Thermally Assisted Spin Hall Effect

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Abstract

The spin polarized charge transport is systematically analyzed as a thermally driven stochastic process. The approach is based on Kramers’ equation describing the semiclassical motion under the inclusion of stochastic and damping forces. Due to the relativistic spin-orbit coupling the damping experiences a relativistic correction leading to an additional contribution within the spin Hall conductivity. A further contribution to the conductivity is originated from the averaged underlying crystal potential, the mean value of which depends significantly on the electric field. We derive an exact expression for the electrical conductivity. All corrections are estimated in lowest order of a relativistic approach and in the linear response regime.

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I. INTRODUCTION

The scattering of an unpolarized electron beam at a likewise unpolarized target leads to a separation of electrons with different spins\(^1\). The reason for that effect is the spin-orbit interaction originated by relativistic corrections to the Schrödinger equation of the order \(c^{-2}\). As a consequence an electric current in a semiconductor should be accompanied by a spin current perpendicular to the conventional current of the charge carriers\(^2\). The generation of a transverse spin current due to an external electric field called as spin Hall effect\(^3\) has attracted much attention recently particularly for realizing spintronic devises\(^4\). In a series of experiments\(^5,6,7,8\) the effect had been observed in different materials. Recently the spin Hall conductivity was measured at room temperature\(^8\), an observation which gives the motivation for the present paper. The transport process is considered as a thermally activated process which is additionally driven by the applied electric field. This field however reveals a direct coupling to the crystal potential in such a manner that also in case of a periodic potential a constant current is maintained. Our approach is based on the Fokker-Planck equation or Kramers’ equation for the semiclassical motion of the charge carriers with damping and coupling to a stochastic source like a heat bath. Thus the charged particles can overcome permanently, but with a certain probability, potential barriers. Even for low temperature one should take into account the coupling of the homogeneous electric field to the potential landscape. Actually as discussed below the averaged force acting on the particles consists of several parts which point at different directions and contribute to the total conductivity. Recently a very promising theory has been proposed\(^9\) by studying the semi-classical deterministic equation of motion. The theoretical approach describing the spin Halle effect goes back to\(^2\) where a mesoscopic equation for the spin density had been proposed. A more phenomenological approach based on an anomalous scattering mechanism in the absence of spin-flip scattering discussed in\(^3\). As a consequence anomalous currents and a finite spin-diffusion length had been studied in\(^10\) where the calculations are based on the Boltzmann equation. In a series of papers\(^11,12,13,14,15\) a quantum approach for the spin Hall conductivity had been discussed. In\(^16\) a classical theory is proposed. In the present paper we consider an extension of the theoretical approach proposed in\(^2,16\) by including systematically a coupling to stochastic forces and friction terms. Because we are in the linear response regime the canonical friction and the strength of the stochastic force
are related by the fluctuation-dissipation theorem. The steady state solution of Kramers’
equation is an appropriate tool to obtain the electrical current. As a novelty we discuss in
detail the influence of the underlying crystal potential. Unlike\(^9\) we get corrections to the
spin Hall conductivity by the averaged crystal potential. Because the mean value over the
crystal potential is performed with the stationary solution of Kramers’ equation and this
solution depends on the electric field there occur additional corrections to the conductivity
in both the linear response regime with respect to the field \(E\) and in lowest order \(e^{-2}\) of
an relativistic approach. Whereas the relation for the conductivity under inclusion of the
crystal potential is an exact result, the real contribution, originated from the potentials,
has to be estimated by model potentials.

II. MODEL

In lowest order of relativistic effects the Hamiltonian has to be supplemented by the
spin-orbit interaction

\[
\mathcal{H} = \frac{p^2}{2m} + U(\mathbf{r}) + \kappa \mathbf{p} \cdot [\mathbf{\sigma} \times \nabla U] \quad \text{with} \quad \kappa = \frac{\hbar}{4m^2c^2}
\]  

(1)

The quantity \(\mathbf{\sigma}\) are Pauli operators which are assumed to be constant. Due to the spin-orbit
interaction the total potential \(U(\mathbf{r})\), related to all forces acting on the charged particles,
appears twofold. In the present paper we incorporate in the potential the intrinsic crystal
potential \(U_{\text{c}}(\mathbf{r})\) and the energy of the homogeneous electric field \(U(\mathbf{r}) = U_{\text{c}}(\mathbf{r}) - e\mathbf{E} \cdot \mathbf{r}\).
Extending the deterministic approach proposed in\(^9\) let us include stochastic forces \(\eta(\mathbf{r}, t)\)
due to other degrees of freedom as imperfections. Additionally, the charged particles are
subjected to an arbitrary damping force \(\Gamma(\mathbf{r}, \mathbf{p})\). Under that conditions the semiclassical
equations of motion read

\[
\dot{\mathbf{r}} = \frac{\mathbf{p}}{m} + \kappa \mathbf{\sigma} \times \nabla U; \\
\dot{\mathbf{p}} = -\nabla U - \kappa \nabla [\mathbf{p} \cdot (\mathbf{\sigma} \times \nabla U)] - \Gamma(\mathbf{r}, \mathbf{p}) + \eta(t).
\]

(2)

Because we are interested in the linear response regime the system is assumed to be nearby
the equilibrium. Therefore it seems to be adequate to assume the stochastic force \(\eta\) dis-
buted by a Gaussian white noise with an arbitrary noise strength \(D: \langle \eta_\alpha(t) \eta_\beta(t') \rangle = \)
2D\alpha\delta(t-t')$. The corresponding Fokker-Planck or Kramers’ equation for the probability density $P(r, p, t)$ is\(^7\)

$$\frac{\partial P}{\partial t} = -\frac{\partial}{\partial r} \left[ \frac{\partial \mathcal{H}}{\partial p} P \right] + \frac{\partial}{\partial p} \left[ \left( \frac{\partial \mathcal{H}}{\partial r} + \Gamma \right) P \right] + D \frac{\partial^2}{\partial p^2} P$$  \hspace{1cm} (3)

It is easy shown that the last equation satisfies the principle of detailed balance and exhibits an equilibrium solution of the form

$$P_e(r, p) \sim \exp\left(-\frac{\mathcal{H}}{k_B T}\right),$$  \hspace{1cm} (4)

provided the arbitrary damping function $\Gamma$ fulfills the relation

$$\Gamma = \frac{D}{k_B T} \frac{\partial \mathcal{H}}{\partial p}.$$  \hspace{1cm} (5)

From here we conclude immediately

$$\Gamma = \gamma \Pi, \text{ with } \Pi = [p + m\kappa(\sigma \times \nabla U(r))].$$  \hspace{1cm} (6)

The quantity $\Pi$ is the canonical momentum whereas the parameter $\gamma$ is the damping constant or the inverse relaxation time, which appears in the conventional Einstein relation $D = m\gamma k_B T$. Due to the linear momentum part in the Hamiltonian $\Pi$ the ‘canonical’ friction includes likewise a relativistic correction, which leads to an additional term in the Drude conductivity discussed below.

### III. STATIONARY CURRENT

Owing to the electric field energy incorporated into the Hamiltonian Eq. $\Pi$, the equilibrium distribution Eq. $\Pi$ may not be appropriate for analyzing the electric current. All charged particles would shift to $-\infty$ to establish an equilibrium state. Such a state is not realized because the equilibrium distribution is not normalizable in that case. Instead of the equilibrium solution one needs a steady state solution. Due to the conservation of the probability Eq. $\Pi$ can be written in form of a continuity equation where the probability current is a function of both, the spatial coordinate and the momentum $j_p(p, r, t)$. Whereas the equilibrium distribution $P_e$ satisfies $j_p = 0$ a steady state solution $P_s$ obeys the weaker
condition $\nabla \cdot \mathbf{j}_p = 0$. The complete evolution equation for the problem reads now

$$\frac{\partial P}{\partial t} = -\frac{\partial}{\partial \mathbf{r}} (A P) - \frac{\partial}{\partial \mathbf{p}} (B P) + D \frac{\partial^2}{\partial \mathbf{p}^2} P \quad \text{with}$$

$$A = \frac{\mathbf{p}}{m} + \kappa \mathbf{\sigma} \times \nabla U$$

$$B = -\nabla U - \kappa \nabla [\mathbf{p} \cdot (\mathbf{\sigma} \times \nabla U)] - \Gamma (\mathbf{r}, \mathbf{p})$$

(7)

From here we conclude

$$\frac{\partial}{\partial t} \langle \Pi \rangle = \langle B \rangle + m \kappa \langle A \cdot \nabla (\mathbf{\sigma} \times \nabla U)(\mathbf{r}) \rangle, \quad \frac{\partial}{\partial t} \langle \mathbf{r} \rangle = \langle A \rangle.$$  

(8)

To maintain a stationary electric current $\mathbf{j}$ the averaged velocity of the charge carriers should be fixed. In according to Eq. (8) this requirement is fulfilled by

$$\mathbf{j} = n e \langle A \rangle, \quad \frac{\partial}{\partial t} \langle \Pi \rangle = 0.$$  

(9)

The quantity $n$ is the density of the charge carriers. The bracket means now the average with the steady state solution $P_s(\mathbf{r}, \mathbf{p}; \mathbf{E}, \kappa)$ of Eq. (7). It is important to note that all averages performed with $P_s$ depends on the electric field $\mathbf{E}$, too. Because we are looking for a solution linear in the relativistic factor $\kappa$ we consider firstly the non-relativistic case $\kappa \equiv 0$. From Eq. (8) combined with Eq. (9) we get

$$\gamma \langle \mathbf{p} \rangle = e \mathbf{E} - \langle \nabla U_c \rangle.$$  

(10)

Since in the non-relativistic case, $\kappa = 0$ the system offers only one preferential direction, namely that one given by the external field $\mathbf{E}$, and furthermore the distribution function of the steady state depends on the electric field, the only possibility is that the averaged force in Eq. (10) point at the field direction. Hence we set

$$\langle \nabla U_c \rangle = \alpha_1 e \mathbf{E},$$

where the dimensionless factor $\alpha_1$ characterizes the influence of the crystal potential. The factor $\alpha_1$ depends on the concrete form of the potential and will be discussed below for a Coulomb potential. Inserting the last relation in Eq. (9) it results in the non-relativistic case

$$\mathbf{j}_0 = \frac{e^2 n}{m \gamma} (1 - \alpha_1) \mathbf{E}.$$  

(11)

The first part is nothing else as the conventional Drude conductivity with the simplest form of a scattering mechanism included in the damping factor $\gamma$. The charge carriers will
follow that law if the influence of the crystal potential is negligible, a situation which should be realized at sufficient high temperatures. In case the lattice potential becomes relevant an additional scattering mechanism is established and the mobility of a charge particle is further reduced leading to a decrease of the conductivity. Now let us take into account the relativistic effects in lowest order in $\kappa$. From Eqs. (8),(9)

$$j = \frac{ne^2}{m\gamma} \left[ E - \frac{1}{e} \langle \nabla U_c \rangle \right] + \frac{2\kappa ne^2 C (1 - \alpha_1)}{m\gamma^2} (\sigma \times E),$$  

(12)

where the parameter $C$ is defined by

$$\left\langle \frac{\partial^2 U_c}{\partial x_\mu \partial x_\nu} \right\rangle = C \delta_{\mu\nu}.$$  

(13)

Notice that the factor $C$ differs by a factor $e$ from that defined in $9$. The last relation is obviously valid for an isotropic crystal. As observed in Eq. (12) the relativistic effect proportional to $\kappa$ yields contributions to the current $j$ pointing toward the field direction $E$ and perpendicular to that one in the $\sigma \times E$ direction. Hence there exists a third direction oriented toward $\sigma \times (\sigma \times E)$. Because the average over the crystal potential has to be fulfilled with the stationary solution of the Kramers equation and this distribution depends on the electric field, the most general expression for the averaged force linear in the field $E$ reads

$$\langle \nabla U_c \rangle = \alpha_1 eE + \kappa e \left[ \alpha_2 (\sigma \times E) + \alpha_3 (\sigma \times (\sigma \times E)) \right] .$$  

(14)

Here the parameters $\alpha_i$, $i = 1, 2, 3$ reflect the influence of the crystal potential. They will be estimated later. As the final result the electric current consists of three parts

$$j = \frac{ne^2}{m\gamma} (1 - \alpha_1)E + \frac{ne^2 \kappa \alpha_3}{m\gamma} [(\sigma \times E) \times \sigma] + \frac{ne^2 \kappa}{m\gamma^2} [2C(1 - \alpha_1) - \alpha_2 \gamma] (\sigma \times E).$$  

(15)

In the subsequent section we discuss the conductivity.

IV. SPIN HALL CONDUCTIVITY

From Eq. (15) one obtains the charge conductivity and the Hall conductivity

$$\sigma_e = \frac{ne^2}{m\gamma} (1 - \alpha_1), \quad \sigma_s = \frac{ne^2 \kappa}{m\gamma^2} [2C(1 - \alpha_1) - \alpha_2 \gamma].$$  

(16)
The parameter $C$ is defined in Eq. (13) whereas the coefficients $\alpha_i$ are introduced in Eq. (14). As already observed in\textsuperscript{9} the ratio

$$\frac{\sigma_s}{\sigma_c} = \frac{\hbar}{4m^2c^2} \frac{2C (1 - \alpha_1) - \alpha_2 \gamma}{(1 - \alpha_1)\gamma}$$

is independent on the concentration of the charge carriers and is determined by the periodic potential. The result is in accordance with microscopic models\textsuperscript{12}. The expression for the electrical current is different from that obtained previously\textsuperscript{9}. However, if all parameters $\alpha_i$ are neglected the ratio in Eq. (17) is in accordance with\textsuperscript{9}. Apart from the thermal activation process as driving force the conventional Drude current is already supplemented by a correction term due to the crystal potential, see $j_0$ in Eq. (11). Otherwise the spin Hall current is likewise corrected twice by the relativistic damping force $\Gamma$ and through the influence of the lattice potential. To discuss the differences in more detail let us estimate the correction coefficients $C, \alpha_i$. The parameter $C$ is originated by the distribution of charge carriers in a cubic lattice. Following the line proposed in\textsuperscript{9} one can estimate the coefficient $C$ using the Poisson equation

$$\nabla^2 U_c(r) = -4\pi \rho e$$

where $\rho$ is the local charge density of the ions. This gives

$$C = \frac{4\pi}{3} Z e n_0$$

Here $-Ze$ is the charge and $n_0$ is the concentration of the ions. Let us notice that the result is correct in linear order of the external field. Using the approach proposed below one can show that corrections to the parameter $C$ due to the field $E$ occur at first in second order. The remaining quantities denoted by $\alpha_i$, may be figured out in a more laborious analysis. In finding out the parameters we have to calculate $\langle \nabla U_c \rangle$ according to Eq. (14). The problem one is confronted with is the fact that the electric field affects the intrinsic crystal potential $U_c(r)$ in such a manner that a constant current is maintained. In particular, the coupling between the external field and the crystal potential becomes important for low excited charge carriers which are subjected strongly to the field. In our approach the influence of the homogeneous field $E$ on the potential is manifested by the explicit field dependence of the steady state solution $P_s(r, p; E, \kappa)$. As a direct consequence the averaged force carried on the charge particles via the crystal potential, depends on $E$ according to Eq. (14). Owing to the pure spatial dependence of the crystal potential the reduced distribution function,
defined by $\rho(\mathbf{r}; \mathbf{E}, \kappa) = \int d\mathbf{p} P_s(\mathbf{r}, \mathbf{p}; \mathbf{E}, \kappa)$ seems to be a more appropriate quantity as $P_s$. However the basis Kramers’ equation (7) allows no exact steady state solution $P_s$. Hence one is relied on a reasonable approximation for the stationary distribution function. We are looking for a solution of Eq. (7) in the linear response regime of the external field and in lowest order of the relativistic factor $\kappa$. Let us make the ansatz for the steady state solution of Eq. (7) in the form

$$P_s(\mathbf{r}, \mathbf{p}; \mathbf{E}, \kappa) = P_0(\mathbf{r}, \mathbf{p}; \mathbf{E}) [1 + \kappa \mathbf{p} \cdot \mathbf{f}(\mathbf{r}, \mathbf{E})],$$

(19)

where $\mathbf{f} = -\frac{1}{\kappa_0 T} \sigma \times \nabla U_c$ in lowest order. Inserting this ansatz in Eq. (7), performing the momentum integration and collecting all terms in linear order in $\mathbf{E}$ and $\kappa$ one obtains

$$\langle \nabla U_c \rangle = \int d\mathbf{r} \left[ \rho(\mathbf{r}, \mathbf{E}, \kappa = 0) + \kappa \mathbf{p}(\mathbf{r}, \mathbf{E}) \cdot \mathbf{f}(\mathbf{r}, \mathbf{E}) \right] \nabla U_c.$$

Here the quantity $\mathbf{p}(\mathbf{r}, \mathbf{E}) = \int d\mathbf{p} P_0(\mathbf{r}, \mathbf{p}; \mathbf{E})$ is the averaged momentum proportional to the current at the coordinate $\mathbf{r}$ for $\kappa = 0$. Assuming that the reduced distribution function $\rho$ obeys the Smoluchowski equation and making the approximation

$$\left\langle \frac{\partial U_c}{\partial x_\alpha} \frac{\partial^2 U_c}{\partial x_\beta \partial x_\gamma} \right\rangle \simeq C \delta_{\beta\gamma} \left\langle \frac{\partial U_c}{\partial x_\alpha} \right\rangle,$$

(20)

we find

$$\langle \nabla U_c \rangle = \alpha_1 e \mathbf{E} + \frac{e\kappa C(1 - \alpha_1)}{\gamma} (\sigma \times \mathbf{E}).$$

Comparing the result with the ansatz made in Eq. (14) we conclude

$$\alpha_2 = \frac{(1 - \alpha_1) C}{\gamma}, \quad \alpha_3 = 0$$

(21)

In lowest order of a relativistic approach there is no current in spin direction. Inserting this result in Eq. (17) one obtains that the ratio of the spin Hall conductivity and the charge conductivity is independent on the lattice potential

$$\frac{\sigma_s}{\sigma_c} = \frac{\hbar C}{4m^2c^2\gamma}. $$

(22)

This expression differs from that obtained in 9 by a factor 2. The reason for the discrepancy is that in the field dependence of the averaged crystal potential is neglected. The spin and the charge current is subjected to the same scattering mechanism by the underlying isotropic crystal potential. If one includes higher order corrections appearing in Eq. (20)
then the ratio should be dependent on the potential. Making a similar approach one can derive the remaining factor \( \alpha_1 \). We find in \( d \) dimensions

\[
\alpha_1 = \frac{1}{V d (k_B T)^2} \int d\mathbf{r} \left( U_c(\mathbf{r}) - \bar{U}_c \right)^2, \quad \bar{U}_c = \frac{1}{V} \int d\mathbf{r} U_c(\mathbf{r})
\]  

(23)

Notice that the result is valid in first order of \( \kappa \) and in the linear response regime. So the problem in finding out the influence of the crystal potential is reduced to calculate the mean square displacement according to Eq. (23). To that aim we have considered a Coulomb potential \( U_c = Z e^2 \sum_{i,j} |\mathbf{r}_i - \mathbf{r}_j|^{-1} \). A straightforward calculation yields

\[
\alpha_1 = \frac{4(Ze^2)^2 n a}{3(k_B T)^2 \pi} \equiv \left( \frac{2\epsilon_A}{\sqrt{3\pi k_B T}} \right)^2
\]

where we have assumed a simple cubic lattice with the lattice spacing \( a \). There occurs a characteristic energy \( \epsilon_A = Z e^2 \sqrt{n a} \). For high temperatures \( \epsilon_A \ll k_B T \) the crystal potential becomes irrelevant, i.e., the motion of the charge carriers is independent on the underlying potential. Otherwise our approach is a classical one which should be restricted to \( \epsilon_A \leq k_B T \).

If the density \( n \) of the charge carriers is of the order \( n \simeq a^{-3} \) then \( \epsilon_A \simeq \frac{Ze^2}{a} \). For a typical electronic system the thermal energy is of the order of the Fermi energy \( k_B T \simeq \epsilon_F \) and therefore

\[
\sigma_c \simeq \frac{ne^2}{m} \left[ 1 - \left( \frac{2\epsilon_A}{\sqrt{3\pi \epsilon_F}} \right)^2 \right].
\]

Even in case that \( \epsilon_A \simeq \epsilon_F \) there is a significant contribution due to the potential. In general the characteristic energy should be smaller than the Fermi energy. Instead of using a Coulomb potential one can also consider a cos-potential \( U_c(\mathbf{r}) = U_0 \sum_{i=1}^d (1 - \cos(q_i x_i)) \).

For this potential one can calculate the conductivity numerically. The ratio of the charge and the spin Hall conductivity versus the rescaled temperature are shown in Fig. 1. For high temperature the potential becomes irrelevant and the classical Drude conductivity is achieved, compare the dashed line in Fig. 1. The reason for the weak deviations of \( \sigma_s/\sigma_c \) from Eq. (22) is originated exclusively by the approximation made in Eq. (20).

V. CONCLUSION

We have presented a thermally driven Drude model under inclusion of the relativistic spin-orbit coupling. The charge carriers are driven by a homogeneous electric field and
a Gaussian white noise. Additionally the charged particles are subjected to an intrinsic periodic crystal potential. Our approach differs from the semiclassical description proposed in\(^9\) in two respects. Firstly, we start consequently from the stochastic Kramers’ equation including canonical friction and white noise terms, and secondly we take into account that the correction terms due to the averaged crystal potential exhibit a pronounced dependence on the electric field and its orientation with respect to the spins. Our approach shows that Spin Hall Effect should also observed for finite temperature as it has reported recently\(^8\). For high temperatures the particles are not influenced by the potential and the conventional Drude conductivity appears. When the temperature is lowered the mobility is reduced owing to the potential. In our approach the interplay between the electric field and the lattice potential is manifested in the field dependence of the averaged force imposed on charged particles.

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1 N. F. Mott, R. Soc. A 124, 425 (1929).
2 M. I. Dyakonov and V. I. Perel, Phys. Lett. A 35, 459 (1971).
3 J. E. Hirsch, Phys. Rev. Lett. 83, 1834 (1999).
4 S.A. Wolf, D.D. Awschalom, R.A. Buhrman, J.M. Daughton, S. von Molnar, M.L. Roukes, A.Y. Chtchelkanova, and D.M. Treger, Science 294, 1488 (2001).
5 Y.K. Kato, R.C. Myers, A.C. Gossard, and D.D. Awschalom, Science 306, 1910 (2004).
6 V. Sih, R.C. Myers, Y.K. Kato, W.H. Lau, A.C. Gossard, and D.D. Awschalom, Nature Phys. 1, 31 (2005).
7 J. Wunderlich, B. Kaestner, J. Sinova, and T. Jungwirth, Phys. Rev. Lett. 94, 047204 (2005).
8 N.P. Stern, S. Ghosh, G. Xiang, M. Zhu, N. Samarth, and D.D. Awschalom, Phys. Rev. Lett. 97, 126603 (2006).
9 E. M. Chudnovsky, Phys. Rev. Lett. 99, 206601 (2007).
10 S. Zhang, Phys, Rev. Lett. 85, 393 (2000).
11 S. Murakami, N. Nagaosa, and S.-C. Zhang, Science, 301, 1348.

12 H.-A. Engel, E. I. Rashba, and B. I. Halperin, arXiv:cond-mat/0603306 (2007).

13 E.M. Hankiewicz and G. Vignale, Phys. Rev. Lett. 100, 026602 (2008).

14 W. Yang, K. Chang, and S.-C. Zhang, Phys. Rev. Lett. 100, 056602 (2008).

15 M-H Liu, S.-H. Chen, and C.-R Chang, arXiv:cond-mat/0802.0366v2 (2008).

16 G.Y. Panasyuk, J.C. Schotland, and V.A. Markel, Phys. Rev. Lett. 100, 047402 (2008).

17 C. W. Gardiner, Handbook of stochastic methods, (Springer, Berlin, 1990).
FIG. 1: The charge conductivity in units of the classical Drude conductivity versus the rescaled temperature (dashed line) and the ratio $\sigma_s/\sigma_c$ in units of $\hbar C/4m^2c^2\gamma$ (full line)