are, respectively, the dispersion relations of the heavy- and light-hole bands. Physically, this transformation corresponds to a change from a spin basis to a helicity basis.

In a realistic 3D system, holes experience scattering by impurities. We assume that this interaction between holes and impurities can be characterized by an isotropic potential,  $V(|\mathbf{p} - \mathbf{k}|)$ , which corresponds to scattering a hole from state  $\mathbf{p}$  to state  $\mathbf{k}$ . In the helicity basis, the scattering potential takes the transformed form,  $\hat{T}(\mathbf{p}, \mathbf{k}) = U_{\mathbf{p}}^\dagger V(|\mathbf{p} - \mathbf{k}|) U_{\mathbf{k}}$ .

We are interested in the spin-Hall current in a bulk hole system driven by a dc electric field  $\mathbf{E}$  along the  $z$  axis. In Coulomb gauge, this electric field can be described by the scalar potential,  $V = -e\mathbf{E} \cdot \mathbf{r}$ , with  $\mathbf{r}$  as the hole coordinate. Without loss of generality, we specifically study a spin current  $J_y^x$  that is polarized along the  $x$  axis and flows along the  $y$  axis. In the spin basis, the conserved single-particle spin-Hall operator  $\check{J}_y^x$  is defined as<sup>24</sup>

$$\check{J}_y^x(\mathbf{p}) = \frac{1}{6} \left\{ \frac{\partial \check{h}_0}{\partial p_y}, P_{\mathbf{p}}^L S_x P_{\mathbf{p}}^L + P_{\mathbf{p}}^H S_x P_{\mathbf{p}}^H \right\}, \quad (2)$$

with  $P_{\mathbf{p}}^L$  and  $P_{\mathbf{p}}^H$ , respectively, as projection operators onto the states of light- and heavy-hole bands:  $P_{\mathbf{p}}^L = \frac{9}{8} - \frac{1}{2p^2} (\mathbf{p} \cdot \mathbf{S})^2$ ,  $P_{\mathbf{p}}^H = 1 - P_{\mathbf{p}}^L$ . Taking a statistical ensemble average, the observed net spin-Hall current is given by

$$J_y^x = \sum_{\mathbf{p}} \text{Tr}[\check{J}_y^x(\mathbf{p}) \check{\rho}(\mathbf{p})], \quad (3)$$

where  $\check{\rho}(\mathbf{p})$  is the distribution function related to the nonequilibrium ‘‘lesser’’ Green’s function,  $\check{G}^<(\mathbf{p}, \omega)$ , as given by  $\check{\rho}(\mathbf{p}) = -i \int \frac{d\omega}{2\pi} \check{G}^<(\mathbf{p}, \omega)$ . Also,  $J_y^x$  can be determined in helicity basis via

$$J_y^x = \sum_{\mathbf{p}} \text{Tr}[\hat{J}_y^x(\mathbf{p}) \hat{\rho}(\mathbf{p})], \quad (4)$$

with  $\hat{J}_y^x(\mathbf{p}) = U_{\mathbf{p}}^\dagger \check{J}_y^x(\mathbf{p}) U_{\mathbf{p}}$  and  $\hat{\rho}(\mathbf{p}) = U^+(\mathbf{p}) \check{\rho}(\mathbf{p}) U(\mathbf{p})$  being the helicity-basis single-particle spin current operator and distribution function, respectively. Explicitly, Eq. (4) can be re-

written as  $[\hat{\rho}_{\mu\nu}(\mathbf{p})]$  are the matrix elements of  $\hat{\rho}(\mathbf{p})$  in helicity basis;  $\mu, \nu = 1, 2, 3, 4$

$$J_y^x = \frac{\sqrt{3} \gamma_2}{m} \sum_{\mathbf{p}} p \{ 4 \cos^2 \phi_p \sin \theta_p \text{Im}[\hat{\rho}_{12}(\mathbf{p}) + \hat{\rho}_{34}(\mathbf{p})] - \sin(2\phi_p) \sin(2\theta_p) \text{Re}[\hat{\rho}_{12}(\mathbf{p}) + \hat{\rho}_{34}(\mathbf{p})] + 2 \cos(2\phi_p) \cos \theta_p \text{Im}[\hat{\rho}_{13}(\mathbf{p}) - \hat{\rho}_{24}(\mathbf{p})] - \sin(2\phi_p) [1 + \cos^2 \theta_p] \text{Re}[\hat{\rho}_{13}(\mathbf{p}) - \hat{\rho}_{24}(\mathbf{p})] \}. \quad (5)$$

Here, the Hermitian property of the distribution function, i.e.,  $\hat{\rho}(\mathbf{p}) = \hat{\rho}^\dagger(\mathbf{p})$ , has been used. It is clear from Eq. (5) that contributions to the spin-Hall current arise only from those elements of the distribution function which describe the interband polarization, such as  $\hat{\rho}_{12}(\mathbf{p})$ ,  $\hat{\rho}_{13}(\mathbf{p})$ ,  $\hat{\rho}_{34}(\mathbf{p})$ , and  $\hat{\rho}_{24}(\mathbf{p})$ . The vanishing of spin-Hall current contributions from the diagonal elements of the distribution function is associated with the helicity degeneracy of the hole bands in  $p$ -type bulk semiconductors. The diagonal elements of the distribution function for holes in same band but with opposite helicities are the same, i.e.,  $\hat{\rho}_{22}(\mathbf{p}) = \hat{\rho}_{33}(\mathbf{p})$  and  $\hat{\rho}_{11}(\mathbf{p}) = \hat{\rho}_{44}(\mathbf{p})$ . However, the corresponding diagonal elements of the single-particle spin current have opposite signs due to opposite helicities,  $(\hat{J}_y^x)_{22}(\mathbf{p}) = -(\hat{J}_y^x)_{33}(\mathbf{p})$  and  $(\hat{J}_y^x)_{11}(\mathbf{p}) = -(\hat{J}_y^x)_{44}(\mathbf{p})$ . As a result, the net contributions to spin-Hall current from the diagonal elements of distribution function are eliminated.

In order to carry out the calculation of spin-Hall current, it is necessary to determine the hole distribution function.<sup>25</sup> Under homogeneous and steady-state conditions, the spin-basis distribution  $\check{\rho}(\mathbf{p})$  obeys a kinetic equation taken in the form

$$e\mathbf{E} \cdot [\nabla_{\mathbf{p}} \check{\rho}(\mathbf{p})] + i[\check{h}_0(\mathbf{p}), \check{\rho}(\mathbf{p})] = -\check{I}, \quad (6)$$

with  $\check{I}$  as a collision term given by

$$\check{I} = \int \frac{d\omega}{2\pi} (\check{\Sigma}_{\mathbf{p}}^r \check{G}_{\mathbf{p}}^< + \check{\Sigma}_{\mathbf{p}}^< \check{G}_{\mathbf{p}}^a - \check{G}_{\mathbf{p}}^r \check{\Sigma}_{\mathbf{p}}^< - \check{G}_{\mathbf{p}}^< \check{\Sigma}_{\mathbf{p}}^a). \quad (7)$$

$\check{G}_{\mathbf{p}}^{r,a,<}$  and  $\check{\Sigma}_{\mathbf{p}}^{r,a,<}$  are, respectively, the nonequilibrium Green’s functions and self-energies. For brevity, hereafter, the argument  $(\mathbf{p}, \omega)$  of these functions will be denoted by a subscript  $\mathbf{p}$ . In the kinetic equation (6) above, the hole-impurity scattering is embedded in the self-energies  $\check{\Sigma}_{\mathbf{p}}^{r,a,<}$ . In present paper, we consider hole-impurity collisions only in the self-consistent Born approximation. It is widely accepted that this is sufficiently accurate to analyze transport properties in the diffusive regime. Accordingly, the self-energies take the forms  $\check{\Sigma}_{\mathbf{p}}^{r,a,<} = n_i \sum_{\mathbf{k}} |V(\mathbf{p} - \mathbf{k})|^2 \check{G}_{\mathbf{k}}^{r,a,<}$ , with impurity density  $n_i$ .

It is most convenient to study the hole distribution function in the helicity basis,  $\hat{\rho}(\mathbf{p}) = U^+(\mathbf{p}) \check{\rho}(\mathbf{p}) U(\mathbf{p})$ , because, there, the unperturbed equilibrium distribution and the equilibrium lesser, retarded, and advanced Green’s functions are all diagonal. To derive the kinetic equation for the helicity-basis distribution  $\hat{\rho}(\mathbf{p})$ , we multiply Eq. (6) from left by  $U_{\mathbf{p}}^\dagger$  and from right by  $U_{\mathbf{p}}$ . Due to the unitarity of  $U_{\mathbf{p}}$ , the collision term in the helicity basis  $\hat{I}$  has a form similar to Eq. (7),

but with the helicity-basis Green's functions and self-energies,  $\hat{G}_p^{r,a,<} = U^+(\mathbf{p})\check{G}_p^{r,a,<}U(\mathbf{p})$  and  $\hat{\Sigma}_p^{r,a,<} = U^+(\mathbf{p})\check{\Sigma}_p^{r,a,<}U(\mathbf{p})$ , respectively, replacing those of the spin basis,  $\check{G}_p^{r,a,<}$  and  $\check{\Sigma}_p^{r,a,<}$ . The left-hand side (LHS) of Eq. (6) is simplified by using the following facts:  $U_p^+\nabla_p\check{\rho}(\mathbf{p})U_p = \nabla_p\hat{\rho}(\mathbf{p}) - \nabla_p U_p^+U_p\hat{\rho}(\mathbf{p}) - \hat{\rho}(\mathbf{p})U_p^+\nabla_p U_p$  and  $\nabla_p U_p^+U_p = -U_p^+\nabla_p U_p$ . Thus the kinetic equation in helicity basis may be written as

$$e\mathbf{E} \cdot \{\nabla_p\hat{\rho}(\mathbf{p}) + [\hat{\rho}(\mathbf{p}), \nabla_p U_p^+U_p]\} + i[\hat{h}_0(p), \hat{\rho}(\mathbf{p})] = -\hat{I}. \quad (8)$$

In this equation, the helicity-basis self-energies  $\hat{\Sigma}_p^{r,a,<}$  take the forms

$$\hat{\Sigma}_p^{r,a,<} = n_i \sum_{\mathbf{k}} \hat{T}(\mathbf{p}, \mathbf{k}) \hat{G}_k^{r,a,<} \hat{T}^+(\mathbf{p}, \mathbf{k}). \quad (9)$$

In this paper, we restrict our considerations to the linear-response regime. In connection with this, all the functions, such as the nonequilibrium Green's functions, self-energies, and distribution, can be expressed as sums of two terms:  $A = A_0 + A_1$ , with  $A$  as the Green's functions, self-energies, or distribution function.  $A_0$  and  $A_1$ , respectively, are the unperturbed part and the linear electric-field part of  $A$ . In this way, the kinetic equation for the linear electric-field part of the distribution  $\hat{\rho}_1(\mathbf{p})$  can be written as

$$e\mathbf{E} \cdot \nabla_p \hat{\rho}_0(\mathbf{p}) - e\mathbf{E} \cdot [\hat{\rho}_0(\mathbf{p}), U_p^+\nabla_p U_p] + i[\hat{h}_0(\mathbf{p}), \hat{\rho}_1(\mathbf{p})] = -\hat{I}^{(1)}, \quad (10)$$

with  $\hat{I}^{(1)}$  as the linear electric-field part of the collision term  $\hat{I}$ :

$$\hat{I}^{(1)} = \int \frac{d\omega}{2\pi} [\hat{\Sigma}_{1p}^r \hat{G}_{0p}^< + \hat{\Sigma}_{1p}^< \hat{G}_{0p}^a - \hat{G}_{1p}^r \hat{\Sigma}_{0p}^< - \hat{G}_{1p}^< \hat{\Sigma}_{0p}^a + \hat{\Sigma}_{0p}^r \hat{G}_{1p}^< + \hat{\Sigma}_{0p}^< \hat{G}_{1p}^a - \hat{G}_{0p}^r \hat{\Sigma}_{1p}^< - \hat{G}_{0p}^< \hat{\Sigma}_{1p}^a]. \quad (11)$$

Further, we employ a two-band generalized Kadanoff-Baym ansatz (GKBA) (Refs. 26 and 27) to simplify Eq. (10). This ansatz, which expresses the lesser Green's function through the Wigner distribution function, has been proven sufficiently accurate to analyze transport and optical properties in semiconductors.<sup>28</sup> To first order in the dc field strength, the GKBA reads

$$\hat{G}_{1p}^< = -\hat{G}_{0p}^r \hat{\rho}_1(\mathbf{p}) + \hat{\rho}_1(\mathbf{p}) \hat{G}_{0p}^a - \hat{G}_{1p}^r \hat{\rho}_0(\mathbf{p}) + \hat{\rho}_0(\mathbf{p}) \hat{G}_{1p}^a, \quad (12)$$

where the equilibrium distribution and retarded and advanced Green's functions are all diagonal matrices:  $\hat{\rho}_0(\mathbf{p}) = \text{diag}[n_F(\varepsilon_H(p)), n_F(\varepsilon_L(p)), n_F(\varepsilon_L(p)), n_F(\varepsilon_H(p))]$  and  $\hat{G}_0^{r,a}(\mathbf{p}) = \text{diag}[(\omega - \varepsilon_H(p) \pm i\delta)^{-1}, (\omega - \varepsilon_L(p) \pm i\delta)^{-1}, (\omega - \varepsilon_L(p) \pm i\delta)^{-1}, (\omega - \varepsilon_H(p) \pm i\delta)^{-1}]$ , with the Fermi function  $n_F(\omega)$ . We note that  $\hat{G}_{1p}^{r,a}$  in the collision term leads to a collisional broadening of the nonequilibrium distribution. In the present transport study, such collisional broadening plays a secondary role and can be ignored. Based on this, the collision term

$\hat{I}^{(1)}$  no longer involves the linear electric-field part of the retarded and advanced Green's functions.

It is obvious that the driving force in Eq. (10) comprises two components: the first of which,  $e\mathbf{E} \cdot \nabla_p \hat{\rho}_0$ , is diagonal, while another one,  $-e\mathbf{E} \cdot [\hat{\rho}_0(\mathbf{p}), U_p^+\nabla_p U_p]$ , has null diagonal elements. In connection with this, we formally split the kinetic equation into two equations with  $\hat{\rho}_1(\mathbf{p}) = \hat{\rho}_1^I(\mathbf{p}) + \hat{\rho}_1^{II}(\mathbf{p})$  as

$$e\mathbf{E} \cdot \nabla_p \hat{\rho}_0(\mathbf{p}) + i[\hat{h}_0(\mathbf{p}), \hat{\rho}_1^I(\mathbf{p})] = -\hat{I}^{(1)}, \quad (13)$$

$$-e\mathbf{E} \cdot [\hat{\rho}_0(\mathbf{p}), U_p^+\nabla_p U_p] + i[\hat{h}_0(\mathbf{p}), \hat{\rho}_1^{II}(\mathbf{p})] = 0, \quad (14)$$

wherein  $\hat{\rho}_1^I(\mathbf{p})$  and  $\hat{\rho}_1^{II}(\mathbf{p})$  can be approximately determined independently, as discussed below. We note that the solution of Eq. (14),  $\hat{\rho}_1^{II}(\mathbf{p})$ , is off-diagonal and independent of impurity scattering. The matrix elements of  $\hat{\rho}_1^{I,II}(\mathbf{p})$  will be denoted by  $(\hat{\rho}_1^{I,II})_{\mu\nu}(\mathbf{p})$ , and from Eqs. (4) and (5), we correspondingly write spin-Hall conductivity contributions based on  $J_y^x = J_y^{xI} + J_y^{xII}$  as

$$(\sigma^J)_{yz}^x = J_y^{xI}/E = \sum_{\mathbf{p}} \text{Tr}[\hat{J}_y^x(\mathbf{p}) \hat{\rho}_1^I(\mathbf{p})];$$

$$(\sigma^J)_{yz}^x = J_y^{xII}/E = \sum_{\mathbf{p}} \text{Tr}[\hat{J}_y^x(\mathbf{p}) \hat{\rho}_1^{II}(\mathbf{p})]. \quad (15)$$

It is evident that the diagonal driving term of Eq. (13),  $e\mathbf{E} \cdot \nabla_p \hat{\rho}_0$ , is free of impurity scattering. Since  $[\hat{h}_0, \hat{\rho}_1^I(\mathbf{p})]$  is off-diagonal, the diagonal parts of this equation lead to diagonal  $\hat{\rho}_1^I(\mathbf{p})$  elements,  $(\hat{\rho}_1^I)_{\mu\mu}(\mathbf{p})$  ( $\mu = 1 \cdots 4$ ), of order of  $(n_i)^{-1}$  in the impurity density. Substituting these diagonal elements,  $(\hat{\rho}_1^I)_{\mu\mu}(\mathbf{p})$ , into the off-diagonal elements of the scattering term  $\hat{I}^{(1)}$  and considering the fact that the terms on the LHS of the off-diagonal components of Eq. (13) are proportional to the off-diagonal elements of  $\hat{\rho}_1^I(\mathbf{p})$ , we find that the leading order of the off-diagonal elements of  $\hat{\rho}_1^I(\mathbf{p})$  in the impurity-density expansion is of order  $(n_i)^0$ , i.e., independent of  $n_i$ . This result implies that, in general, there always exists a contribution to the spin-Hall current which is disorder related but independent of impurity density within the diffusive regime. On the other hand, the off-diagonal impurity-density-independent  $\hat{\rho}_1^I(\mathbf{p})$  elements, as well as all the nonvanishing elements of  $\hat{\rho}_1^{II}(\mathbf{p})$ , make contributions to the scattering term,  $\hat{I}^{(1)}$ , which are linear in the impurity density, while the  $\hat{I}^{(1)}$  terms involving diagonal elements  $(\hat{\rho}_1^I)_{\mu\mu}(\mathbf{p})$  are independent of  $n_i$ . Hence the contributions to  $\hat{I}^{(1)}$  from off-diagonal elements of  $\hat{\rho}_1(\mathbf{p})$  can be ignored and  $\hat{I}^{(1)}$  effectively involves only the diagonal elements of the distribution. Correspondingly, Eqs. (13) and (14) are approximately independent of each other and can be solved separately.

## B. Disorder-independent spin-Hall effect

The disorder-independent spin-Hall current is associated with  $\hat{\rho}_1^{II}(\mathbf{p})$ , the solution of Eq. (14). The nonvanishing elements of this function are given by

$$\begin{aligned}
(\hat{\rho}_1^H)_{12}(\mathbf{p}) &= -(\hat{\rho}_1^H)_{21}(\mathbf{p}) = (\hat{\rho}_1^H)_{34}(\mathbf{p}) = -(\hat{\rho}_1^H)_{43}(\mathbf{p}) \\
&= \frac{\sqrt{3}m}{4\gamma_2 p^3} i e E \sin \theta_{\mathbf{p}} [f_0^H(p) - f_0^L(p)], \quad (16)
\end{aligned}$$

with  $f_0^H(p) = n_F[\varepsilon_H(p)]$  and  $f_0^L(p) = n_F[\varepsilon_L(p)]$ , while its remaining elements, such as  $(\hat{\rho}_1^H)_{13}(\mathbf{p})$ ,  $(\hat{\rho}_1^H)_{24}(\mathbf{p})$ , etc. vanish. Substituting  $\hat{\rho}_1^H(\mathbf{p})$  into Eq. (5), we find that the disorder-independent contribution to intrinsic spin-Hall current  $J_y^x|I$  can be written as

$$J_y^x|I = \frac{eE}{6\pi^2} \int_0^\infty [f_0^H(p) - f_0^L(p)] dp. \quad (17)$$

This result agrees with that obtained in Ref. 24.

Obviously, the nonvanishing of  $J_y^x|I$  is associated with the nonzero driving term on the LHS of Eq. (14), which is just the interband electric dipole moment between the heavy- and light-hole bands. Thus the disorder-independent spin-Hall effect arises essentially from the polarization process between two hole bands directly induced by the dc electric field. Such a polarization can also be interpreted as a two-band quantum interference process. It should be noted that this polarization process affects only those off-diagonal  $\hat{\rho}_1^H(\mathbf{p})$  elements which describe dc-field induced transitions between hole states in the light- and heavy-hole bands. Of course, such transition processes are not restricted only to hole states in the vicinity of the Fermi surface: they contribute from all the hole states below the Fermi surface. As a result, the disorder-independent spin-Hall current given by Eq. (17) is a function of the entire unperturbed equilibrium distribution  $n_F(\omega)$ , not just of its derivative  $\partial n_F(\omega)/\partial \omega$ , at the Fermi surface.

### C. Disorder-related spin-Hall effect

To simplify Eq. (13), we first analyze symmetry relations between the elements of the distribution function  $\hat{\rho}_1^I(\mathbf{p})$  in the self-consistent Born approximation. Since the distribution function is a Hermitian matrix, only the independent elements  $(\hat{\rho}_1^I)_{\mu\nu}(\mathbf{p})$  with  $\mu, \nu = 1-4$  and  $\mu \leq \nu$  need to be considered. We know that  $(\hat{\rho}_1^I)_{11}(\mathbf{p})$  and  $(\hat{\rho}_1^I)_{44}(\mathbf{p})$  describe the distributions of the heavy holes having spins  $S_z = 3/2$  and  $S_z = -3/2$ , respectively. In equilibrium, heavy hole populations in degenerate states with  $S_z = 3/2$  and  $S_z = -3/2$  distribute equally. Out of equilibrium, the dc electric field action on these hole populations is also the same. Hence the nonequilibrium distribution of the heavy holes with  $S_z = 3/2$  is the same as that of the heavy holes with  $S_z = -3/2$ , i.e.,  $(\hat{\rho}_1^I)_{11}(\mathbf{p}) = (\hat{\rho}_1^I)_{44}(\mathbf{p})$ . An analogous relation for light holes is also expected to be valid:  $(\hat{\rho}_1^I)_{22}(\mathbf{p}) = (\hat{\rho}_1^I)_{33}(\mathbf{p})$ . Indeed, substituting these symmetrically related diagonal elements of the distribution  $\hat{\rho}_1^I(\mathbf{p})$  into the scattering term, we find  $\hat{I}_{11}^{(1)} = \hat{I}_{44}^{(1)}$ ,  $\hat{I}_{22}^{(1)} = \hat{I}_{33}^{(1)}$ , and  $\hat{I}_{23}^{(1)} = \hat{I}_{32}^{(1)} = \hat{I}_{14}^{(1)} = \hat{I}_{41}^{(1)} = 0$ , which are consistent with the elements on the LHS of Eq. (13). As another consequence of these relations  $[(\hat{\rho}_1^I)_{11}(\mathbf{p}) = (\hat{\rho}_1^I)_{44}(\mathbf{p})$  and  $(\hat{\rho}_1^I)_{22}(\mathbf{p}) = (\hat{\rho}_1^I)_{33}(\mathbf{p})]$ , we also obtain symmetry relations between the remaining off-diagonal elements of  $\hat{I}^{(1)}$ :  $\hat{I}_{12}^{(1)} = -\hat{I}_{34}^{(1)}$  and  $\hat{I}_{13}^{(1)} = \hat{I}_{24}^{(1)}$ , which result in symmetry relations for the  $\hat{\rho}_1^I(\mathbf{p})$  ele-

ments as  $(\hat{\rho}_1^I)_{12}(\mathbf{p}) = (\hat{\rho}_1^I)_{34}(\mathbf{p})$  and  $(\hat{\rho}_1^I)_{13}(\mathbf{p}) = -(\hat{\rho}_1^I)_{24}(\mathbf{p})$ . Hence to determine the disorder-related spin-Hall effect, one only needs to evaluate the diagonal elements,  $(\hat{\rho}_1^I)_{11}(\mathbf{p})$  and  $(\hat{\rho}_1^I)_{22}(\mathbf{p})$ , and the off-diagonal elements,  $(\hat{\rho}_1^I)_{12}(\mathbf{p})$  and  $(\hat{\rho}_1^I)_{13}(\mathbf{p})$ .

From Eq. (13), it follows that the diagonal  $\hat{\rho}_1^I(\mathbf{p})$  elements are determined by the integral equation

$$\begin{aligned}
-e\mathbf{E} \cdot \nabla_{\mathbf{p}} n_F[\varepsilon_\mu(p)] &= \pi \sum_{\mathbf{k}} |V(\mathbf{p}-\mathbf{k})|^2 \{a_1(\mathbf{p}, \mathbf{k}) [(\hat{\rho}_1^I)_{\mu\mu}(\mathbf{p}) \\
&\quad - (\hat{\rho}_1^I)_{\mu\mu}(\mathbf{k})] \Delta_{\mu\mu} + a_2(\mathbf{p}, \mathbf{k}) [(\hat{\rho}_1^I)_{\mu\mu}(\mathbf{p}) \\
&\quad - (\hat{\rho}_1^I)_{\bar{\mu}\bar{\mu}}(\mathbf{k})] \Delta_{\mu\bar{\mu}}\}. \quad (18)
\end{aligned}$$

Here,  $\mu = 1, 2$ , respectively, correspond to the heavy- and light-hole bands:  $\varepsilon_1(p) \equiv \varepsilon_H(p)$ ,  $\varepsilon_2(p) \equiv \varepsilon_L(p)$ ,  $\bar{\mu} = 3 - \mu$ ,  $\Delta_{\mu\nu} = \delta[\varepsilon_\mu(p) - \varepsilon_\nu(k)]$ . The factors  $a_1(\mathbf{p}, \mathbf{k})$  and  $a_2(\mathbf{p}, \mathbf{k})$  are associated only with the momentum angles:

$$\begin{aligned}
a_1(\mathbf{p}, \mathbf{k}) &= \frac{1}{4} \{2 + 6 \cos^2 \phi_{pk} [\sin^2 \theta_{\mathbf{p}} - \cos^2 \theta_{\mathbf{k}}] \\
&\quad + 6 \cos^2 \theta_{\mathbf{p}} \cos^2 \theta_{\mathbf{k}} [1 + \cos^2 \phi_{pk}] \\
&\quad + 3 \cos \phi_{pk} \cos(2\theta_{\mathbf{p}}) \cos(2\theta_{\mathbf{k}})\}, \quad (19)
\end{aligned}$$

$$a_2(\mathbf{p}, \mathbf{k}) = 2 - a_1(\mathbf{p}, \mathbf{k}), \quad (20)$$

where  $\phi_{pk} \equiv \phi_{\mathbf{p}} - \phi_{\mathbf{k}}$ . From Eq. (18), we see that we may remove the dependence of  $(\hat{\rho}_1^I)_{\mu\mu}(\mathbf{p})$  on momentum angle  $\phi_{\mathbf{p}}$  by redefining the angular integration variable as  $\phi_{\mathbf{k}} \rightarrow \phi_{pk} = \phi_{\mathbf{p}} - \phi_{\mathbf{k}}$ , taken jointly with the facts that the left hand side does not depend on  $\phi_{\mathbf{p}}$  and the potential  $V(\mathbf{p}-\mathbf{k})$ , as well as the factors  $a_1(\mathbf{p}, \mathbf{k})$  and  $a_2(\mathbf{p}, \mathbf{k})$ , depends on  $\phi_{\mathbf{p}}$  and  $\phi_{\mathbf{k}}$  only through the combination  $\phi_{pk}$ .

Analyzing the components of the scattering term in the kinetic equation for the off-diagonal elements,  $(\hat{\rho}_1^I)_{12}(\mathbf{p})$  and  $(\hat{\rho}_1^I)_{13}(\mathbf{p})$ , we find that these elements of the distribution  $\hat{\rho}_1^I(\mathbf{p})$  are similarly effectively independent of  $\phi_{\mathbf{p}}$ . In connection with this, contributions to the disorder-related spin-Hall current  $J_y^x|I$  from  $(\hat{\rho}_1^I)_{13}(\mathbf{p})$  and  $\text{Re}[(\hat{\rho}_1^I)_{12}(\mathbf{p})]$  vanish under the  $\phi_{\mathbf{p}}$  integration in Eq. (5), and only the imaginary part of  $(\hat{\rho}_1^I)_{12}(\mathbf{p})$  makes a nonvanishing contribution to  $J_y^x|I$ . Hence

$$J_y^x|I = \frac{8\sqrt{3}\gamma_2}{m} \sum_{\mathbf{p}} p \{ \cos^2 \phi_{\mathbf{p}} \sin \theta_{\mathbf{p}} \text{Im}[(\hat{\rho}_1^I)_{12}(\mathbf{p})] \}, \quad (21)$$

with

$$\begin{aligned}
\text{Im}[(\hat{\rho}_1^I)_{12}(\mathbf{p})] &= \frac{\sqrt{3}\pi m}{4\gamma_2 p^2} \sum_{\mathbf{k}, \mu=1,2} |V(\mathbf{p}-\mathbf{k})|^2 a_3(\mathbf{p}, \mathbf{k}) \\
&\quad \times (-1)^\mu \{ \Delta_{\mu\mu} [(\hat{\rho}_1^I)_{\mu\mu}(\mathbf{p}) - (\hat{\rho}_1^I)_{\mu\mu}(\mathbf{k})] \\
&\quad - \Delta_{\mu\bar{\mu}} [(\hat{\rho}_1^I)_{\mu\mu}(\mathbf{p}) - (\hat{\rho}_1^I)_{\bar{\mu}\bar{\mu}}(\mathbf{k})] \}, \quad (22)
\end{aligned}$$

and

$$\begin{aligned}
a_3(\mathbf{p}, \mathbf{k}) &= -\frac{1}{2} \{ \sin(2\theta_{\mathbf{p}}) [\cos^2 \theta_{\mathbf{k}} - \sin^2 \theta_{\mathbf{k}} \cos^2 \phi_{pk}] \\
&\quad + \sin(2\theta_{\mathbf{k}}) \cos \phi_{pk} [1 - 2 \cos^2 \theta_{\mathbf{p}}] \}. \quad (23)
\end{aligned}$$

From Eqs. (18) and (22) we see that  $J_y^x|I$  is independent of impurity density. In contrast to the disorder-independent case, the disorder-related spin-Hall current involves only the derivative of the equilibrium distribution function, i.e.,  $\partial n_F(\omega)/\partial\omega$ . This implies that  $J_y^x|I$  is constituted of contributions arising only from hole states in the vicinity of the Fermi surface, or in other words, from hole states involved in longitudinal transport. Physically, the holes participating in transport experience impurity scattering, producing diagonal  $\hat{\rho}_1^I(\mathbf{p})$  elements of order of  $n_i^{-1}$ . Moreover, the scattering of these perturbed holes by impurities also gives rise to an interband polarization, which no longer depends on impurity density within the diffusive regime. It is obvious that in such a polarization process the disorder plays only an intermediate role. It should be noted that  $J_y^x|I$  generally depends on the form of the hole-impurity scattering potential, notwithstanding its independence of impurity density in the diffusive regime.

The fact that the total spin-Hall current,  $J_y^x = J_y^x|I + J_y^x|II$ , consists of two parts associated with hole states below and near the Fermi surface, respectively, is similar to the well-known result of Středa<sup>29</sup> in the context of the 2D charge Hall effect. In 2D electron systems in a normal magnetic field, the off-diagonal conductivity usually arises from two terms, one of which is due to electron states near the Fermi energy and the other is related to the contribution of all occupied electron states below the Fermi energy. A similar picture has also recently emerged in studies of the anomalous Hall effect.<sup>30,31</sup>

### III. RESULTS AND DISCUSSIONS

To compare our results with the short-range result presented in Ref. 21, we first consider a short-range hole-impurity scattering potential described by  $V(\mathbf{p}-\mathbf{k}) \equiv u$ , with  $u$  as a constant. Substituting Eq. (22) into Eq. (5) and performing integrations with respect to the angles of  $\mathbf{p}$  or  $\mathbf{k}$ , respectively, for terms involving  $(\hat{\rho}_1^I)_{\mu\mu}(\mathbf{k})$  or  $(\hat{\rho}_1^I)_{\mu\mu}(\mathbf{p})$ , we find that the contribution of short-range disorder to the spin-Hall current vanishes, i.e.,  $J_y^x|I = 0$ . This implies that for short-range hole-impurity collisions, the total spin-Hall current is just the disorder-independent one,  $J_y^x = J_y^x|II$ . This result agrees with that obtained in Ref. 21.

Furthermore, we perform a numerical calculation to investigate the effect of long-range hole-impurity collisions on the spin-Hall current in a GaAs bulk semiconductor. The long-range scattering is described by a screened Coulombic impurity potential  $V(p)$ :  $V(p) = e^2/(\epsilon_0\epsilon)[p^2 + 1/d_D^2]^{-1}$  with  $\epsilon$  as a static dielectric constant.<sup>32</sup>  $d_D$  is a Thomas-Fermi-Debye-type screening length:

$$d_D^2 = \pi^2 \epsilon_0 \epsilon / (e^2 \sqrt{2m^3 E_F} 2^{-1/3}) \\ \times [(\gamma_1 + 2\gamma_2)^{-3/2} + (\gamma_1 - 2\gamma_2)^{-3/2}]^{-2/3},$$

with  $E_F = (3\pi^2 N_p/2)^{2/3}/(2m)$ . The material parameters  $\gamma_1$  and  $\gamma_2$  are chosen to be 6.85 and 2.5, respectively.<sup>33</sup> In our calculation, the momentum integration is computed by the Gauss-Legendre scheme.

In the present paper, we address the spin-Hall effect at zero temperature,  $T=0$ . In this case, the disorder-independent spin-Hall current can be obtained analytically from Eq. (17):

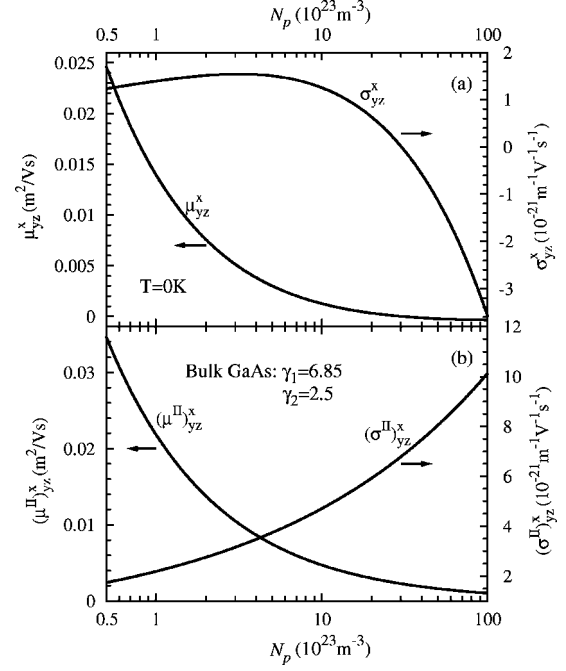


FIG. 1. Hole-density dependencies of (a) total  $\sigma_{yz}^x$  and  $\mu_{yz}^x$ , and (b) disorder-independent  $(\sigma_{yz}^II)^x$  and  $(\mu_{yz}^II)^x$ , in a bulk GaAs semiconductor. The material parameters for GaAs are  $\gamma_1=6.85$  and  $\gamma_2=2.5$ . The lattice temperature is  $T=0$  K.

$J_y^x|II = eE[k_F^H - k_F^L]/(6\pi^2)$ , with  $k_F^H$  and  $k_F^L$  as the Fermi momenta for heavy- and light-hole bands, respectively. In order to investigate the disorder-related spin-Hall effect, we need to compute the distribution function  $\hat{\rho}_1^I(\mathbf{p})$  at the Fermi surface. In this calculation, we employ a “singular value decomposition” method<sup>34</sup> to solve the integral equation, Eq. (18), for the diagonal  $\hat{\rho}_1^I(\mathbf{p})$  elements. The obtained diagonal elements are then employed to determine  $\text{Im}[(\hat{\rho}_1^I)_{12}(\mathbf{p})]$  using Eq. (22). Following that, we obtain the disorder-related spin-Hall current from Eq. (21), performing the momentum integration.

In Fig. 1, the calculated total and disorder-independent spin-Hall conductivities,  $\sigma_{yz}^x = J_y^x/E$  and  $(\sigma_{yz}^II)^x = J_y^x|II/E$ , and the total and disorder-independent spin-Hall mobilities,  $\mu_{yz}^x = \sigma_{yz}^x/N_p$  and  $(\mu_{yz}^II)^x = (\sigma_{yz}^II)^x/N_p$ , are shown as functions of the hole density. The spin-Hall mobility, analogous to the mobility of charge transport, characterizes the average mobility of a single spin driven by the external field. This quantity has the same units in 2D and 3D systems.

From Fig. 1, we see that, with increasing hole density, the total spin-Hall conductivity first increases and then decreases and even becomes negative as the hole density becomes larger than  $N_{pc} = 3 \times 10^{24} \text{ m}^{-3}$ . This behavior of the hole-density dependence of total spin-Hall conductivity is the result of a competition between the disorder-independent and disorder-related processes. The contributions to spin-Hall conductivity from these two processes always have opposite signs and their absolute values increase with increasing hole density. Considering total spin-Hall conductivity, the disorder-related part,  $(\sigma_{yz}^II)^x$ , is dominant for high hole density, while  $(\sigma_{yz}^I)^x$  is important in the low hole-density regime.

Notwithstanding this hole-density dependence of  $\sigma_{yz}^x$ , the total spin-Hall mobility  $\mu_{yz}^x$  as well as the disorder-independent one, monotonically decreases with increasing hole density.

It should be noted that the total spin-Hall mobility in bulk systems has the same order of magnitude as that in 2D hole systems. We know that the spin-Hall conductivity in 2D hole systems is of order of  $e/\pi$ .<sup>19</sup> For a typical 2D hole density,  $n_p^{(2D)} = 1 \times 10^{12} \text{ cm}^{-2}$ , the corresponding spin-Hall mobility is about  $0.05 \text{ m}^2/\text{Vs}$ .

In the present paper, we have ignored the effect of collisional broadening on spin-Hall current. Since  $J_y^{x||}$  is associated only with the hole states in the vicinity of the Fermi surface, the neglect of broadening in the disorder-related spin-Hall current is valid for  $\varepsilon_F \tau > 1$  ( $\varepsilon_F$  is the Fermi energy and  $\tau$  is the larger of the relaxation times for holes in the different bands at the Fermi surface,  $\tau_L(\varepsilon_F)$  and  $\tau_H(\varepsilon_F)$ :  $\tau = \max[\tau_L(\varepsilon_F), \tau_H(\varepsilon_F)]$ ). This condition coincides with the usual restriction on transport in the diffusive regime and is satisfied for  $p$ -type bulk GaAs with mobility approximately larger than  $1 \text{ m}^2/\text{Vs}$  (for  $N_p > 5 \times 10^{22} \text{ m}^{-3}$ ). On the other hand, the disorder-independent spin-Hall conductivity involves contributions from all hole states in the Fermi sea and hence it may be strongly affected by collisional broadening. To estimate the broadening effect on the disorder-independent SHE, we add an imaginary part to  $\hat{h}_0(\mathbf{p})$  and use  $\hat{h}_0(\mathbf{p}) + i\hat{\gamma}(\mathbf{p})$  instead of  $\hat{h}_0(\mathbf{p})$  in Eq. (14) [ $\hat{\gamma}(\mathbf{p})$  is a diagonal matrix describing the broadening:  $(\hat{\gamma})_{11}(\mathbf{p}) = (\hat{\gamma})_{44}(\mathbf{p}) = 1/2\tau_H(\varepsilon_H(p))$  and  $(\hat{\gamma})_{22}(\mathbf{p}) = (\hat{\gamma})_{33}(\mathbf{p}) = 1/2\tau_L(\varepsilon_L(p))$ ]. In this way,  $J_y^{x||}$  takes a form similar to Eq. (17) but with an additional factor,  $(2\gamma_2 p^2)^2 / \{ [2\gamma_2 p^2]^2 + [1/2\tau_H(\varepsilon_H(p)) - 1/2\tau_L(\varepsilon_L(p))]^2 \}$ , in the momentum integrand. Performing a numerical calculation, we find that, in the studied regime of hole density, the effect of collisional broadening on the disorder-independent spin-Hall current is less than 1% for  $p$ -type bulk GaAs semiconductors with mobility approximately larger than  $5 \text{ m}^2/\text{Vs}$ . Thus, in such systems, the effect of collisional broadening on the total spin-Hall conductivity can be ignored. It should be noted that in our calculations, we computed  $\tau_{L,H}(\varepsilon)$  by considering short-range hole-impurity scattering:  $1/\tau_{L,H}(\varepsilon) = 2\pi n_i u^2 \nu_{L,H}(\varepsilon)$  with the densities of hole states in the light- and heavy-hole bands taken as  $\nu_{L,H}(\varepsilon) = 2\sum_{\mathbf{p}} \delta[\varepsilon - \varepsilon_{L,H}(p)]$ . The quantity  $n_i u^2$  is determined from the mobility of the system:  $\mu = e[N_p^L \tau_L(\varepsilon_F)/m_L + N_p^H \tau_H(\varepsilon_F)/m_H]/N_p$ , where  $m_L = m/(\gamma_1 + 2\gamma_2)$  and  $m_H = m/(\gamma_1 - 2\gamma_2)$  are the effective masses of holes and  $N_p^L/N_p^H = [(\gamma_1 - 2\gamma_2)/(\gamma_1 + 2\gamma_2)]^{3/2}$  with  $N_p^L$  and  $N_p^H$  being the hole

densities in the light- and heavy-hole bands, respectively.

On the other hand, in our considerations, the impurities are taken to be so dense that we can use a statistical average over the impurity configuration. This requires that  $L_D < L$  ( $L$  is the characteristic size of the sample and  $L_D$  is the larger of the diffusion lengths of holes in the light- and heavy-hole bands). Failing this, the behavior of the holes would become ballistic, with transport properties depending on the specific impurity configuration.

#### IV. CONCLUSIONS

We have employed a nonequilibrium Green's function kinetic equation approach to investigate disorder effects on the spin-Hall current in the diffusive regime in  $p$ -type bulk Luttinger semiconductors. Long-range hole-impurity scattering has been considered within the framework of the self-consistent Born approximation. We have found that, in contrast to the null effect of short-range disorder on the spin-Hall current, long-range scattering produces a nonvanishing contribution to the spin-Hall current, independent of impurity density in the diffusive regime. This contribution has its sign opposite to that of the disorder-independent one, leading to a sign change of the total spin-Hall current as the hole density varies. We also made clear that the disorder-independent spin-Hall effect arises from a dc-field-induced polarization associated with all hole states in the Fermi sea, while the disorder-related one is produced by a disorder-mediated polarization and relates to only those hole states in the vicinity of the Fermi surface. The numerical calculation indicates that with increasing hole density, the total spin-Hall mobility monotonically decreases, whereas the spin-Hall conductivity first increases and then falls.

In addition to  $J_y^x$ , we also examined other components of the spin current. We found that the previously discovered "basic spintronics relation,"<sup>23</sup> which relates the  $i$ th component of the spin current along the direction  $j$ ,  $J_j^i$ , and the applied electric field  $E_k$  by  $J_j^i = \sigma_s \epsilon_{ijk} E_k$  with  $\epsilon_{ijk}$  as a totally antisymmetric tensor, still holds in the presence of spin-conserving hole-impurity scattering.

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