Theory of spin Hall effect

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An extension of Drude model is proposed that accounts for spin and spin-orbit interaction of charge carriers. Spin currents appear due to combined action of the external electric field, crystal field and scattering of charge carriers. The expression for spin Hall conductivity is derived for metals and semiconductors that is independent of the scattering mechanism. In cubic metals, spin Hall conductivity $\sigma_s$ and charge conductivity $\sigma_r$ are related through $\sigma_s = [2\pi\hbar/(3mc^2)]\sigma_r^2$ with $m$ being the bare electron mass. Theoretically computed value is in agreement with experiment.

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It has been a common knowledge in atomic physics that due to spin-orbit interaction the spatial separation of electrons with different spin projections can be achieved through scattering of an unpolarized electron beam by an unpolarized target [1]. Dyakonov and Perel were the first to notice that in the presence of the electric current the scattering of charge carriers by impurities in a semiconductor is independent of the mechanism. It was subsequently called the spin Hall effect [2] and observed in semiconductors [3, 4] and metals [5]. A number of microscopic models have been developed that explain spatial separation of spin polarizations by various “extrinsic” (due to impurities) and “intrinsic” (impurity-free) mechanisms, see for review Ref. 7. While these models provide valuable insight into microscopic origin of the spin Hall effect, they are lacking universality of, e.g., Drude model of charge conductivity [6]. The Drude model, in spite of its simplicity, is independent of the scattering mechanism. In cubic metals, spin Hall effect appears due to combined action of the external electric field, quadrupole crystal electric field and scattering of charge carriers. Same as for charge conductivity, all details of the scattering mechanism are absorbed into the momentum relaxation time $\tau$. We will show that this crude model provides correct values of spin Hall conductivity in both metals and semiconductors.

For certainty we will speak about electrons but the model will equally apply to holes. The non-relativistic limit of the Dirac Hamiltonian for spin-1/2 particle is [9]

$$\mathcal{H} = \frac{p^2}{2m} + U(\mathbf{r}) + \frac{\hbar c}{4m^2} \sigma \cdot \nabla \times \mathbf{p}. \quad (1)$$

Here $U(\mathbf{r})$ represents the action of microscopic electric field on charge carriers. It incorporates effects of electrostatic crystal potential $\Phi_c$, potential due to imperfections of the crystal lattice $\Phi_i$, and external potential $\Phi_e$,

$$U(\mathbf{r}) = e\Phi_0(\mathbf{r}) + e\Phi_i(\mathbf{r}) + e\Phi_e(\mathbf{r}). \quad (2)$$

The last term in Eq. 1 is the spin-orbit interaction, with $\sigma$ being Pauli matrices. Hamiltonian mechanics for canonically conjugated variables $p$ and $r$ is described by the equations

$$\dot{r} = \frac{\partial \mathcal{H}}{\partial p} = \frac{p}{m} + \frac{\hbar c}{4m^2} \left[ \sigma \times \frac{\partial U}{\partial r} \right] \quad (3)$$

$$\dot{p} = -\frac{\partial \mathcal{H}}{\partial r} = -\frac{\partial U}{\partial r} - \frac{\hbar c}{4m^2} \frac{\partial}{\partial r} \left[ \sigma \times \frac{\partial U}{\partial r} \right] \cdot \mathbf{p} \quad (4)$$

(These equations can also be derived from quantum-mechanical relations: $i\hbar \dot{r} = [r, \mathcal{H}]$, $i\hbar \dot{p} = [p, \mathcal{H}]$, $[r_i, p_j] = i\hbar \delta_{ij}$.) From Eq. 3 one has

$$p = m\dot{r} - \frac{\hbar c}{4m^2} \left[ \sigma \times \frac{\partial U}{\partial r} \right] \quad (5)$$

$$\dot{p} = m\dot{\mathbf{r}} - \frac{\hbar c}{4m^2} \left( \dot{\mathbf{r}} \cdot \frac{\partial}{\partial r} \right) \left[ \sigma \times \frac{\partial U}{\partial r} \right] \quad (6)$$
The second term in the expression for the momentum, Eq. (5), that is proportional to the cross product of the electron magnetic moment and the electric field, is the so-called “hidden mechanical momentum” associated with the momentum of the electromagnetic field, see e.g. Ref. [10] and references therein.

Substitution of Eqs. (5) and (6) into Eq. (4) yields the following form of the second equation of Newton’s law for charge carriers:

$$m\ddot{r} = -\frac{\partial U}{\partial r} + F_\sigma(r, \dot{r}),$$

where the spin-dependent force is given by

$$F_\sigma(r, \dot{r}) = \frac{\hbar}{4mc^2} \times \left\{ (\dot{r} \cdot \frac{\partial}{\partial r}) [\sigma \times \frac{\partial U}{\partial r}] - \frac{\partial}{\partial r} \left( \dot{r} \times [\sigma \times \frac{\partial U}{\partial r}] \right) \right\}.$$

Here we neglected the term proportional to $1/c^4$ that exceeds the accuracy of Eq. (11) and took into account that $\dot{r}$ in the second line of Eq. (8), that originates from the expression for $p$ in Eq. (5), should not be differentiated on $r$ because $p$ and $r$ in Eqs. (3) and (4) are independent canonically conjugated variables. Note that the force in Eq. (8) is equivalent to the Lorentz force,

$$F_\sigma = (e/c)(\dot{r} \times B_\sigma),$$

acting on a particle of charge $e$ in the magnetic field

$$B_\sigma = \nabla \times A_\sigma, \quad A_\sigma = \frac{\hbar}{4mc} (\sigma \times E_{\text{tot}}),$$

with $E_{\text{tot}}$ being the total electric field, $eE_{\text{tot}} = -\partial U/\partial r$. One can trace this force to the fact that with an accuracy to $c^{-2}$ the Hamiltonian (11) can be written as

$$\mathcal{H} = \frac{1}{2m} \left( p - \frac{e}{c} A_\sigma \right)^2 + U(r).$$

Crystal field creates a non-zero average of this force any time the charge carriers have a non-zero drift velocity, $\langle \dot{r} \rangle \neq 0$. It is this effective Lorentz force that is responsible for the spin Hall effect. Our conclusion is similar to the conclusion of Hirsch [12] who studied the force exerted on a line of moving magnetic dipoles by the electrostatic field of charges arranged in a cubic lattice. For a cubic lattice (see below) our result for the effective Lorentz force coincides up to a factor of 2 with the result obtained by Hirsch. As in our approach, Hirsch found that the effective Lorentz force is generated by the second derivative of the crystal field. In computing this force he replaced moving magnetic dipoles with stationary electric dipoles that produce an equivalent electric field. This eliminated the hidden momentum responsible for the first term in the second line of Eq. (8). The absence of this term in Hirsch’s model accounts for the above mentioned difference by a factor of 2.

In the spirit of the Drude model we shall now add to Eq. (7) the drag force $-m\dot{r}/\tau$. Then Eq. (11) becomes

$$m\ddot{r} = -\frac{\partial U}{\partial r} - \frac{m}{\tau} \dot{r} + F_\sigma(r, \dot{r}).$$

Here we assume that to the first approximation the velocity relaxation of charge carriers is independent of their spin, that is, $\tau$ is independent of $\sigma$. Since the relaxation is due to imperfections of the crystal lattice, in order not to count their effect twice, we should now think of $U(r)$ in Eqs. (11) and (8) as a sum of the ideal periodic potential of the crystal lattice, $e\Phi_0$, and the potential produced by the externally applied voltage, $e\Phi_r$. Due to relativistic smallness of the spin-dependent force [5] one can treat $F_\sigma(r, \dot{r})$ in Eq. (11) as a perturbation. Then the solution of Eq. (11) can be written in the form $\dot{r} = r_0 + \dot{r}_1$, where $\dot{r}_1$ is a small spin-dependent part of the velocity proportional to $c^{-2}$. In the presence of a constant external electric field $E = -\partial \Phi_r/\partial r$, with the linear accuracy on $E$, one obtains from Eqs. (11) and (8)

$$\langle \dot{r}_0 \rangle = -\frac{\tau}{m} \left( \frac{\partial U}{\partial r} \right) = \frac{e\tau}{m} E$$

$$\langle \dot{r}_1 \rangle = \frac{\tau}{m} \langle F_\sigma(r_0, \dot{r}_0) \rangle = -\frac{\hbar e^2 \tau^2}{4mc^2} E \times \left( \frac{\partial}{\partial \dot{r}} \times \left( \sigma \times \frac{\partial \Phi_r}{\partial r} \right) \right).$$

In deriving Eq. (13) we have made an assumption that

$$\langle F_\sigma(r_0, \dot{r}_0) \rangle \equiv \frac{e}{c} \langle \dot{r}_0 \times B_\sigma(r_0) \rangle = \frac{e}{c} \langle \dot{r}_0 \rangle \times \langle B_\sigma \rangle.$$

Some justification of this assumption is provided by the following argument. By symmetry, the only reason for $\langle F_\sigma \rangle$ to be different from zero would be $\langle \dot{r}_0 \rangle \neq 0$. Consequently, $\langle F_\sigma \rangle$ should be first order on $\langle \dot{r}_0 \rangle$. Being perpendicular to the velocity, the force $F_\sigma = (e/c)(\dot{r} \times B_\sigma)$ does not do mechanical work on the charge. Neither should $\langle F_\sigma \rangle$ with respect to $\langle \dot{r}_0 \rangle$, rendering the form $\langle F_\sigma \rangle = (e/c)(\langle \dot{r}_0 \rangle \times B_{eff})$. Since the trajectory of the particle $r_0(t)$ does not have strong correlation with the quadrupole component of the crystal electric field, the above factorization of the average with the choice $B_{eff} = \langle B_\sigma \rangle$ should not deviate strongly from the exact average.

The right hand side of Eq. (13) contains the volume average of $\nabla \nabla \Phi_r(r)$. In what follows we will study the spin Hall effect in a cubic lattice. Generalization to other lattices is straightforward and will be considered elsewhere. The case of a cubic lattice, besides simplicity, is interesting because experiments performed to date have been done in cubic semiconductors and in aluminum that is also cubic [4, 5, 6]. In the cubic case the only in-
variant permitted by symmetry is
\[ \langle \frac{\partial^2 \Phi}{\partial r_i \partial r_j} \rangle = A \delta_{ij}, \] (15)

where \( A \) is a constant to be determined later. With the help of Eq. (15) one obtains from Eq. (13):
\[ \langle \mathbf{\hat{r}}_1 \rangle = \frac{\hbar e^2 \tau^2 A}{2m^2 c^2} [\sigma \times \mathbf{E}]. \] (16)

Let us now introduce the vector of spin polarization of the electron fluid, \( \xi = \langle \sigma \rangle \), which absolute value lies between 0 and 1,
\[ \xi = \frac{n_+ - n_-}{n_+ + n_-}. \] (17)

Here \( n_\pm \) are concentrations of charge carriers with spins parallel and antiparallel to \( \xi \) respectively, with \( n_+ + n_- = n \) being the total concentration of charges carrying the electric current. For a ferromagnet, \( \xi \neq 0 \) is the equilibrium state of charge carriers below the Curie temperature, while for a small non-magnetic conductor a significant value of \( \xi \) can be achieved through injection of spin-polarized charge carriers from a magnetic conductor, see for review Ref. [14]. The density matrix of the charge carriers in the spin space (normalized to their total concentration \( n \)) can be written as
\[ N = \frac{1}{2} n (1 + \xi \cdot \sigma). \] (18)

The electric current is
\[ \mathbf{j} = e \langle N \mathbf{r} \rangle = e \langle N (\mathbf{r}_0 + \mathbf{r}_1) \rangle. \] (19)

Substituting here equations (12) and (10) one obtains
\[ \mathbf{j} = \sigma_s \mathbf{E} + \sigma_c [\xi \times \mathbf{E}], \] (20)

where charge conductivity and spin Hall conductivity are given by
\[ \sigma_c = \sigma_D = \frac{e^2 n \tau}{m}, \] (21)
\[ \sigma_s = \frac{\hbar e^3 n \tau^2 A}{2m^2 c^2}. \] (22)

An interesting observation is that the ratio
\[ \frac{\sigma_s}{\sigma_c} = \frac{\hbar e \tau A}{2m^2 c^2} \] (23)
is independent of the concentration of charge carriers. This result also follows from microscopic models of spin Hall effect [13, 15]. It explains why this ratio has the same order of magnitude in metals and semiconductors [4, 6] despite very different concentrations of charge carriers. Note that according to Eq. (23) the temperature dependence of the ratio of spin Hall and charge conductivities is determined by the temperature dependence of the relaxation time \( \tau \). Consequently, in metals one should observe monotonic temperature dependence of spin Hall conductivity, \( \sigma_s(T) \propto \sigma_c^2(T) \), while in semiconductors \( \sigma_s(T) \propto n(T)\tau^2(T) \) may exhibit maximum on temperature [16].

Eq. (13) shows that quantitative analysis of the spin Hall effect requires knowledge of the volume average of the quadrupole component of the crystal electric field, \( \langle \partial^2 \Phi_0/\partial r_i \partial r_j \rangle \). For a specific crystal it can be computed by methods of density functional theory. For a cubic crystal \( \langle \partial^2 \Phi_0/\partial r_i \partial r_j \rangle \) reduces to a single constant \( A \), see Eq. (15). Here we will provide a simple estimate of this constant. In a metal the electrostatic potential created by the crystal lattice of positively charged ions satisfies Maxwell equation
\[ \nabla^2 \Phi_0 = -4\pi \rho(x, y, z), \] (24)

where \( \rho(x, y, z) \) is the local charge density of ions. The volume average of this equation is
\[ \langle \frac{\partial^2 \Phi_0}{\partial x^2} \rangle + \langle \frac{\partial^2 \Phi_0}{\partial y^2} \rangle + \langle \frac{\partial^2 \Phi_0}{\partial z^2} \rangle = 3A = -4\pi \langle \rho(x, y, z) \rangle \] (25)

Due to the periodicity of the crystal field, it is sufficient to compute this average over the unit cell of the crystal. This gives
\[ A = \frac{4\pi}{3} Z n e n_0, \] (26)

where \( -Ze \) and \( n_0 \) are the charge and the concentration of ions respectively. The sign in \( \langle \rho \rangle = -Ze n_0 \) is determined by our choice of the negative charge \( e \) of the charge carriers. In the accurate quantum-mechanical calculation of the parameter \( A \) produced by the distribution of charges in a cubic lattice, \( Z \) should come out as a number of order unity when \( n_0 \) is chosen as the inverse volume of the unit cell. This should be true for both metals and semiconductors.

Substitution of Eq. (26) into Eq. (23) gives
\[ \frac{\sigma_s}{\sigma_c} = \frac{2\pi \hbar e^2}{3m^2 c^2} Z n_0 \tau. \] (27)

At \( n_0 \sim 10^{22} \text{cm}^{-3} (10^{23} \text{cm}^{-3}) \) and \( \tau \sim 10^{-13} \text{s} (10^{-14} \text{s}) \) this ratio is of order \( 10^{-4} \) which is in agreement with recent experimental findings in metals and semiconductors [4, 6]. According to our model such a value of \( \sigma_s/\sigma_c \) is not universal though. In pure conductors, when scattering of charge carriers is dominated by phonons, large \( \tau \) at low temperature can provide much greater values of the ratio of spin Hall and charge conductivities.

For the absolute value of spin Hall conductivity one obtains from Eq. (22)
\[ \sigma_s = \frac{2\pi \hbar e^4}{3m^3 c^2} Z n_0 \tau^2. \] (28)
In metals, when $Z$ is identified with the ion valence, one can replace $Zn_0$ with $n$ and write Eq. (28) as
\[ \sigma_s = \frac{2\pi \hbar}{3mc^2} \sigma^\epsilon. \] (29)

This relation between spin Hall and charge conductivities permits comparison with experimental data without any fitting parameters. Such a comparison with the data on aluminum [6] is shown in Table I (Note that conductivity in Gauss units that have been used to derive Eq. (29), equals conductivity in units of $\Omega^{-1}m^{-1}$ times $9 \times 10^9$.)

| Conductivity | Experiment ($\Omega^{-1}m^{-1}$) | Theory ($\Omega^{-1}m^{-1}$) |
|--------------|--------------------------------|-----------------------------|
| $\sigma_s$ (12nm) | $1.05 \times 10^9$ | 1.05 $\times 10^9$ |
| $\sigma_s$ (12nm) | $(3.4 \pm 0.6) \times 10^9$ | $2.6 \times 10^9$ |
| $\sigma_s$ (25nm) | $1.7 \times 10^9$ | $1.7 \times 10^9$ |
| $\sigma_s$ (25nm) | $(2.7 \pm 0.6) \times 10^9$ | $6.9 \times 10^8$ |

TABLE I: Comparison of Eq. (29) with experimental data [6] on charge and spin Hall conductivities in Al strips of 12-nm and 25-nm thickness.

We can, therefore, serve as a simple physical picture of spin Hall conductivity. Throughout our derivations we did not distinguished between the effective mass and the bare mass of charge carriers. To account for their difference we notice that one of the masses in the spin-orbit term with $m^*$ in front should be replaced by $m^*$. After these replacements are made and followed down to Eq. (29), $m^2$ gets absorbed into $\sigma^\epsilon$ while $1/m$ in front of $\sigma^\epsilon$ can be traced to the expression for the Bohr magneton, $\mu_B = |e|\hbar/(2mc)$. Thus the coefficient in front of $\sigma^\epsilon$ in Eq. (29) contains the bare electron mass. We used this fact for computing numerical values of $\sigma_s$ presented in Table I.

The theory of spin Hall effect developed in this Letter should also apply to the anomalous Hall effect observed in ferromagnets. According to Eq. (10) the weak flow of charge carriers with opposite spin polarizations in the opposite (perpendicular to $E$) directions occurs regardless of the average polarization $\xi$ given by Eq. (17). When the time of spin relaxation of charge carriers is sufficiently long, this will lead to the spin polarization of the boundaries of a small conductor even when $\xi = 0$. On the contrary, the spin Hall current given by the second term in Eq. (29) is proportional to $\xi$. In non-magnetic metals and semiconductors, large spin polarization is not easy to achieve but in a ferromagnetic metal $\xi$ can be of order unity, resulting in the noticeable current, $\sigma_s[\xi \times \mathbf{E}]$, that is normal to $\mathbf{E}$ and normal to the magnetization.

In Conclusion, we have presented a simple extension of Drude model of conductivity to the case of charge carriers that have spin and spin-orbit interaction. Spin Hall effect appears naturally in such a theory as a combined action of the external voltage, crystal electric field, and scattering of charge carriers. The expression for spin Hall conductivity is independent of the mechanism of scattering. Theoretical values of spin Hall conductivity computed within such a model are in agreement with experimental data on metals and semiconductors. The model can, therefore, serve as a simple physical picture of spin Hall effect.

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