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Kinetic investigation of the extrinsic spin Hall effect induced by skew scattering

J L Cheng and M W Wu¹

Hefei National Laboratory for Physical Sciences at the Microscale and Department of Physics,
University of Science and Technology of China, Hefei, Anhui, 230026,
People's Republic of China

E-mail: mwwu@ustc.edu.cn

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Abstract

A study of the kinetics of the extrinsic spin Hall conductivity induced by skew scattering is performed using the fully microscopic kinetic spin Bloch equation approach to the (001) GaAs symmetric quantum well. In the steady state, the extrinsic spin Hall current/conductivity vanishes for the linear \mathbf{k} dependent spin-orbit coupling and is very small for the cubic \mathbf{k} dependent spin-orbit coupling. The spin precession induced by the Dresselhaus/Rashba spin-orbit coupling plays a very important role in the vanishing of the extrinsic spin Hall conductivity in the steady state. An in-plane spin polarization is induced by the skew scattering, with the help of the spin-orbit coupling. This spin polarization is very different from the current-induced spin polarization.

Generating and manipulating the spin polarization in semiconductors is one of the important prerequisites for the realization of the new spintronic devices [1]. The spin Hall effect (SHE) is considered as a convenient method for generating spin polarization, in addition to the traditional methods such as the external magnetic field, the circular/linear polarized laser [2, 3], the spin-galvanic effect [4] and spin injection from ferromagnetic metal to semiconductor [5]. The SHE is induced by intrinsic or extrinsic spin-orbit coupling (SOC) [6] which gives rise to a spin current perpendicular to the charge current without applying an external magnetic field and/or spin accumulation at sample edges [7–9]. Experimentally, the spin Hall conductivity (SHC) is estimated indirectly from the spin accumulation at the sample edges [10–14], or the charge current with a transverse magnetic field applied in a gyrotropic system [15–17]. Recently, a direct electronic measurement of the SHE was given by Valenzuela and Tinkham for the metallic conductor [18]. All these effects are explained as the intrinsic [6, 19–27] and/or the extrinsic SHE [6, 7, 28–38] theoretically by using the Kubo formula [19, 20, 30, 31] or the Boltzmann equation [6, 7, 23, 34, 36] with only the carrier-impurity scattering included.

The intrinsic SHE is induced by the intrinsic SOC (i.e., the Dresselhaus [39] and/or the Rashba [40] SOC)

with the applied external electric field and the resulting SHC was at first thought a dissipationless one in perfect crystals [19, 20]. Later investigations proved that this kind of SHC disappears even for infinitesimal impurity density with the vertex correction [22, 23, 41–44] in the Rashba model or the linear Dresselhaus model in quantum wells [45], but remains a finite value for the cubic SOC [46]. However, the spin current is not an observable quantity. Laughlin's gauge gedanken experiment indicates that the intrinsic SHE cannot lead to any spin accumulation at sample edges [24, 25], except in a mesoscopic system. In addition to the Dresselhaus and the Rashba SOC, the mixing between the valence and the conduction bands gives rise to two corrections. One is the additional spin dependent electron-impurity [2, 48] or the electron-phonon [16, 17] skew scattering. The extrinsic SHE induced by the skew scattering alone has been widely studied by using both the Kubo formula and the Boltzmann equation method [6, 7, 28–30, 34–36], and the nonzero extrinsic SHC is obtained. Lately, Tse and Das Sarma [31] have proved the vanishing of the extrinsic SHC by considering the vertex correction of the linear SOC in the Kubo formula. However, a fully microscopic calculation of the extrinsic SHC via the kinetic equation approach is still missing and the vanishing of the extrinsic SHC caused by the vertex correction from the Kubo approach needs to be verified using the kinetic approach. The other correction arises from the additional spin dependent

¹ Author to whom any correspondence should be addressed.

position and velocity operators, which bring about a correction to the definition of the spin current, referred to as the side-jump mechanism [6]. Here two corrections to the definition should be specified. The first comes from the electrical potential which gives an intrinsic-like contribution and again cannot contribute to the spin accumulation according to [24, 25, 47]. The second comes from the spin dependent scattering in which high order correlations between different wavevectors need to be considered [6, 34]. It is hard to include the second correction in the Boltzmann equation approach [6], though it also gives rise to the extrinsic SHE, together with the skew scattering. In the following, we concentrate on the extrinsic SHE induced by the skew scattering.

The spin polarization is not only accumulated at the sample edges due to the extrinsic SHE, but also observed simultaneously inside the samples, induced by the charge current [10, 11, 13, 49–52]. By comparing the experiments in [10, 13, 51], it is easy to find that the two spin polarizations are of the same order. From theory, Engel *et al* [49] and Trushin and Schliemann [52] attributed the current-induced spin polarization (CISP) in the homogeneous system as a result of the current-induced effective magnetic field (EMF) from the SOC [51]. Tarasenko showed that the spin-flip phonon scattering in asymmetric quantum wells can also induce this kind of spin polarization [50]. However, the spin-conserving skew scattering in two-dimensional GaAs semiconductor can also induce spin polarization inside the sample due to the extrinsic SHE. This effect has not been studied in the literature. Moreover, a fully microscopic kinetic investigation on the extrinsic SHE is also missing in the literature.

In this paper, we focus on the kinetic process of the extrinsic SHE induced by the skew scattering in a symmetric GaAs(001) quantum well using the kinetic spin Bloch equation (KSBE) approach [53, 54]. We demonstrate the important role of the spin precession induced by the (intrinsic) Dresselhaus/Rashba SOC to the SHE and show that it is inadequate to study the extrinsic SHE from the Kubo formalism approach without considering the Dresselhaus/Rashba SOC from the literature. We further show that the extrinsic SHE can generate spin polarizations in homogeneous system.

By using the non-equilibrium Green function method and the generalized Kadanoff–Baym ansatz [55], we construct the KSBE [53, 54] for electrons as follows:

$$\frac{\partial \rho_{\mathbf{k}}(t)}{\partial t} - eE \frac{\partial \rho_{\mathbf{k}}}{\partial k_x} + \left. \frac{\partial \rho_{\mathbf{k}}}{\partial t} \right|_{\text{coh}} + \left. \frac{\partial \rho_{\mathbf{k}}}{\partial t} \right|_{\text{scat}} + \left. \frac{\partial \rho_{\mathbf{k}}}{\partial t} \right|_{\text{ss}} = 0. \quad (1)$$

Here, $\rho_{\mathbf{k}}(t) = \begin{pmatrix} f_{\mathbf{k}\uparrow} & \rho_{\mathbf{k}\uparrow\downarrow} \\ \rho_{\mathbf{k}\downarrow\uparrow} & f_{\mathbf{k}\downarrow} \end{pmatrix}$ is the electron density matrix with wavevector \mathbf{k} at time t . The applied electric field E is assumed along the x axis and the magnetic field B is across the x – y (well) plane. The coherent term describes the spin precession along the magnetic/effective magnetic field and is given by $\left. \frac{\partial \rho_{\mathbf{k}}}{\partial t} \right|_{\text{coh}} = i[\frac{1}{2}(\Omega^D(\mathbf{k}) + g\mu_B \mathbf{B}) \cdot \boldsymbol{\sigma}, \rho_{\mathbf{k}}(t)]$, where $\Omega^D(\mathbf{k}) = \gamma(k_x(k_y^2 - (\frac{\pi}{a})^2), k_y((\frac{\pi}{a})^2 - k_x^2), 0)$ represents the EMF from the Dresselhaus SOC [39] with γ standing for the material-determined SOC strength [56, 57] and a being the well width. An infinite-well-depth assumption is adopted here

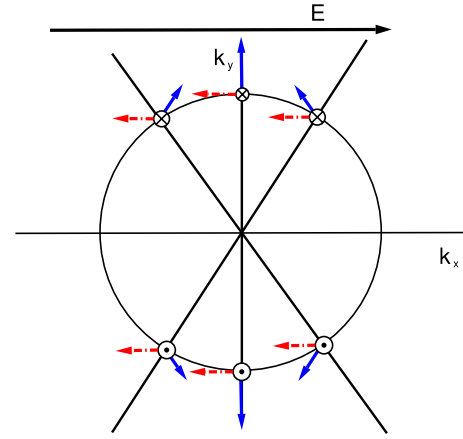


Figure 1. The schematic diagram of the skew scattering and the intrinsic spin–orbit coupling in the \mathbf{k} space. \odot (\otimes) stands for the spin-up (spin-down) polarization. The blue solid arrows give the direction of the EMF from the Dresselhaus SOC which rotates the spin polarization to the direction indicated by the red dashed arrows. (This figure is in colour only in the electronic version)

and only the lowest subband is taken into account due to the small well width. The spin-conserving scattering $\left. \frac{\partial \rho_{\mathbf{k}}}{\partial t} \right|_{\text{scat}}$ is given by the spin-conserving electron–impurity scattering, the electron–phonon scattering and the electron–electron Coulomb scattering which are given in detail in [58].

The skew scattering is given by the third-order expansion of the electron–impurity scattering and reads [6, 30, 31]

$$\left. \frac{\partial \rho_{\mathbf{k}}}{\partial t} \right|_{\text{ss}} = -2\pi^2 N_i \lambda \gamma^2 \sum_{\mathbf{k}_1 \mathbf{k}_2; q_1 q_2} \delta(\varepsilon_{\mathbf{k}_2} - \varepsilon_{\mathbf{k}}) \delta(\varepsilon_{\mathbf{k}_1} - \varepsilon_{\mathbf{k}}) \times V(\mathbf{k} - \mathbf{k}_1, q_1) V(\mathbf{k}_1 - \mathbf{k}_2, q_2) V(\mathbf{k}_2 - \mathbf{k}, -q_1 - q_2) \times \{(\mathbf{k} - \mathbf{k}_1) \times (\mathbf{k}_2 - \mathbf{k}) \cdot \boldsymbol{\sigma}, \rho_{\mathbf{k}_2}\}. \quad (2)$$

Here $\lambda \gamma^2 = \frac{\eta(2-\eta)}{2m^* E_g (3-\eta)}$ is the strength of the skew scattering with $\eta = \frac{\Delta}{\Delta + E_g}$ [2]. E_g and Δ are the band gap and the spin–orbit splitting of the valence band respectively. $V(\mathbf{q}, q_z) = \frac{-e^2}{q^2 + q_z^2 + \kappa^2} I(\frac{q_z a}{2\pi})$ with $I(x) = e^{i\pi x} \frac{\sin(\pi x)}{\pi x (1-x^2)}$ being the form factor and κ denoting the Debye–Hückel screening constant. This term produces an asymmetric spin-conserving scattering of electrons so that the spin-up/down electrons prefer to be scattered to the left/right side. A schematic diagram of the skew scattering is given in figure 1 for a left moving electron.

We first analyse the KSBE for some simple cases. After carrying out the summation over \mathbf{k} , one gets the equation of continuity for the spin density $\mathbf{S} = \sum_{\mathbf{k}} s_{\mathbf{k}} = \sum_{\mathbf{k}} \text{Tr}[\rho_{\mathbf{k}} \boldsymbol{\sigma}]$ as

$$\frac{\partial \mathbf{S}(t)}{\partial t} - \sum_{\mathbf{k}} \Omega^D(\mathbf{k}) \times s_{\mathbf{k}}(t) - g\mu_B \mathbf{B} \times \mathbf{S}(t) = 0. \quad (3)$$

The summation of the spin-conserving scattering is naturally zero. The summation of the skew scattering in equation (2) for the two-dimensional system is also zero because it can only skew the spin-up and spin-down electrons separately instead of flip them. Equation (3) is consistent with the result in [44] which is obtained by using the general operator commutation relations. When only the linear \mathbf{k} term in $\Omega^D(\mathbf{k})$ is retained,

for the steady state one obtains

$$J_y^z = \frac{eg\mu_B B_y}{\gamma m^* ((\pi/a)^2 - \langle k_x^2 \rangle)} S^z. \quad (4)$$

Here $\mathbf{J}^z = -e \sum_{\mathbf{k}} \hbar \mathbf{k} / m^* (f_{\mathbf{k}\uparrow} - f_{\mathbf{k}\downarrow})$ is the spin current which is the simplest but the most widely used definition [6] without considering the contribution from the side-jump effect. The SHC is given as $\sigma_y^z = J_y^z / E$. In the derivation, we also take the approximation $\sum_{\mathbf{k}} k_x k_y^2 s_{\mathbf{k}}^z = -\frac{m^*}{e} \langle k_y^2 \rangle J_x^z$ and $\sum_{\mathbf{k}} k_y k_x^2 s_{\mathbf{k}}^z = -\frac{m^*}{e} \langle k_x^2 \rangle J_y^z$ with $\langle k_{x/y}^2 \rangle$, the average value of $k_{x/y}^2$. If the strain-induced SOC $H_s = \alpha(k_y \sigma_x - k_x \sigma_y)$ (with the same expression for the Rashba SOC) is taken into account, equation (4) changes into

$$J_y^z = \frac{\gamma((\frac{\pi}{a})^2 - \langle k_y^2 \rangle) B_y - 2\alpha B_x}{\gamma^2((\frac{\pi}{a})^2 - \langle k_x^2 \rangle)((\frac{\pi}{a})^2 - \langle k_y^2 \rangle) - 4\alpha^2} \frac{eg\mu_B}{m^*} S^z. \quad (5)$$

Without the external magnetic field, equations (4) and (5) give $J_y^z = 0$, which verifies the zero extrinsic SHC given by [31] from the Kubo approach. However, the skew scattering does generate spin currents when the electric field is applied (in figure 1), but it is just dynamic. To make clear how the spin current disappears, we rewrite the x component of equation (3) as

$$\partial S^x / \partial t = m^* \gamma [(\pi/a)^2 - \langle k_z^2 \rangle] J_y^z / e. \quad (6)$$

It is hence easy to find that the spin Hall current is converted to the spin polarization along the x axis and it tends to zero in the steady state. This can further be understood from figure 1: after the spin current is excited by the skew scattering, the spin polarization distributes (\odot and \otimes) anti-symmetrically at $\pm k_y$. However the y components of the EMF due to the SOC (the blue solid arrows) have the same symmetry and rotate the spin polarizations to the $-x$ direction (the red dashed arrows). Therefore, the spin Hall current is converted to the in-plane spin polarization.

Now we show the time evolution of the SHC σ_y^z and the spin polarization $P_x = S^x / N_e$ calculated by numerically solving the KSBE with all the scattering explicitly included at $T = 200$ K in figure 2. The parameters in the calculation are taken as the following: the electron and impurity densities $N_e = N_i = 4 \times 10^{11} \text{ cm}^{-2}$; $a = 7.5 \text{ nm}$; $E = 0.1 \text{ kV cm}^{-1}$; $\gamma = 11.4 \text{ eV \AA}^3$; and $\sqrt{\lambda} \gamma = 2.07 \text{ \AA}$. From the figure, the SHC increases with time first from the zero value to a maximum one in nearly 1 ps, then decreases slowly to a very small value (instead of zero due to the inclusion of the Dresselhaus SOC with the cubic \mathbf{k} terms) on a characteristic timescale of about 50 ps. The spin polarization is along the $-x$ axis and increases from zero to its steady state $P_x = 1.2 \times 10^{-4}$.

The above evolution is easy to understand with the help of the schematic diagram in figure 1. When the positive electric field is applied, the skew scattering scatters the spin-down electrons to the upper panel of the \mathbf{k} space and the spin-up ones to the lower panel. This leads to the spin currents flowing along the y direction. The strength of the skew scattering is determined by the shift of the electron distribution, so the SHC increases fast to its maximum value $\sigma_y^z \sim 2.5 \times 10^{-3} \frac{e^2}{h}$ at the timescale of the charge current (see the dashed curve in

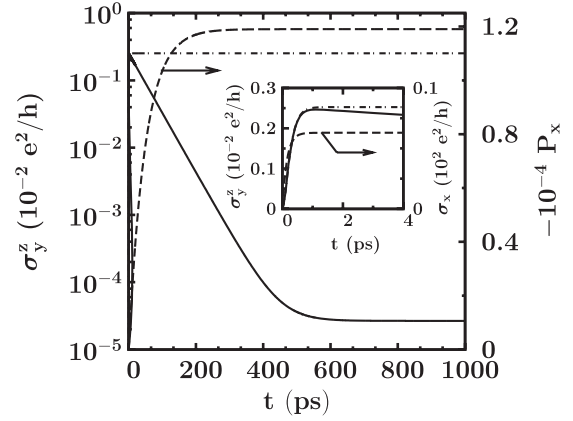


Figure 2. Time evolution of the SHC with (solid curve)/without (chain curve) coherent terms and the time evolution of the spin polarization (dashed curve) along the x axis at $T = 200$ K. $N_i = N_e = 4 \times 10^{11} \text{ cm}^{-2}$ and the electric field $E = 0.1 \text{ kV cm}^{-1}$. The corresponding time evolutions of the SHC of the first 4 ps are shown in the inset, together with the charge conductivity σ_x . It is noted that the scales of the spin polarization/charge conductivity are on the right-hand side of the frames.

the inset of figure 2). Then the spin polarization precesses along the y components of the EMF from the SOC to the $-x$ direction to generate the in-plane spin polarization. Due to the symmetry, the spin polarizations along the y and z axes are zero.

It is interesting to see that the SHC obtained in the steady state is orders of magnitude smaller than the one obtained from the Kubo formula widely used in the literature where only the lowest order diagram is considered [30]. With only the impurity scattering included at zero temperature, the Kubo formula gives the extrinsic SHC [30] as $\frac{2\pi m^* \lambda \gamma^2 e_F}{\hbar^2} \sigma_x \sim 3.37 \times 10^{-3} \sigma_x$ with the charge conductivity $\sigma_x = \frac{ne^2 \tau}{m}$. This value is orders of magnitude larger than our result $\sigma_y^z \sim 4.1 \times 10^{-8} \sigma_x$, obtained from the fully microscopic KSBE. The difference is caused by the inhomogeneous broadening [59] in spin precession due to the Dresselhaus/Rashba SOC. To show this effect, we drop the coherent term and plot the time evolution of the SHC as chain curves in figure 2. We find that the steady SHC $\sigma_y^z \sim 0.4 \times 10^{-3} \sigma_x$ is much closer to the one above, given by the Kubo formula at 0 K. Therefore, we conclude that it is not appropriate to calculate the extrinsic SHC without considering the spin precession. Furthermore, the side-jump mechanism gives a time independent contribution as $\sigma_y^z = -2\lambda \gamma^2 e^2 N_e \sim -2 \times 10^{-3} e^2/h$ with the sign opposite to the one from the skew scattering.

It is further noted that although the spin precession induced by the EMF leads to the vanishing of the SHC, it plays a very important role in generating the spin polarization. From the discussion above, it is easy to see that the skew scattering alone cannot generate any spin polarization due to the anti-symmetrical spin polarization at $\pm k_y$. Unlike for the CISP [49] where the SOC is used to provide a current-induced EMF [10, 58], here the SOC acts as an anti-symmetrical precession field, which is the same as the spin polarization induced by the spin dependent phonon

scattering [3]. We further note that the spin polarization induced by the skew scattering is very different from the CISP. (i) The spin polarization induced by current-induced EMF favours a small well width which gives a large EMF [49], whereas the one induced by the skew scattering and the spin precession favours a large well width. The later can be seen as follows: from figure 2, the evolution of the extrinsic spin Hall current can be written as $J_y^z(t) = J_{y,0}^z e^{-t/\tau_s}$ with the relaxation time τ_s . $J_{y,0}^z$ approximates to the maximum value which is only determined by the skew scattering. Therefore $S^x = m^* \tau_s \gamma ((\pi/a)^2 - \langle k_x^2 \rangle) J_{y,0}^z / e$. For the D'yakonov-Perel' mechanism [60], $\tau_s \propto [\gamma ((\pi/a)^2 - \langle k_x^2 \rangle)]^{-2}$. Hence $S^x \propto \gamma ((\pi/a)^2 - \langle k_x^2 \rangle)^{-1}$. (ii) When the electric field is along the x axis, for the Dresselhaus SOC, the CISP is along the x direction, while the polarization induced by the skew scattering is along the $-x$ direction. However, for the strain-induced or the Rashba SOC, the spin polarizations from the two mechanisms are along the same direction. (iii) The CISP decreases with the impurity density [49] because high impurity density reduces the EMF effectively. However, the skew-scattering-induced spin polarization increases with the impurity density as the skew scattering is proportional to the impurity density.

In summary, we investigated the SHC and the spin polarization induced by the \mathbf{k} -asymmetric spin-conserving skew scattering in a symmetrical (001) GaAs quantum well using the fully microscopic KSBE approach at high temperature with all the scattering explicitly included. We find that the spin precession induced by the Dresselhaus/Rashba SOC has a very important effect on the extrinsic SHC and verify the vanishing of the SHC for linear \mathbf{k} dependent SOC. We also show that the SHC induced by the skew scattering calculated from the Kubo formula in the literature is inadequate without considering the spin precession. Finally we show that with the joint effects from the skew scattering and the spin precession, an in-plane spin polarization can be generated which can be further rotated to the z direction by applying an external in-plane magnetic field.

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