Spin Hall Effect in Doped Semiconductor Structures

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In this Letter we present a microscopic theory of the extrinsic spin Hall effect based on the diagrammatic perturbation theory. Side-jump and skew-scattering contributions are explicitly taken into account to calculate the spin Hall conductivity, and we show that their effects scale as $\sigma_{xy}^{\mathrm{SJ}}/\sigma_{xy}^{\mathrm{SS}} \sim (\hbar/\tau)/\varepsilon_F$, with τ being the transport relaxation time. Motivated by recent experimental work we apply our theory to n- and p-doped 3D and 2D GaAs structures, obtaining $\sigma_s/\sigma_c \sim 10^{-3}$–$10^{-4}$, where $\sigma_{s(c)}$ is the spin Hall (charge) conductivity, which is in reasonable agreement with the recent experimental results of Kato *et al.* [Science **306**, 1910 (2004)] in n-doped 3D GaAs system.

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The spin Hall effect (SHE) is an intriguing phenomenon, theoretically predicted [1,2] in 1971, where the application of a longitudinal electric field creates a transverse motion of spins, with the spin-up and spin-down carriers transversing in perpendicular directions with respect to the electric field opposite to each other, leading to a transverse spin current and presumably to spin accumulation at the edges of a bulk sample. There have been enormous recent interest and activity in this topic due to a number of reasons: (1) the emergence of the subject of ''spintronics'' [3] where active control and manipulation of spin dynamics in electronic materials leads to conceptually new functionalities and projected novel device applications; (2) the rediscovery [4] of the original prediction of SHE, and the theoretical prediction and controversy [5–7] surrounding a new type of SHE, called the ''intrinsic'' SHE [5]; and (3) recent reports of the experimental observation [8–10] of SHE in n- and p-doped semiconductor structures by two experimental groups. The fact that the two experimental groups report SHE observations differing by orders of magnitude in strength coupled with claims and counterclaims on whether the experimentally observed effects are the original (in this context referred to as ''extrinsic'') SHE [1,2] or the new intrinsic [5] SHE has made the subject of SHE one of the most intensively studied current topics in electronic solid state physics. The theory of SHE is in flux—although the original extrinsic SHE (arising from the spin-orbit coupling effect in impurity scattering) is on fairly firm conceptual ground, its magnitude has often been claimed to be minuscule (and far too weak to be of any experimental consequence), whereas the very existence of the intrinsic SHE (which arises from the intrinsic spin-orbit coupling effects in the band structure) has often been questioned. Therefore, taking the most pessimistic (optimistic) view of the theoretical literature an impartial observer could reasonably conclude that the SHE is essentially zero (very large in magnitude) always (often).

It is therefore quite important to provide not just general theoretical frameworks but concrete theoretical calculations relating to the specific experimental SHE measurements. In this Letter we provide one such concrete calculation [11] for the recent experimental measurements [8–10] using entirely the extrinsic SHE perspective, completely ignoring any intrinsic SHE considerations [12]. The fact that we get reasonable qualitative agreement with the experimental SHE data from one group [8,9], but not the other [10], is significant in the context of the continuing debate and controversy in the SHE. In particular, our results support the claim [8,9] that the observed SHE in n-doped GaAs is the extrinsic and not the intrinsic SHE. In Ref. [13] the extrinsic SHE is treated in metallic systems. We also emphasize that the extrinsic SHE is always present in a doped semiconductor structure (since it arises from impurity scattering) although its magnitude can be small [12] depending on the strength of the spin-orbit coupling.

In this Letter we confine ourselves to the extrinsic spin Hall effect, which arises from the effects of impurity scattering [1,2]. Drawing similarity with the well-studied anomalous Hall effect [14], we calculate the spin Hall conductivity using diagrammatic perturbation theory. In particular, we derive general expressions for the side-jump and the skew-scattering contributions using the Kubo-Greenwood formula, and then apply the theory, within simplified model approximations, to 3D and 2D doped semiconductor systems obtaining simple analytical formulas for the magnitude of the extrinsic SHE. In two dimensions, we find the spin Hall conductivity to be formally equivalent to the corresponding anomalous Hall conductivity.

The single-particle Hamiltonian, $H = H_0 + H_{\mathrm{SO}} + V$, in the presence of spin-orbit (SO) scattering due to impurities is

$$H = \frac{|\boldsymbol{p} + e\boldsymbol{A}/c|^2}{2m} - \frac{\lambda_0^2}{4}[\boldsymbol{\sigma} \times \boldsymbol{\nabla} V(\boldsymbol{r})] \cdot \boldsymbol{p} + V(\boldsymbol{r}), \quad (1)$$

where m is the carrier effective mass, λ_0 is a length characterizing the strength of SO interaction, $\boldsymbol{A}$ is the vector potential, and all other notations are standard. We note that the SO coupling strength parameter λ_0 is greatly enhanced in the solid state GaAs environment over its free-electron vacuum value of $\hbar/m_e c$, the Compton wavelength. This could be construed as a band-structure-induced renormalization of the effective Compton wavelength (just as the effective mass and the background lattice dielectric constant are modified) in the semiconductor environment. In GaAs this renormalization of the Compton length over its vacuum value is by as much as a factor of 10^3 (or larger), reflecting the much stronger (by 10^6) SO coupling in semiconductors over the corresponding vacuum effect. This leads to a much more enhanced extrinsic SHE in GaAs than the corresponding vacuum estimate. The inclusion of this band structure effect in the SO coupling is the key to understanding the extrinsic SHE in recent experiments [8,9], as has also been emphasized recently by Engel *et al.* [11] in the context of a Boltzmann theory calculation.

We model the impurity scattering potential $V(\boldsymbol{r})$ as a short-range white noise disorder with $\langle V(\boldsymbol{r}_1)V(\boldsymbol{r}_2)\rangle = n_i v_0^2 \delta(\boldsymbol{r}_1 - \boldsymbol{r}_2)$ and $\langle V(\boldsymbol{r}_1)V(\boldsymbol{r}_2)V(\boldsymbol{r}_3)\rangle = n_i v_0^3 \delta(\boldsymbol{r}_1 - \boldsymbol{r}_2)\delta(\boldsymbol{r}_2 - \boldsymbol{r}_3)$. Notice that the third order moment of V is required since the skew-scattering effect shows up only in the third order of the impurity potential. Here n_i is the impurity density, and v_0 is the Fourier component of $V(\boldsymbol{r})$ at $q = 0$, which is related to the scattering amplitude $f(\theta)$ as

$$v_0 = \int d^3 r V(\boldsymbol{r}) = -(4\pi\hbar^2/m) f(\theta = 0). \tag{2}$$

The extrinsic spin Hall effect results from the SO coupling in two ways: the antisymmetry of the matrix element $\langle \boldsymbol{k}|H_{\mathrm{SO}}|\boldsymbol{k}'\rangle$ with respect to interchanging $\boldsymbol{k}$ and $\boldsymbol{k}'$ gives rise to the skew scattering, while the noncommutativity of $\boldsymbol{r}$ and H_{SO}, which results in an extra term—the anomalous current, gives rise to the side jump leading to a renormalization of the current vertex. This is similar to the anomalous Hall effect (AHE) since the same physics underlies both AHE and SHE.

In the following, we proceed to calculate the vertex correction of the spin current (i.e., the side-jump contribution). The spin current $\boldsymbol{j}_s = -e\{\sigma_z, \boldsymbol{u}\}/4$ is calculated as

$$\boldsymbol{j}_s = -e\left[\frac{1}{2m}\left(\boldsymbol{p} + \frac{e}{c}\boldsymbol{A}\right)\sigma_z - \frac{\lambda_0^2}{8}\hat{z} \times \boldsymbol{\nabla} V(\boldsymbol{r})\right], \tag{3}$$

where $\boldsymbol{u} = (i/\hbar)[H, \boldsymbol{r}]$ is the velocity. Here, following standard practice, we have multiplied the conventional definition of the spin current by the electronic charge $-e$ (where $e > 0$) so that it has the same units and dimensions as the charge current. Notice that the second term in Eq. (3) is the "anomalous" contribution to the spin current.

Expressing all quantities from now on in the momentum representation the Hamiltonian in the second quantized form, $H = \int d^3 r \psi^\dagger(\boldsymbol{r}) H \psi(\boldsymbol{r})$, can be written as (we use the same notation H to express the Hamiltonian in the first and the second quantized notations)

$$H = \sum_{\boldsymbol{k}\boldsymbol{k}'} \psi_{\boldsymbol{k}}^\dagger \left\{ \frac{1}{2m} \left| \hbar\boldsymbol{k} + \frac{e}{c}\boldsymbol{A} \right|^2 \delta_{\boldsymbol{k}\boldsymbol{k}'} + V_{\boldsymbol{k}-\boldsymbol{k}'}\left[1 - \frac{i\lambda_0^2}{4}(\boldsymbol{k} \times \boldsymbol{k}') \cdot \boldsymbol{\sigma}\right]\right\}\psi_{\boldsymbol{k}'}, \tag{4}$$

from which the SO vertex correction to the Green function is identified as

$$\langle \boldsymbol{k}|\delta H_{\mathrm{SO}}|\boldsymbol{k}'\rangle = -(i\lambda_0^2/4)(\boldsymbol{k} \times \boldsymbol{k}') \cdot \boldsymbol{\sigma}. \tag{5}$$

The spin current in second quantized form, $\boldsymbol{J}_s = \int d^3 r \psi^\dagger(\boldsymbol{r}) \boldsymbol{j}_s \psi(\boldsymbol{r})$, is

$$\boldsymbol{J}_s = -e \sum_{\boldsymbol{k}\boldsymbol{k}'} \psi_{\boldsymbol{k}}^\dagger \left\{ \frac{\hbar\boldsymbol{k}}{2m}\sigma_z \delta_{\boldsymbol{k}\boldsymbol{k}'} - \frac{i\lambda_0^2}{8} V_{\boldsymbol{k}-\boldsymbol{k}'}[\hat{z} \times (\boldsymbol{k} - \boldsymbol{k}')]\right\}\psi_{\boldsymbol{k}'}, \tag{6}$$

from which the SO vertex renormalization for the spin current can be identified as

$$\delta j_{s,l} = (ie\lambda_0^2/8)\epsilon_{lmz}(k_m' - k_m)V_{\boldsymbol{k}-\boldsymbol{k}'}. \tag{7}$$

The charge current vertex renormalization can also be obtained as

$$\delta j_{c,l} = (ie\lambda_0^2/4)\epsilon_{lmn}(k_m' - k_m)\sigma_n V_{\boldsymbol{k}-\boldsymbol{k}'}. \tag{8}$$

From the Kubo-Greenwood formula, the spin Hall conductivity can be calculated from the spin current-charge current correlation function, which can be represented schematically as a bubble diagram with one spin current vertex and one charge current vertex (Fig. 1).

The retarded and advanced bare Green functions (i.e., without the SO scattering potential) at zero frequency are diagonal matrices with the diagonal elements $G^{R,A}_{\boldsymbol{k}\uparrow\uparrow,\downarrow\downarrow} = [\varepsilon_{F\uparrow,\downarrow} - \varepsilon_{\uparrow,\downarrow}(k) \pm i\hbar/2\tau_{\uparrow,\downarrow}]^{-1}$, where $\uparrow,\downarrow$ signifies spin-up and spin-down species, $\varepsilon_{F\uparrow,\downarrow}$ their Fermi levels, $\varepsilon_{\uparrow,\downarrow} = \hbar^2 k_{\uparrow,\downarrow}^2/2m$ the corresponding kinetic energies. $\tau_{\uparrow,\downarrow}$ are the relaxation times for spin-up and spin-down carriers in the first-order Born approximation given analytically for our short-range scattering as $\tau_{\uparrow,\downarrow} = \hbar/2\pi N_{\uparrow,\downarrow} n_i v_0^2$, with $N_{\uparrow,\downarrow}$ the density of states of the spin-up and spin-down carriers at their respective Fermi levels. Now taking into account of

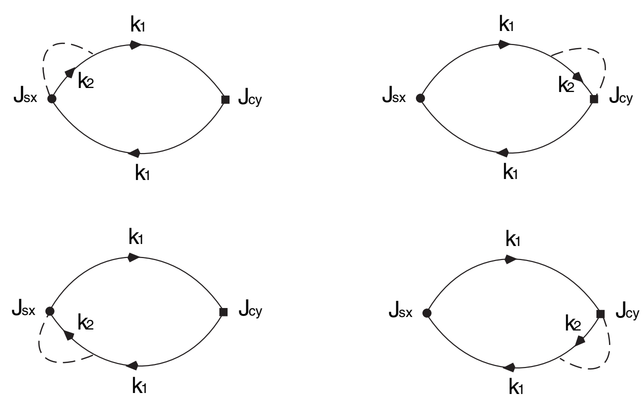

FIG. 1. Diagrams for the side-jump contribution. The vertex correction for the spin current Eq. (7) is denoted by a solid circle connected to a dashed line on the left-side vertex; and the vertex correction for the charge current Eq. (8) by a solid square connected to a dashed line on the right-side vertex. The solid circle or square without a connecting dashed line implies a bare vertex.

the vertex renormalizations of both spin and charge currents (Fig. 1), we find the side-jump contribution as

$$\sigma_{xy}^{\mathrm{SJ}} = \frac{ie^2\lambda_0^2}{8\pi m} n_i v_0^2 \,\mathrm{tr} \sum_{\boldsymbol{k}_1\boldsymbol{k}_2} [k_{1y}^2 G_{\boldsymbol{k}_1}^R G_{\boldsymbol{k}_1}^A (G_{\boldsymbol{k}_2}^R - G_{\boldsymbol{k}_2}^A)]. \quad (9)$$

The skew-scattering contribution can be obtained by keeping up to third order in the scattering potential (Fig. 2). Summing both diagrams in Fig. 2, we obtain

$$\sigma_{xy}^{\mathrm{SS}} = -\frac{ie^2\hbar^2\lambda_0^2}{16\pi m^2} n_i v_0^3 \,\mathrm{tr} \sum_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3} [k_{1x}^2 G_{\boldsymbol{k}_1}^R G_{\boldsymbol{k}_1}^A k_{2y}^2 G_{\boldsymbol{k}_2}^R G_{\boldsymbol{k}_2}^A \times (G_{\boldsymbol{k}_3}^R - G_{\boldsymbol{k}_3}^A)]. \quad (10)$$

Evaluating the integral in Eqs. (9) and (10) for the cases of three dimensions and two dimensions gives

$$\sigma_{xy}^{\mathrm{SJ}} = \begin{Bmatrix} e^2\hbar/12m \\ e^2\hbar/8m \end{Bmatrix} \lambda_0^2 (k_{F\uparrow}^2 N_\uparrow + k_{F\downarrow}^2 N_\downarrow). \quad \begin{matrix} (3\mathrm{D}) \\ (2\mathrm{D}) \end{matrix} \quad (11)$$

$$\sigma_{xy}^{\mathrm{SS}} = \begin{Bmatrix} \pi e^2\hbar^2/36m^2 \\ \pi e^2\hbar^2/16m^2 \end{Bmatrix} \lambda_0^2 v_0 \{k_{F\uparrow}^4 N_\uparrow^2 \tau_\uparrow + k_{F\downarrow}^4 N_\downarrow^2 \tau_\downarrow\}. \quad \begin{matrix} (3\mathrm{D}) \\ (2\mathrm{D}) \end{matrix} \quad (12)$$

In spin Hall effect, one observes the deflection of opposite spins from an unpolarized electron beam, so we set $n_\uparrow = n_\downarrow = n/2$. Here the density of states per spin is $N_{\uparrow,\downarrow} = mk_F/2\pi^2\hbar^2$ for three dimensions and $m/2\pi\hbar^2$ for two dimensions. Equations (11) and (12) are our important extrinsic SHE results for 2D and 3D semiconductor structures within the short-range impurity scattering model. We believe that these analytic formulas would approximately apply even when the impurity scattering is not strictly zero range, e.g., for screened ionized scattering. Assuming the dominant impurities in the semiconductor to be randomly distributed screened ionized impurity centers, we can further simplify our SHE formulas for 2D and 3D doped semiconductor systems. In the first-order Born approximation, the scattering amplitude of the screened Coulomb potential (assuming Thomas-Fermi screening) is $f(\theta) = (2me^2/\hbar^2\epsilon_m)(q^2 + q_{\mathrm{TF}}^2)^{-1}$ in three dimensions, and $f(\theta) = (me^2/\hbar^2\epsilon_m)(q + q_{\mathrm{TF}})^{-1}$ in two dimensions, where ϵ_m is the dielectric constant of the material and $q = 2k\sin(\theta/2)$ is the momentum transfer. The Thomas-Fermi screening wave number is given by $q_{\mathrm{TF}} = \sqrt{6\pi ne^2/\epsilon_m\varepsilon_F}$ for three dimensions and $q_{\mathrm{TF}} = 2\pi ne^2/\epsilon_m\varepsilon_F$ for two dimensions. Using these formulas for the cases of two dimensions and three dimensions, it is then straightforward to calculate the extrinsic SHE contributions using Eqs. (11) and (12) within this simplifying approximation scheme. Accordingly, the side-jump contribution is found to be

$$\sigma_{xy}^{\mathrm{SJ}} = (e^2\lambda_0^2/4\hbar)n, \quad (13)$$

for both 3D and 2D cases, whereas for skew scattering we find

$$\sigma_{xy}^{\mathrm{SS}} = \begin{Bmatrix} -\pi m\lambda_0^2\varepsilon_F/3\hbar^2 \\ -\pi m\lambda_0^2\varepsilon_F/2\hbar^2 \end{Bmatrix} \frac{ne^2\tau}{m}. \quad \begin{matrix} (3\mathrm{D}) \\ (2\mathrm{D}) \end{matrix} \quad (14)$$

We note that the side-jump and the skew-scattering contributions scale as $\sigma_{xy}^{\mathrm{SJ}}/\sigma_{xy}^{\mathrm{SS}} \sim (\hbar/\tau)/\varepsilon_F$. Typically, $\tau \sim 10^{-13}$–10^{-12} s, so the side-jump contribution is approximately comparable to the skew-scattering contribution when the Fermi energy $\varepsilon_F \sim 1$–10 meV.

Some order-of-magnitude estimates from Eqs. (13) and (14) are in order. We choose $\lambda_0 = 4.7 \times 10^{-8}$ cm (which is a factor of 10^3 enhancement over the vacuum electron Compton wavelength of 3.9×10^{-11} cm) in n-GaAs consistent with the expected electronic spin-orbit coupling strength in GaAs [15], which is thus enhanced by 6 orders of magnitude over the corresponding Thomas term in the free-electron vacuum case. For three dimensions, we employ the parameters from the experiment of Kato *et al.* [8,9], where the electron density is $n = 3 \times 10^{16}$ cm^{-3} and the longitudinal conductivity $\sigma_{xx} \simeq 3 \times 10^3\ \Omega^{-1}\,\mathrm{m}^{-1}$. For two dimensions, we take $n = 10^{11}$ cm^{-2} and $\sigma_{xx} = 10^{-4}\ \Omega^{-1}$. In the following, we invert the sign of our calculated values of the spin Hall conductivity for comparison with experimental results where e instead of $-e$ [8] is used in the definition of the spin current Eq. (3). We then get for three dimensions $\sigma_{xy}^{\mathrm{SJ}} = -0.375\ \Omega^{-1}\,\mathrm{m}^{-1}$ and $\sigma_{xy}^{\mathrm{SS}} = 2.97\ \Omega^{-1}\,\mathrm{m}^{-1}$; whereas for two dimensions $\sigma_{xy}^{\mathrm{SJ}} = -1.25 \times 10^{-8}\ \Omega^{-1}\,\mathrm{m}^{-1}$ and $\sigma_{xy}^{\mathrm{SS}} = 10^{-7}\ \Omega^{-1}\,\mathrm{m}^{-1}$. This gives, for three dimensions and two dimensions, respectively, the spin Hall conductivity as $2.6\ \Omega^{-1}\,\mathrm{m}^{-1}$ and $8.8 \times 10^{-8}\ \Omega^{-1}$; and the ratios of the spin Hall conductivity $\sigma_{xy}^{\mathrm{SH}}$ to the longitudinal conductivity σ_{xx} as 8.65×10^{-4} and 8.75×10^{-4}. The experimental SHE quoted in Ref. [8] is about $0.7\ \Omega^{-1}\,\mathrm{m}^{-1}$, which is a factor of ~4 smaller than our estimate. Here we content ourselves with this order-of-magnitude agreement; a more detailed comparison of any theoretically calculated value with the existing experimental values [8] of the spin Hall conductivity should not be taken too seriously, for the spin Hall conductivity was not a directly measured but instead an estimated quantity based on fitting the measured spin accumulation data with a simple assumed spin density profile. We also emphasize our results are only approximate given that the real impurity potential of the scattering centers is not strictly zero range. In addition, we note the crucial point that our calculated SHE is directly proportional to the SO coupling strength λ_0^2, which is only approximately known in GaAs—any inaccuracy in the knowledge [16] of the pre-

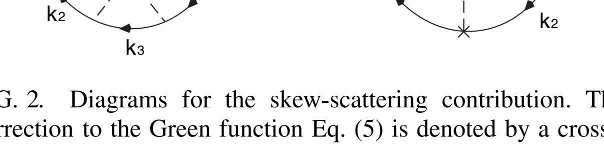

FIG. 2. Diagrams for the skew-scattering contribution. The correction to the Green function Eq. (5) is denoted by a cross.

cise SO coupling is directly reflected in our estimate of the extrinsic SHE. We also point out that the net SHE in our theory is a sum of a positive (side-jump) and a negative (skew-scattering) contribution, further leading to the possibility of quantitative errors. However, the order-of-magnitude agreement of the ratio $\sigma_{xy}^{\mathrm{SH}}/\sigma_{xx}$ between our calculated result and the experiment [8] suggests that the measured effect is indeed extrinsic [12].

Now we briefly extend our discussion to the case of 2D holes using the experimental parameters from the experiment of Wunderlich *et al.* [10], where the hole density is $p = 2 \times 10^{12}$ cm^{-2} and longitudinal conductivity $\sigma_{xx} \simeq 1.09 \times 10^{-3}\ \Omega^{-1}$. We obtain, assuming the same spin-orbit coupling strength λ_0 as in the electron case, $\sigma_{xy}^{\mathrm{SJ}} = -1.55 \times 10^{-8}\ \Omega^{-1}$ and $\sigma_{xy}^{\mathrm{SS}} = 1.36 \times 10^{-6}\ \Omega^{-1}$, giving the total spin Hall conductivity $1.34 \times 10^{-6}\ \Omega^{-1}$ and its ratio to the longitudinal conductivity as 1.23×10^{-3}. This is an order of magnitude lower than the intrinsic value estimated in Ref. [10]. We note, however, that the SO coupling strength parameter for holes is expected to be larger than that for electrons, and therefore the possibility (at least as a matter of principle) that the 2D hole experiment in Ref. [10] is also a measurement of the extrinsic SHE cannot be completely ruled out.

We finally discuss the formal connection between the spin Hall effect and the anomalous Hall effect. First, the side-jump contribution of the anomalous Hall conductivity $\tilde{\sigma}_{xy}^{\mathrm{AH}}$ for both three dimensions and two dimensions can formally be expressed as $\tilde{\sigma}_{xy}^{\mathrm{SJ}} = (e^2\lambda_0^2/2\hbar)s$, where $s = n_\uparrow - n_\downarrow$ is the spin density. Except for the appearance of s instead of n, this formula is very similar to that for the spin Hall effect, Eq. (13). The skew-scattering contribution can be written as $\tilde{\sigma}_{xy}^{\mathrm{SS}} = -(\pi m\lambda_0^2\varepsilon_F/\hbar^2)(2se^2\tau_{\mathrm{eff}}/3m)$ in three dimensions and $-(\pi m\lambda_0^2\varepsilon_F/\hbar^2)(se^2\tau/m)$ in two dimensions, where we have defined $\tau_{\mathrm{eff}} = (k_{F\uparrow}^6\tau_\uparrow - k_{F\downarrow}^6\tau_\downarrow)/(k_{F\uparrow}^6 - k_{F\downarrow}^6)$ for the case of three dimensions to be an effective relaxation time. Now we note that both the skew-scattering and the side-jump contributions for the anomalous Hall effect and the spin Hall effect appear in very similar forms, except for an extra factor of 2 which comes from $\sigma_z/2$ in the definition of the spin Hall current Eq. (3). In the particular case of two dimensions, the relaxation times for spin-up and spin-down carriers are equal, $\tau_\uparrow = \tau_\downarrow$ (since the density of states per spin is a constant); we have the equality between the spin Hall mobility and the anomalous Hall mobility (except for a factor of 2 as explained above): $\sigma_{xy}^{\mathrm{SH}}/n = \tilde{\sigma}_{xy}^{\mathrm{AH}}/2$ s.

In summary, we have obtained analytic formulas for the extrinsic spin Hall effect in 2D and 3D doped semiconductor structures using a Kubo formula-based diagrammatic perturbation theory. Our theory explicitly manifests the formal connection between the SHE and the AHE. We find that the recent experimental results of Kato *et al.* [8] are consistent with our (admittedly crude) estimate of the extrinsic SHE, whereas the experimental results of Wunderlich *et al.* [10], while being larger than our estimate, are not impossibly large given the uncertainty in the precise knowledge of the SO coupling strength. We therefore suggest the possibility, at least as a matter of principle, that the recent experimental observations of the SHE in GaAs are the confirmation of a beautiful prediction [1,2] going back more than thirty years.

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