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Kane model parameters and stochastic spin current

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ABSTRACT

The spin current and spin conductivity is computed through thermally driven stochastic process. By evaluating the Kramers equation and with the help of $\vec{k}.\vec{p}$ method we have studied the spin Hall scenario. Due to the thermal assistance, the Kane model parameters get modified, which consequently modulate the spin orbit coupling (SOC). This modified SOC causes the spin current to change in a finite amount.

1. Introduction

Today's condensed matter research mainly relies on the study of the spin related issues of different materials. This put forward the concept of "Spintronics" [1,2], which unveils the importance of the spin degrees of freedom of electron for improved spin based devices. In this context, the development in the arena of semiconductor spintronics attracts the attention of many theoreticians as well as experimentalists. Spin Hall effect (SHE) [3,4] and spin orbit coupling (SOC) are the most important candidates for many theoretical understanding in the realm of semiconductor spintronics. The spin Hall effect is the spin analogue of charge Hall effect with some differences as well. In spin Hall effect, external magnetic field is redundant for separating spin up and down spin electrons. The candidate responsible for the separation is SOC, which effectively generates a magnetic field in the rest frame of the electron and as a consequence we have spin current in this system. SOC, which is the relativistic coupling between orbital and spin degrees of freedom of electron can be obtained through the Foldy–Wouthuysen (FW) transformation [5] of the Dirac equation in the presence of the external electric field. Alternatively, synthetic SOC can be generated via the strain parameter or with mechanical parameters like acceleration and rotation or via topological defects [6–8].

Besides, in semiconductor, the spin dynamics is influenced by the $\vec{k}.\vec{p}$ perturbation theory [9]. The semiconductor band structure, close to band edges, can be very well described by the $\vec{k}.\vec{p}$ method. It is possible to explain the spin dynamics of semiconductor by taking into account the interband mixing via $\vec{k}.\vec{p}$ perturbation theory. In [6], we have demonstrated that when band structure of semiconductor is considered, the free electron SOC parameter gets modified by the Kane model parameters. The inclusion of this renormalized SOC parameter makes the theory of electron in semiconductor more accurate.

Finite temperature effects are very important issues in different aspects of spin physics [10]. This gives the birth of spincaloritronics [11]. Very recently, the spin Hall conductivity is demonstrated in room temperature [12], which motivates us to study the thermally activated spin related issues. We are considering here the Fokker–Planck equation for analyzing the semi-classical motion of charge carriers. We have incorporated the additional constraints like damping force and also have included stochastic force arising due to the coupling of the system with a stochastic source of heat bath. In our formalism, the temperature correction is arising through the damping force. Besides, in the presence of temperature the Kane model parameters are affected as well. This consequently affects the spin orbit coupling and electron "g" factor. SOC is an important ingredient to have control over different physical parameters like spin current, conductivity, Berry curvature, spin relaxation time [13], etc. In this paper, we theoretically have investigated the thermally driven spin current in a semiconductor on the basis of $\vec{k}.\vec{p}$ perturbation theory from a generalized spin orbit Hamiltonian, which includes the stochastic force and arbitrary damping force. Here the Fokker–Planck or Kramer's equation is employed to calculate the spin current. Furthermore, the effect of the crystal symmetry is also taken care of. At first, we have

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considered the temperature correction due to scattering mechanism through the damping constant γ. Secondly, the temperature dependence of the Kane model parameters is appraised. Our goal is to examine the expression of the thermally assisted spin current and spin conductivity in semi-conducting system.

The organization of the paper is as follows: in Section 2 we build our model Hamiltonian considering the $\vec{k}.\vec{p}$ coupling between the Γ_6 conduction band and Γ_8 and Γ_7 valance bands. In Section 3, the semi-classical equation of motion is calculated applying Kramer's equation. We incorporate the effect of temperature through damping constant in this section and have computed the spin current. In Section 4, the renormalization of the Kane model parameters through temperature is taken care of, which modifies the SOC parameters as well. This renormalization of the SOC parameter alters the spin current in a different manner than that of the previous case. The conclusion is presented in Section 5.

2. The model Hamiltonian

The Pauli–Schrödinger Hamiltonian with the effect of spin orbit coupling due to an external electric field can be written as [6–8]

$$H = \frac{i\hbar^2 \vec{k}^2}{2\,\mathrm{m}} + qU(\vec{r}) + q\lambda\vec{\sigma}.(\vec{k}\times\vec{E}) + g\mu\vec{\sigma}.\vec{B}, \tag{1}$$

where the first and second terms are the kinetic term with m as the free electron mass and the potential of the external electric field respectively. The third term is the spin orbit coupling term and the forth term denotes the Zeeman term appearing as a consequence of external magnetic field. The free electron Hamiltonian in Eq. (1) modifies significantly when we consider the whole picture within a semiconductor, where one should incorporate the (8×8) Kane model [14] to include the effect of energy bands. The Hamiltonian for the (8×8) Kane model can be written as [6,9]

$$H_{8\times 8} = \begin{pmatrix} H_{6c6c} & H_{6c8v} & H_{6c7v} \\ H_{8v6c} & H_{8v8v} & H_{8v7v} \\ H_{7v6c} & H_{7v8v} & H_{7v7v} \end{pmatrix} \tag{2}$$

$$H_{8\times 8} = \begin{pmatrix} (E_c+eU)I_2 & \sqrt{3}P\vec{T}.\vec{k} & -\frac{P}{\sqrt{3}}\vec{\sigma}.\vec{k} \\ \sqrt{3}P?\vec{T}^{\dagger}.\vec{k} & (E_v+eU)I_4 & 0 \\ -\frac{P}{\sqrt{3}}\vec{\sigma}.\vec{k} & 0 & (E_v-\Delta_0+eU)I_2 \end{pmatrix}, \tag{3}$$

$\vec{T}$ matrices are given as

$$T_x = \frac{1}{3\sqrt{2}}\begin{pmatrix} -\sqrt{3} & 0 & 1 & 0 \\ 0 & -1 & 0 & \sqrt{3} \end{pmatrix},\quad T_y = -\frac{i}{3\sqrt{2}}\begin{pmatrix} \sqrt{3} & 0 & 1 & 0 \\ 0 & 1 & 0 & \sqrt{3} \end{pmatrix},$$

$$T_z = \frac{\sqrt{2}}{3}\begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix} \tag{4}$$

and I_2, I_4 are unit matrices of size 2 and 4 respectively. $U = V_e(\vec{r}) + V_c(r)$ is the total potential of the system which contains potential due to the external electric field $V_e(\vec{r})$ and crystal potential $V_c(r)$. E_c and E_v denote the energies at the conduction and valence band edges respectively. Δ_0 is the spin orbit gap, P is the Kane momentum matrix element which couples s like conduction bands with p like valence bands. This Kane Momentum matrix element remains almost constant for group III–V semiconductors, whereas Δ_0 and $E_G = E_c - E_v$ varies with materials. Here E_G denotes the energy gap between the conduction and valance band. The parameters P, Δ_0 and E_G are known as the Kane model parameters.

The Hamiltonian (3) can now be reduced to an effective Hamiltonian of the conduction band electron states [6,9] as

$$H_{kp} = \frac{P^2}{3}\left(\frac{2}{E_G}+\frac{1}{E_G+\Delta_0}\right)k^2 + eV(\vec{r}) - \frac{P^2}{3}\left(\frac{1}{E_G}-\frac{1}{(E_G+\Delta_0)}\right)\frac{ie}{\hbar}\vec{\sigma}.(\vec{k}\times\vec{k})$$
$$+ e\frac{P^2}{3}\left(\frac{1}{E_G^2}-\frac{1}{(E_G+\Delta_0)^2}\right)\vec{\sigma}.(\vec{k}\times\vec{E}) \tag{5}$$

Now to find out the total Hamiltonian, we must add up the Hamiltonian Eq. (1) with Eq. (5). The total Hamiltonian for the electron in the conduction band edges can be written as [9]

$$H_{tot} = \frac{\hbar^2\vec{k}^2}{2m^*} + eV(\vec{r}) + e(\lambda+\delta\lambda)\vec{\sigma}.(\vec{k}\times\vec{E}) + \left(1+\frac{\delta g}{2}\right)\mu\vec{\sigma}.\vec{B}, \tag{6}$$

where $\left(\frac{1}{m^*} = \frac{1}{m} + \frac{2P^2}{3\hbar^2}\left(\frac{2}{E_G}+\frac{1}{E_G+\Delta_0}\right)\right)$ is the effective mass and $(\vec{E} = -\vec{\nabla}V_e(\vec{r}))$ is the effective total electric field and $(\lambda = \frac{\hbar^2}{4m^2c^2})$ is the spin orbit coupling strength as considered in vacuum. Furthermore, the perturbation parameters $(\delta\,\lambda)$ and $(\delta\,g)$ are given by [9]

$$\delta\lambda = +\frac{P^2}{3}\left(\frac{1}{E_G^2}-\frac{1}{(E_G+\Delta_0)^2}\right)$$
$$\delta g = -\frac{4m}{\hbar^2}\frac{P^2}{3}\left(\frac{1}{E_G}-\frac{1}{E_G+\Delta_0}\right). \tag{7}$$

The $\delta\lambda$ parameter is responsible for the renormalization of spin orbit coupling and the δg term modifies the electron g factor considerably. It is possible to show that this extra term in the electron g factor can produce a shift in the ESR frequency. The Hamiltonian equation (6) can be rewritten neglecting the effect of Zeeman term as

$$H_{tot} = \frac{\hbar^2k^2}{2m^*} + eU + e\lambda_{eff}\vec{\sigma}.(\vec{k}\times\vec{E}), \tag{8}$$

where $\lambda_{eff} = \lambda + \delta\lambda$ is the effective SOC term. The Hamiltonian in Eq. (8) is our system Hamiltonian, where the first term is the kinetic term, second term is the potential energy term and the third term denotes the SOC term. The renormalization of the mass and the SOC indicates that when we consider the electron within a semiconductor, we must take care of these Kane model parameters as well.

The renormalized SOC parameter λ_{eff} must influence the spin dynamics in of electron [6]. Our job is to find the spin current from Eq. (8). One can note that SOC is very important term in explaining the spin Hall effect. Here due to the interband mixing, the SOC term is changed. As a consequence the spin Hall current should modify as well. But how this SOC parameter is related to thermal corrections, is an important observation and we proceed to find this in Section 4. But before that in Section 3 we want to find out the spin current without incorporating the thermal corrections of SOC.

3. Fokker–Planck equation and spin current

Considering Hamiltonian in equation (8), it is possible to calculate the semi-classical equations of motion by evaluating $\vec{r}$ *and* $\vec{p}$ via Heisenberg algebra. Before doing that, let us include the stochastic forces $\zeta(r,t)$, which appears as a consequences of other degrees of freedom as imperfection. One can also incorporate an arbitrary damping force κ(r,p). Including all these forces, we can write the semi-classical equation of motion as

$$\vec{r} = \frac{1}{i\hbar}[r, H_{tot}] = \frac{\vec{p}}{m^*} + e\lambda_{eff}(\vec{\sigma}\times\vec{\nabla}U)$$