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SPIN CURRENT IN SPIN–ORBIT COUPLING SYSTEMS

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We present a simple and pedagogical derivation of the spin current as the linear response to an external electric field for both Rashba and Luttinger spin–orbital coupling Hamiltonians. Except for the adiabatic approximation, our derivation is exact to the linear order of the electric field for both models. The spin current is a direct result of the difference in occupation levels between different bands. Moreover, we show a general topological spin current can be defined for a broad class of spin–orbit coupling systems.

Keywords: Spin current; spin–orbital coupling; adiabatic approximation.

1. Introduction

Spintronics aims to manipulate spins of particles. As such, an essential step in the field is the generation of a reliable spin current. The injection of spin polarized electron current from a ferromangetic metal is not favorable because polarization is lost at the interface due to the conductance mismatch.[1,2] Injections from ferromagnetic semiconductors into nonmagnetic semiconductors have been successfully developed in recent several years.[3–5] The theory of spin transport in the fore-mentioned cases depends on the detailed mechanism of spin relaxation, where spin transport generally is a dissipative process.

Recently, Murakami, Nagaosa and Zhang[6] have discovered a dissipationless and topological spin Hall current in the hole doped semiconductors with strong spin–orbit coupling. These authors studied the effective Luttinger Hamiltonian[12]

$$H_L = \frac{1}{2m}\left[\left(\gamma_1 + \frac{5}{2}\gamma_2\right)P^2 - 2\gamma_2 (P\cdot S)^2\right] \tag{1}$$

which describes conventional semiconductors such as Si, Ge, GaAs and InSb. The geometrical structure of the effect is such that for an electric field applied on the z

direction, a y-polarized spin current will flow in the x direction. The electric field induced spin current can be summarized by the following formula

$$J_j^i = \sigma_s \epsilon_{ijk} E_k \,, \tag{2}$$

where ϵ_{ijk} is the antisymmetric tensor. Unlike the ordinary Ohm's law, this equation has the remarkable property of time reversal symmetry.[6,7] This effect also has a deep topological origin,[6,7] related to the topological structure of the four-dimensional quantum Hall effect.[13]

In an independent work, Sinova *et al.* also suggested[8] that the dissipationless, or the intrinsci spin current can exist in the two-dimensional Rashba system, described by the Hamiltonian[11,10]

$$H_R = \frac{P^2}{2m} + \gamma(P_x S_y - P_y S_x) \,. \tag{3}$$

In this case, the spin current is polarized in the direction perpendicular to the two-dimensional plane and flowing in a planar direction perpendicular to the direction of the charge current. Surprisingly, the spin conductance in these systems turns out to be independent of the spin orbit coupling and given by:

$$\sigma_s = \frac{e}{8\pi} \,. \tag{4}$$

In both of the above models, the intrinsic spin current is induced by an external electric field. The authors of Refs. 6 and 8 have argued that the spin current is dissipationless because the spin conductance is invariant under time-reversal operations. However, the approaches taken by the authors of Refs. 6 and 8 are markedly different. In the first two-dimensional model,[8] a semi-classical approach is used to derive the spin current, while in the second three-dimensional model,[6] the spin current is derived as a topological effect in momentum space. It therefore appears that the physics of the spin current in these two models is different. In fact, in the first model, there is no known topological structure. However, from a purely theoretical point of view, we should be able to derive the results and understand the physics in one unified approach.

2. Derivation of Spin Current for the Rashba and Luttinger Models

The aim of this article is to present a simple, pedagogical and unified derivation of the spin current for both models. The derivation of Murakami *et al.*[6,7] emphasizes on the momentum space topology which requires some advanced mathematical knowledge. The semi-classical derivations presented in Refs. 6, 8 and 9 may not be familiar to general readers. In view of the importance of the effect, we feel that the general reader could benefit from a simple derivation based on the standard time dependent perturbation theory within single particle quantum mechanics. As in Refs. 6 and 8, we work within the adiabatic approximation. Since there is no interaction between particles, the result derived here is exact only as far as the linear response to the external electric field in the adiabatic limit is concerned. Moreover, general conclusions about the spin current can be manifestly drawn in this approach. Following the common definition of the spin current, we show that the spin current is always a direct result of the difference in occupation levels between different bands in the models. Part of the spin current can be interpreted as topological spin current. In fact, we present an analysis and derivation of the topological spin current for a broad class of spin–orbital coupling models.

In the following, we first calculate the spin current in the Rashba and Luttinger models and then discuss the topological part of the spin current. For the Luttinger Hamiltonian, we show that the expectation value for the spin current in the heavy hole and light hole states differs by exactly a minus sign. This result leads to the conclusion that the contributions to the spin current from the heavy hole and light hole bands should be exactly opposite and differ by the Fermi velocities of two bands. The total spin current gives a quantum correction to the semiclassical result of Ref. 6. The nature of the quantum correction can be manifestly understood in our calculation, and has also been discussed in Ref. 7. For the Rashba Hamiltonian, our approach gives the same spin current as the Ref. 8 if the same definition of the spin current is taken.

In our calculation, the spin current is defined by the velocity times the spin, which is a rank two tensor. However, the velocity operator in general does not commute with the spin operator in a model with spin–orbit coupling. In order to define the spin current tensor as a Hermitian operator, we have to symmetrize it:

$$J_i^j = \frac{1}{2}\left(S_i \frac{\partial H}{\partial P_j} + \frac{\partial H}{\partial P_j} S_i\right) . \tag{5}$$

2.1. *Adiabatic approximation and Kubo formula*

Let us consider a general spin–orbit coupling model described by the many-body Hamiltonian $H(P, S)$. In the presence of a constant external electric field, we choose the vector potential $\mathbf{A} = -\mathbf{E}t$. The total Hamiltonian becomes time dependent, $H(t) = H(P - e\mathbf{E}t, S)$. Let $|G, t\rangle$ be an instantaneous ground state eigenstate of the time-dependent Hamiltonian,

$$H(t)|G, t\rangle = E_G(t)|G, t\rangle . \tag{6}$$

The many-body ground state wavefunction $\Psi_G(t)$ of the Hamiltonian satisfies the Schrodinger equation,

$$i\frac{d}{dt}\Psi_G(t) = H(t)\Psi_G(t) . \tag{7}$$

By first-order time-dependent perturbation theory, we have

$$|\Psi_G(t)\rangle = \exp\left\{-i\int_0^t dt' E_G(t')\right\}$$
$$\times\left\{|G,t\rangle + i\sum_n \frac{|n,t\rangle\langle n,t|\frac{\partial}{\partial t}|G,t\rangle}{E_n(t)-E_G(t)}(1-e^{i(E_n(t)-E_G(t))t})\right\}, \quad (8)$$

where $|n,t\rangle$ are the instantaneous excited eigenstates.

The second term in the RHS of the expression above contains a fast oscillation term which averages to zero, and which we neglect below. For the non-interacting Fermi system, the above expression can be simplified into summation over all instantaneous single particle eigenstates. Then for an arbitrary operator O, the difference of expectation values between the perturbed and unperturbed states is given in Ref. 14

$$\langle\Psi_G,t|\hat{O}|\Psi_G,t\rangle$$
$$= i\sum_{\epsilon_{\lambda,P}<E_f<\epsilon_{\lambda',P}}$$
$$\times\frac{\langle\lambda,P(t)|\hat{O}|\lambda',P(t)\rangle\langle\lambda',P(t)|\frac{\partial}{\partial t}|\lambda,P(t)\rangle + \langle\lambda,P(t)|\frac{\partial}{\partial t}|\lambda',P(t)\rangle\langle\lambda',P(t)|\hat{O}|\lambda,P(t)\rangle}{\epsilon_{\lambda',P(t)}-\epsilon_{\lambda,P(t)\rangle}},$$
$$(9)$$

where $|\lambda,P(t)\rangle$ is the instantaneous eigenstate with polarization λ of the single particle Hamiltonian.

The entire calculation of the spin current that follows relies on the above Kubo formula. However, when the Hamiltonian has degenerate states, we use the following convention: if a set of states, $\{|\lambda,P(t)\rangle\}$, are degenerate in energy, we can always choose a complete orthogonal basis of states in the set, $\{|\alpha,P(t)\rangle\}$, such that, for any two new different orthogonal states $|\alpha_1,P(t)\rangle$ and $|\alpha_2,P(t)\rangle$, we have,

$$\langle\alpha_1,P(t)|\frac{\partial}{\partial t}|\alpha_2,P(t)\rangle = 0\,. \quad (10)$$

In this case, the summation index in the formula does not include the degenerate states and therefore, the formula is well defined.

2.2. *Spin current in the Rashba spin–orbital coupling model*

Let us now consider the particular case of the Rashba Hamiltonian in an external electric field. The time dependent Rashba Hamiltonian is given by

$$H_R(t) = \frac{P(t)^2}{2m} + \gamma(P_x(t)S_y - P_y(t)S_x)\,. \quad (11)$$

For a given $P(t)$, the instantaneous eigenstates are given by

$$|\lambda,P(t)\rangle = U_R|\lambda\rangle\,, \quad (12)$$

with

$$\epsilon(P(t)) = \frac{P^2(t)}{2m} + \gamma\lambda|P(t)|\,,$$

$$U_R = e^{-i\phi(t)S_z}\,,$$

$$\phi(t) = \tan^{-1}\frac{P_y(t)}{P_x(t)}$$

the azimuthal angle, and $|\lambda\rangle$ is the eigenstate of S_y with $S_y|\lambda\rangle = \lambda|\lambda\rangle$. Therefore,

$$\frac{\partial}{\partial t}|\lambda, P(t)\rangle = -i\frac{d\phi(t)}{dt}S_z|\lambda, P(t)\rangle\,, \tag{13}$$

with

$$\frac{d\phi(t)}{dt} = e\epsilon_{ij}E_i\frac{P_j(t)}{P^2(t)}\,,$$

where ϵ_{ij} is rank-2 antisymmetric tensor. By applying the Kubo formula, for any Hermitian operator $\hat{O}$, we obtain

$$\langle\lambda, P(t)|\hat{O}|\lambda, P(t)\rangle = 2e\epsilon_{ij}E_i\frac{P_j(t)}{|P(t)|^3} \times \sum_{\lambda'\neq\lambda}\langle\lambda', P(t)|S_z|\lambda, P(t)\rangle\frac{\mathrm{Re}(\langle\lambda, P(t)|\hat{O}|\lambda', P(t)\rangle)}{\gamma(\lambda'-\lambda)}\,. \tag{14}$$

For the spin one half particles, the above formula is simplified to

$$\left\langle \pm\frac{1}{2}, P(t)|O|\pm\frac{1}{2}, P(t)\right\rangle = \pm C_o\epsilon_{ij}E_i\frac{P_j(t)}{P(t)^3} \tag{15}$$

where

$$C_o = \frac{e}{\gamma}\mathrm{Re}\left\langle\frac{1}{2}\middle|\,\hat{O}(t)\,\middle|-\frac{1}{2}\right\rangle\,.$$

The spin current operator when the spin is polarized in the perpendicular direction to the xy plane is given by

$$J_i^z = \frac{P_i}{m}S_z + \frac{\gamma}{2}\epsilon_{ij}(S_zS_j + S_jS_z)\,. \tag{16}$$

It is easy to show that

$$\mathrm{Re}\left\langle\frac{1}{2}\middle|\,\hat{J}_i(t)\,\middle|-\frac{1}{2}\right\rangle = \frac{P_i}{m}\left\langle\frac{1}{2}\middle|\,S_z\,\middle|-\frac{1}{2}\right\rangle = \frac{P_i}{2m}\,.$$

Considering the whole Fermi surface, we can easily calculate the total spin current. Let us take the electric field is in x direction and consider the current J_y.

$$J_y = \frac{e}{8\pi\gamma m}\Delta P_f \tag{17}$$

where the ΔP_f is the difference of the fermi velocity for the two bands. In this model, $\Delta P_f = m\lambda$. This yields the result of the Eq. (4).

2.3. *Spin current in the Luttinger model*

We now turn to the discussion of the effective Luttinger Hamiltonian. In the presence of the external electric field, the time dependent effective Luttinger Hamiltonian is

$$H_L(t) = \frac{1}{2m}\left[\left(\gamma_1 + \frac{5}{2}\gamma_2\right)(P(t))^2 + 2\gamma_2(P(t)\cdot S)^2\right]. \tag{18}$$

For a given $P(t)$, the Hamiltonian has four instantaneous eigenstates,

$$\begin{aligned} H(t)|P(t),\lambda\rangle &= \epsilon_\lambda(P(t))|P(t),\lambda\rangle\,, \\ \frac{P(t)\cdot S}{|P(t)|}|P(t),\lambda\rangle &= \lambda|P(t),\lambda\rangle\,, \end{aligned} \tag{19}$$

where

$$\epsilon_\lambda(P(t)) = \frac{P^2(t)}{2m}\left(\gamma_1 + \left(\frac{5}{2} - 2\lambda^2\right)\gamma_2\right).$$

For $\lambda = \pm\frac{3}{2}$ and $\lambda = \pm\frac{1}{2}$, they are referred to as the heavy hole band and light hole band respectively. The eigenstates can be explicitly written as

$$|P(t),\lambda\rangle = U_L|\lambda\rangle\,, \quad U_L = e^{-i\phi(t)S_z}e^{-i\theta(t)S_y}|\lambda\rangle\,, \tag{20}$$

where $\tan(\phi(t)) = P_y(t)/P_x(t)$, $\cos(\theta(t)) = P_z(t)/|P(t)|$ and $S_z|\lambda\rangle = \lambda|\lambda\rangle$.

Since the eigenstates are degenerate, we have to choose an orthogonal basis and satisfy the Eq. (10) in order to use the Kubo formula. Without loss of generality, we choose the electric field in the z direction. In this case, ϕ is time-independent. Therefore,

$$\langle P(t),\lambda'|\frac{\partial}{\partial t}|P(t),\lambda\rangle - i\frac{d\theta(t)}{dt}\langle\lambda'|S_y|\lambda\rangle\,. \tag{21}$$

From this equation, we obtain that for the states with the helicity equal to $\pm\frac{3}{2}$, the matrix element $\langle P(t),-\frac{3}{2}|\partial_t|P(t),\frac{3}{2}\rangle$ vanishes. The only states for which we have to find an orthogonal base are in the helicity $\pm\frac{1}{2}$. Let us define

$$\begin{aligned} |P(t),+\rangle &= \left(\frac{1}{\sqrt{2}}\left|P(t),\frac{1}{2}\right\rangle + i\left|P(t),-\frac{1}{2}\right\rangle\right), \\ |P(t),-\rangle &= \frac{1}{\sqrt{2}}\left(\left|P(t),\frac{1}{2}\right\rangle - i\left|P(t),-\frac{1}{2}\right\rangle\right), \end{aligned} \tag{22}$$

which satisfy $\langle P(t),+|\partial_t|P(t),-\rangle = 0$.

For an arbitrary operator $\hat{O}$, let $\hat{O}(t) = U_L^+\hat{O}U_L$. Applying the Kubo formula, we obtain the expectation value for an arbitrary Hermitian operator,

$$\langle\Psi_{\frac{3}{2}}(t)|\hat{O}|\Psi_{\frac{3}{2}}(t)\rangle = \frac{\sqrt{3}m}{2\gamma_2P^2}\frac{d\theta(t)}{dt}\mathrm{Im}\left(\left\langle\frac{1}{2}\right|\hat{O}(t)\left|\frac{3}{2}\right\rangle\right) \tag{23}$$

and

$$\langle \Psi_+(t)|\hat{O}|\Psi_+(t)\rangle = \frac{\sqrt{3}m}{4\gamma_2 P^2}\frac{d\theta(t)}{dt}\left\{\mathrm{Im}\left(\left\langle \frac{3}{2}\left|\hat{O}(t)\right|\frac{1}{2}\right\rangle + \left\langle -\frac{1}{2}\left|\hat{O}(t)\right|-\frac{3}{2}\right\rangle\right)\right.$$
$$\left. + \mathrm{Re}\left(\left\langle -\frac{1}{2}\left|\hat{O}(t)\right|\frac{3}{2}\right\rangle + \left\langle \frac{1}{2}\left|\hat{O}(t)\right|-\frac{3}{2}\right\rangle\right)\right\}. \tag{24}$$

The spin current operator where the spin is polarized in y direction and flows in x direction is given by

$$\hat{J}^y_x = \frac{\gamma_1 + \frac{5}{2}\gamma_2}{m}P_x S_y - \frac{\gamma_2}{2m}[S_y((P\cdot S)S_x + S_x(P\cdot S)) + h.c.]\,. \tag{25}$$

The matrix element $\mathrm{Im}\,\langle\frac{3}{2}|\hat{J}^y_x(t)|\frac{1}{2}\rangle$ is calculated to be

$$\mathrm{Im}\left\langle \frac{3}{2}\right|\hat{J}^y_x(t)\left|\frac{1}{2}\right\rangle = \frac{\sqrt{3}P}{2m}\sin\theta(\gamma_1\cos^2\phi + 2\gamma_2\sin^2\phi)\,. \tag{26}$$

We thus obtain,

$$\langle \Psi_{\frac{3}{2}}(t)|J^y_x|\Psi_{\frac{3}{2}}(t)\rangle = -\langle \Psi_+(t)|J^y_x|\Psi_+(t)\rangle$$
$$= \frac{3e}{4\gamma_2 P^4}(\gamma_1 P_x^2 + 2\gamma_2 P_y^2)E \tag{27}$$

where we used $d\theta(t)/dt = eE\sin(\theta(t))/|P(t)$.

For the states $|P(t), -\frac{3}{2}\rangle$ and $|P(t), -\rangle$, the expectation values for spin current are the same as $|P(t), \frac{3}{2}\rangle$ and $|P(t), +\rangle$ respectively. Therefore the total spin current by including all the particles in the two bands is given by

$$J^y_x = \frac{eE(\gamma_1 + 2\gamma_2)}{4\pi^2\gamma_2}\Delta P_f\,, \tag{28}$$

where ΔP_f is the Fermi momentum difference between the heavy and light hole bands. Once again, we show that the spin current comes from the occupation difference between two bands. The above result has been independently obtained by Murakami, Nagaosa and Zhang through a slightly different derivation based on Kubo formula too.[7]

3. Topological Spin Current and Conclusion

This full quantum mechanical calculation gives a quantum correction to the original semiclassical result.[6] In fact, the difference comes from the definition of spin current operator. In Ref. 6, an effective Hamiltonian was derived by introducing a monopole in momentum space. The spin current is thought of as a topological effect of the monopole. In the heavy hole states, the gauge potential is Abelian while in the light hole states, the gauge potential is non-Abelian. However, the field strength in both bands is Abelian. For each helicity states, the field strength is given by

$$F_{ij} = [D_i, D_j] = \lambda\left(\lambda^2 - \frac{7}{2}\right)\epsilon_{ijk}\frac{P_k}{P^3}\,, \tag{29}$$

where

$$D_j = P_{h(l)}(U_L^+ \partial_{p_j} U_L)$$

($P_{h(l)}$ is the projection onto heavy (light) hole bands). This gauge field modifies the semiclassical equation of motions as

$$v_{i,\lambda} = \dot{X}_{i,\lambda} = \frac{P_i}{m_\lambda} + F_{ik} E_k \,. \tag{30}$$

In Ref. 6, the spin current is derived by replacing the spin operator by its expectation value in the helicity states compared to the definition in the Eq. (5). If we use the same replacement, it is straightforward to show that the spin current from the perturbation theory is the same as from Ref. 6. Namely, for a given helicity state $|\lambda, P(t)\rangle$, the expectation value of $\langle v_i \rangle_\lambda$ in the adiabatic approximation from the perturbation theory is given by $\frac{\partial P_j}{\partial t}\langle\lambda|F_{ij}|\lambda\rangle$.

However, the above calculation does not underline the topological nature. Several questions still remain. The first is how the topological spin current can be separated from the general spin current formula in the Eq. (5). The second is that since the calculation is performed on a specific model, it is not clear whether the topological arguments can be applied to more general cases such as realistic anisotropic, inversion-symmetry breaking semiconductors. The recent work of Murakami, Nagaosa and Zhang[7] have answered some of these questions from the Kubo formula for the isotropic Luttinger Hamiltonian. Here we give an independent argument based on our formalism.

Let us review Eq. (5) and discuss a general case. Let us assume a general unitary transformation U which is a function in the momentum space and diagonalizes a general Hamiltonian H. For any operator O, let $O(U) = U^+ O U$. Therefore, $H_0 = H(U)$ is diagonal and

$$J_i^j(U) = \frac{-i}{2}[S_i(U)[X_j(U), H_0] + [X_j(U), H_0]S_i(U)] \,. \tag{31}$$

Let us write

$$S_i(U) = S_i^p(U) + S_i^c(U) \,,$$

$$X_j(U) = X_j^p(U) + X_j^c(U) \,,$$

where $O^p(U)$ keeps the elements of $O(U)$ which are only between the degenerate eigenvalues of $H(U)$ for a given operator O; namely, it is the projection onto the degenerate bands. $O^c(U)$ is the leftover part. Now we can define the total spin current operator into $J_i^j(U) = T_i^j(U) + A_i^j(U)$, where the first part $T_i^j(U)$ is defined

$$T_i^j(U) = \frac{-i}{2}([S_i^p(U)X_j(U) + X_j S_i^p(U), H_0] + [S_i(U)X_j^p(U) + X_j^p S_i(U), H_0]) \tag{32}$$

and

$$A_i^j(U) = \frac{-i}{2}[S_i^c(U)[X_j^c(U), H_0] + [X_j^c(U), H_0]S_i^c(U)] \,. \tag{33}$$

where the relations $[S_i^p(U), H_0] = 0$ and $[X_j^p(U), H_0] = 0$ have been used in the above equations. It is clear that $A_i^j(U)$ is the band crossing contribution to the spin current. $T_i^j(U)$ can be considered as the topological part of the spin current. This statement is true for any models with arbitrary number of bands and with arbitrary degeneracy in each bands caused by spin orbit coupling. The proof is straightforward from the perturbation theory.

Without loss of generality, we assume that H_0 is the diagonal matrix,

$$H_0 = \begin{pmatrix} E_1 I_{m_1} & 0 & 0 & \cdots \\ 0 & E_2 I_{m_2} & 0 & \cdots \\ \cdots & \cdots & \cdots & \cdots \end{pmatrix},$$

where m_1, $m_2, \ldots$ are the number of degeneracies of each of the bands. By a direct calculation from the Eq. (5), the spin current contribution from $T_i^j(U)$ is given by

$$\langle T_i^j \rangle = i\,\mathrm{Tr}\{S_i^p(U)[X_j^p(U), X_k^p(U)]\}\frac{\partial P_k(t)}{\partial t}\,. \tag{34}$$

The above equation is independent of U for all of unitary matrixes which $U^+HU = H_0$. Therefore, the symmetry group for U is $SU(m_1) \bigotimes SU(m_2) \bigotimes \cdots$. The above formula is manifestly gauge invariant if we view the symmetry group as a gauge group in momentum space as described in Ref. 6.

From the above analysis, we see that the topological spin current exists in much broader spin–orbit coupling systems. However, it requires the degeneracy of the bands, namely the non-Abelian gauge structure in momentum space. The direct consequences from this result is that for a realistic anisotropic Luttinger Hamiltonian, the topological part of spin current will still exist, and that for the Rashba Hamiltonian there is no topological part of the spin current since there is only a $U(1)$ gauge.

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