Semiclassical Spin Transport in Spin-Orbit-Coupled Bands

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Motivated by recent interest in novel spintronics effects, we develop a semiclassical theory of spin transport that is valid for spin-orbit coupled bands. Aside from the obvious convective term in which the average spin is transported at the wave packet group velocity, the spin current has additional contributions from the wave packet's spin and torque dipole moments. Electric field corrections to the group velocity and carrier spin contribute to the convective term. Summing all terms we obtain an expression for the intrinsic spin-Hall conductivity of a hole-doped semiconductor, which agrees with the Kubo formula prediction for the same quantity. We discuss the calculation of spin accumulation, which illustrates the importance of the torque dipole near the boundary of the system.

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Electrical control of spins in systems with spin-orbit interactions is of basic interest and has great potential in semiconductor spintronics [1–3]. In recent years, steady progress has been made towards realization of convenient semiconducting ferromagnets and spin injection into semiconductors from ferromagnetic metals [4–9]. The spin transport theory presented in this Letter is motivated generally by current interest in novel spin-related transport effects in semiconductors, and particularly by interest in various schemes that generate spin-polarized currents [10–16]. Using a semiclassical wave packet approach, we find that the spin current can be expressed as the sum of several physically transparent terms which are grouped together in a Kubo formula description. As an example, we use our theory to derive an expression for the intrinsic spin-Hall conductivity [10,11] of a hole-doped semiconductor.

Semiclassical formulations of transport theory exploit the smooth variation of transport fields on atomic length scales. Previous semiclassical theories of *spin* transport [13,17–20] have not accounted explicitly for intrinsic spin-orbit interaction in the crystal apart from, occasionally, its role in the relaxation of nonequilibrium spin polarizations. In this Letter, we apply the wave packet approach introduced by Sundaram and Niu [21], which captures the consequences of the wave vector dependence of the Bloch spinors, to treat spin transport in spin-orbit coupled bands. This wave packet approach has already been successful in describing the anomalous Hall effect in ferromagnetic semiconductors [22] and transition metals [23], interpreting it as a consequence of the Berry-phase correction to the group velocity induced by the intrinsic spin-orbit interaction. We show here that the Hall spin current in response to an electric field is nonzero even in paramagnetic systems and that, in addition to the Berry phase term evaluated in a recent paper [10], other contributions must be taken into account. First of all, there is a contribution from the electric field correction to the average spin orientation of a wave packet. In addition, there are also contributions from the spin dipole and torque dipole of a carrier, which arise from the fact that spin and torque distribution within a wave packet generally differ from that of the charge. Including all these contributions, we obtain a total semiclassical spin current which is in agreement with the Kubo formula expression for the same quantity. We show that nonequilibrium spin polarization near the sample edge is driven not by the spin current alone but by the sum of the spin current and torque dipole density.

The semiclassical dynamics of each spin-charge carrier in a nondegenerate band is described by a wave packet, whose charge centroid has coordinates $(\mathbf{r}_c, \mathbf{k}_c)$. Wave packet construction is thoroughly explained in [21,24]. When expanded in the basis of Bloch eigenstates, the wave packet has the form

$$|w\rangle = \int d^3k\, a(\mathbf{k}, t) e^{i\mathbf{k}\cdot\hat{\mathbf{r}}} |u(\mathbf{r}_c, \mathbf{k}, t)\rangle. \tag{1}$$

In the above, the wave functions $|u\rangle$ contain [25] corrections linear in the electric field. They form a complete set and retain the Bloch periodicity. The function $a(\mathbf{k}, t)$ is a narrow distribution sharply peaked at $\mathbf{k}_c$, and its phase specifies the center of charge position $\mathbf{r}_c$. The size of the wave packet in k space must be considerably smaller than that of the Brillouin zone. In real space, this implies that the wave packet must stretch over many unit cells.

In the presence of a uniform electric field, the semiclassical equations of motion for a nondegenerate band read [21]

$$\hbar\dot{\mathbf{r}}_c = \frac{\partial\varepsilon}{\partial\mathbf{k}_c} - e\mathbf{E}\times\mathbf{\Omega} \quad \text{and} \quad \hbar\dot{\mathbf{k}}_c = e\mathbf{E}, \tag{2}$$

where e is the carrier charge, ε is the band dispersion, and $\mathbf{\Omega}$ is the Berry curvature of the Bloch state [21]. Henceforth, $\mathbf{k}_c$ will be abbreviated to $\mathbf{k}$. The effect of the electric field is thus twofold: It drives the center of the wave packet in k space, and it gives rise to a nonadiabatic correction to the wave functions, which mixes the bands at each $\mathbf{k}$.

Following the strategy of Boltzmann transport theory, we consider a collection of particles described by a phase space distribution $f(\mathbf{r}_c, \mathbf{k}, t)$. This distribution can drift according to the semiclassical equations of motion (2), and can also change due to collisions:

$$\frac{\partial f}{\partial t} + \dot{\mathbf{r}}_c\cdot\frac{\partial f}{\partial\mathbf{r}_c} + \dot{\mathbf{k}}\cdot\frac{\partial f}{\partial\mathbf{k}} = \frac{df}{dt}\bigg|_{\text{coll}}. \tag{3}$$

The collision term on the right-hand side may be modeled by relaxation times or more accurately by collision integrals as usual.

The spin density distribution is defined as

$$S(\mathbf{r}, t) \equiv \iint d^3k\, d^3r_c\, f(\mathbf{r}_c, \mathbf{k}, t)\langle\delta(\mathbf{r}-\hat{\mathbf{r}})\hat{s}\rangle, \tag{4}$$

where $\hat{s}$ is an arbitrary component of the spin operator, and the bracket indicates quantum mechanical average over the wave packet with charge centroid $(\mathbf{r}_c, \mathbf{k})$. Further analysis of this distribution will be facilitated by making the analogy with the standard coarse graining of electrodynamics in material media [26]. Our wave packets play the role of "molecules," whose size will be taken as much smaller than the length scale of the distribution function. We are thus allowed to view the δ function in the above definition of the spin density as a sampling function with a width somewhere between the microscopic scale of the wave packets and the macroscopic scale of the distribution function. We can therefore write it as $\delta[(\mathbf{r}-\mathbf{r}_c) - (\hat{\mathbf{r}}-\mathbf{r}_c)]$ and expand it around $\mathbf{r}_c$, keeping only the first order term. Performing the integration over $\mathbf{r}_c$, the spin density can be reexpressed in the following form:

$$S = \int d^3k\, f\langle\hat{s}\rangle - \nabla\cdot\int d^3k\, f\mathbf{p}^s, \tag{5}$$

where $f = f(\mathbf{r}, \mathbf{k}, t)$, and $\mathbf{p}^s = \langle(\hat{\mathbf{r}}-\mathbf{r}_c)\hat{s}\rangle|_{\mathbf{r}_c=\mathbf{r}}$ is the spin dipole. The two terms can be regarded as monopole and dipole contributions. The second term is analogous to the contribution to the charge density in electrodynamics from the divergence of the polarization.

Spin is in general not conserved, and for what follows it will be useful to define a quantity, which we shall call the torque density, in order to include the rate of change of spin into our discussion of transport:

$$\mathcal{T}(\mathbf{r}, t) \equiv \iint d^3k\, d^3r_c\, f(\mathbf{r}_c, \mathbf{k}, t)\langle\delta(\mathbf{r}-\hat{\mathbf{r}})\hat{\tau}\rangle, \tag{6}$$

in which $\hat{\tau}$ is understood as $\frac{i}{\hbar}[\hat{H}, \hat{s}]$ and $\hat{H}$ is the Hamiltonian. Following the steps outlined above, the torque density becomes

$$\mathcal{T} = \int d^3k\, f\langle\hat{\tau}\rangle - \nabla\cdot\int d^3k\, f\mathbf{p}^\tau, \tag{7}$$

with the torque dipole $\mathbf{p}^\tau = \langle(\hat{\mathbf{r}}-\mathbf{r}_c)\hat{\tau}\rangle|_{\mathbf{r}_c=\mathbf{r}}$.

We evaluate the spin-current using the microscopic spin-current operator and the semiclassical distribution function:

$$\mathbf{J}^s(\mathbf{r}, t) \equiv \iint d^3k\, d^3r_c\, f(\mathbf{r}_c, \mathbf{k}, t)\langle\delta(\mathbf{r}-\hat{\mathbf{r}})\dot{\hat{\mathbf{r}}}\hat{s}\rangle. \tag{8}$$

Throughout this paper, symmetrization of products of noncommuting operators is implied. After expanding, the spin current takes the form

$$\mathbf{J}^s = \int d^3k\, f\langle\dot{\hat{\mathbf{r}}}\hat{s}\rangle - \nabla\cdot\int d^3k\, f\langle(\hat{\mathbf{r}}-\mathbf{r})\dot{\hat{\mathbf{r}}}\hat{s}\rangle. \tag{9}$$

For a homogeneous system, where the distribution function is independent of position, the gradient term vanishes, and it is permissible to use Bloch states (which may be regarded as the limit of very wide wave packets) to evaluate the carrier spin current $\langle\dot{\hat{\mathbf{r}}}\hat{s}\rangle$. Since the Bloch states contain first order correction in the field, this can in general yield an overall linear-in-field spin current even with the equilibrium distribution function. This intrinsic spin current has been evaluated for a number of systems recently, and identical results are obtained with the semiclassical approach developed here.

To illuminate the underlying physics, we decompose the carrier spin current into a number of terms:

$$\mathbf{J}^s = \int d^3k\, f\left(\dot{\mathbf{r}}_c\langle\hat{s}\rangle + \frac{d\mathbf{p}^s}{dt} - \mathbf{p}^\tau\right). \tag{10}$$

The first contribution is convective, arising from the fact that the total spin is transported as the wave packet moves. The second comes from the rate of change of the spin dipole, while the third is from the torque dipole. This decomposition makes it possible to compare the Kubo formula result with those based on various heuristic arguments. The authors of [10] restricted their scope to the convective term and considered only the Berry phase contribution to the charge center velocity $\dot{\mathbf{r}}_c$. The present semiclassical decomposition allows us to recognize the missing terms due to the spin and torque dipoles, as well as a field correction to the carrier spin in the convective term. The approach of [10] would give a zero result for the Rashba model, whereas the Kubo formula approach of [11], which agrees with (10), yields a nonzero spin-Hall current for this model. Interestingly, the spin Hall current in the Rashba model can be obtained exactly from a heuristic argument based on a velocity and field dependent correction to the carrier spin as discussed in [11].

This approach is, however, applicable only to single-band models with wave-vector-dependent Zeeman coupling.

The spin density and current satisfy the following equation of continuity:

$$\frac{\partial S}{\partial t} + \nabla \cdot \mathbf{J}^s = \mathcal{T} + \int d^3k \frac{df}{dt} \langle \hat{s} \rangle. \tag{11}$$

It is seen that the torque density appears in the source, accounting for the spin nonconserving terms in the Hamiltonian, and acting as a bulk mechanism for spin generation. The second term accounts for the effect of collisions.

The source can be decomposed into intrinsic and extrinsic contributions, depending on the equilibrium and nonequilibrium parts of the distribution, respectively. If we restrict our attention to homogeneous systems, the torque density is simply $f\langle \hat{\tau} \rangle$. We find that this term is always first order in the electric field, and is given by $f \frac{e}{\hbar} \mathbf{E} \cdot \frac{\partial \langle \hat{s} \rangle}{\partial \mathbf{k}}$. We are thus justified in replacing f by its equilibrium value f_0, in which case this term is purely intrinsic. The second term in the source, which depends on the nonequilibrium shift in the distribution function, is entirely extrinsic.

Our formalism thus far applies to independent nondegenerate bands, and for the Rashba model its predictions are in agreement with [11]. There exists a parallel formalism for coupled degenerate bands, which yields the same results as given above [25]. In this case, the distribution function becomes a density matrix, while $\langle \hat{s} \rangle$, $\langle \hat{\tau} \rangle$, $\dot{\mathbf{r}}_c$, $\mathbf{p}^s$, and $\mathbf{p}^\tau$ are replaced by matrices. To find the macroscopic expectation values, one traces over the density matrix. This formalism can be applied, for example, to the spherical four-band Luttinger Hamiltonian,

$$H_0 = \frac{\hbar^2}{2m} \left[\left(\gamma_1 + \frac{5}{2} \gamma_2 \right) k^2 - 2\gamma_2 (\mathbf{k} \cdot \hat{\mathbf{J}})^2 \right], \tag{12}$$

where $\hat{\mathbf{J}}$ is the operator for angular momentum $3/2$ and γ_1, γ_2 are the Luttinger parameters. The Bloch states are eigenstates of the angular momentum projection in the $\mathbf{k}$ direction, $\hat{J}_k$. The four bands are split (for finite k) into two degenerate manifolds with $\hat{J}_k = \pm 3/2$ (heavy holes) and $\hat{J}_k = \pm 1/2$ (light holes).

Let us take a closer look at the source term, using the four-band model as an illustration. This discussion applies to either of the heavy- and light-hole manifolds. In equilibrium, the density matrix is diagonal and equal to f_0 for each band. The mean spin in the z direction is $\langle \hat{s}_z \rangle_{\pm 3/2} = \pm[(\hbar k_z)/(2k)]$ for the heavy holes, and it is $\langle \hat{s}_z \rangle_{\pm 1/2} = \pm[(\hbar k_z)/(6k)]$ for the light holes. The spin expectation values have opposite signs in the two bands, so that, when averaged over the equilibrium density matrix, the intrinsic term in the source, $f\langle \hat{\tau} \rangle$, will vanish. The intrinsic source $\mathcal{T}$ therefore vanishes in the bulk for this system.

In the relaxation time approximation, the collision term in (3) is given by [27]

$$\left. \frac{df}{dt} \right|_{\rm coll} = \frac{f_0 - \frac{1}{2}\mathrm{Tr} f}{\tau_p} I - \frac{\mathrm{Tr}(f\boldsymbol{\sigma}) \cdot \boldsymbol{\sigma}}{\tau_s}, \tag{13}$$

where τ_p and τ_s are the momentum and spin relaxation times, respectively, I is the identity matrix, and $\boldsymbol{\sigma}$ is the vector of Pauli spin matrices. In the extrinsic term in the source, the part depending on the momentum relaxation time will also cancel between the two bands, leaving us with just the contribution coming from the second term on the right-hand side of (13). The equation of continuity is then

$$\frac{\partial S}{\partial t} + \nabla \cdot \mathbf{J}^s = \frac{-S}{\tau_s} - \nabla \cdot \mathbf{P}^\tau, \tag{14}$$

where $\mathbf{P}^\tau = \int d^3k f \mathbf{p}^\tau$ is the torque dipole density. The two divergences will vanish in the bulk if the sample is homogeneous.

We will now take a closer look at the spin current, making further use of the four-band model for the spin-orbit coupled valence bands of a zinc blende semiconductor. In previous work [13–15], extensive discussions have been devoted to the extrinsic part of the spin current, which is given by the zero-field carrier velocity and spin integrated over the nonequilibrium part of the distribution. Here we will concentrate on the intrinsic part of the spin current, coming from the field correction to the carrier spin current integrated over the equilibrium distribution. In order for this term to be dominant, scattering must be strong enough to keep the distribution function close to its equilibrium value, and weak enough to limit interband mixing. This is therefore opposite to the limit of Dyakonov-Perel [28] relaxation of spin in the weakly spin-orbit split bands of crystals.

The twofold degeneracy of both the heavy- and light-hole manifolds implies that, in the presence of an electric field, however weak it may be, mixing within the degenerate manifold will occur in general. Fortunately, for the heavy holes the $\hat{J}_k = \pm 3/2$ bands do not mix to first order in the electric field, and we can apply the nondegenerate band formalism. The s_z dipole moment for the heavy holes is found to be $\mathbf{p}_h^{s_z} = -\frac{\hbar \mathbf{k} \times \hat{\mathbf{z}}}{4k^2}$. The torque dipole is, after an angular average, $\mathbf{p}_h^{\tau_z} = -\frac{e\mathbf{E} \times \hat{\mathbf{z}}}{6k^2}$. The spin and torque dipoles are equal for both heavy-hole bands. For the convective part of carrier spin current, in addition to a field correction to the carrier velocity due to the Berry phase [10], we obtain a term which is due to the change in the spin expectation value induced by the electric field and has the form $\frac{1}{\hbar} \frac{\partial \varepsilon}{\partial \mathbf{k}} \mathbf{E} \cdot \frac{\partial \langle \hat{s} \rangle}{\partial \mathbf{E}}$. Using these results, we find the current for the spin-z component of a heavy-hole carrier to be

$$\mathbf{j}_h^s = \left(\frac{1}{4k^2} - \frac{\hbar^2}{6m_h \Delta} - \frac{1}{12k^2} + \frac{1}{6k^2} \right) e\mathbf{E} \times \hat{\mathbf{z}}, \tag{15}$$

where $\Delta = \epsilon_h - \epsilon_l$ is the energy difference between the heavy and light holes. The first two terms come from the convective part due to field corrections to the carrier velocity and spin, respectively. The third term comes from the rate of change of the spin dipole, while the last one comes from the torque dipole. The heavy-hole carrier spin current can be simplified to

$$\mathbf{j}_h^s = \frac{e\mathbf{E} \times \hat{\mathbf{z}}}{3k^2} \frac{1}{1 - \frac{m_l}{m_h}}. \tag{16}$$

For the light holes, we must consider field induced mixing between the two degenerate bands. The details of this calculation will be deferred to a future publication [25]; we quote only the final result here which is very simple. The spin current per carrier in the light-hole manifold has the same form as for the heavy holes, and differs only by a minus sign. Integrating over k and summing the contributions from all four bands, we arrive finally at the following expression for the total spin current: $\mathbf{J}^s = \sigma_{SH}\mathbf{E} \times \hat{\mathbf{z}}$, where the spin-Hall conductivity is given by

$$\sigma_{SH} = \frac{e}{3\pi^2} \frac{k_h - k_l}{1 - \frac{m_l}{m_h}} = \frac{e}{3\pi^2} \frac{k_h}{1 + \sqrt{\frac{m_l}{m_h}}}, \tag{17}$$

where k_h and k_l are the Fermi wave vectors for the heavy and light holes, respectively. Separate calculations based on the Kubo formula by the present authors and by Murakami *et al.* [29] yield the same results.

Finally, we comment on the relationship between bulk spin currents and spin accumulation near the edge of the sample. A theory of spin accumulation must start from the spin density continuity Eq. (14). If the torque dipole density $\mathbf{P}^\tau$ were absent from this equation, then in the steady state the spin accumulation would be due only to the spin current. The presence of the torque dipole density modifies the expression for the spin accumulation, giving that

$$\int S\, dx = \tau_s(J_x^s + P_x^\tau). \tag{18}$$

We have already discussed the response of the spin current to an electric field, and after a similar calculation for the torque density we find that

$$J_x^s + P_x^\tau = \frac{eE_y}{3\pi^2} \frac{k_h}{1 + \sqrt{\frac{m_l}{m_h}}} \left(\frac{1}{2} - \frac{m_l}{2m_h} - \sqrt{\frac{m_l}{m_h}}\right). \tag{19}$$

Using $n = 2.4 \times 10^{11}$ cm^{-2} and an electric field of 20 000 V/cm as typical values, the spin current is -10^{25} spins per unit area per second. We take the spin relaxation time to be $\tau_s = 30$ ps [30] and a unit cell size of 6.3 Å, and we obtain a spin accumulation of 1.2×10^{-4} spins per *unit cell area*. This is a measurable effect as discussed in [10,11].

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