Proper Definition of Spin Current in Spin-Orbit Coupled Systems

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The conventional definition of spin current is incomplete and unphysical in describing spin transport in systems with spin-orbit coupling. A proper and measurable spin current is established in this study, which fits well into the standard framework of near-equilibrium transport theory and has the desirable property to vanish in insulators with localized orbitals. Experimental implications of our theory are discussed.

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A central theme of spintronics research is on how to generate and manipulate spin current as well as to exploit its various effects [1,2]. In the ideal situation where spin (or its projection along a direction) is conserved, spin current is simply defined as the difference between the currents of electrons in the two spin states. This concept has served well in the early study of spin-dependent transport effects in metals. The ubiquitous presence of spin-orbit coupling inevitably makes the spin nonconserved, but this inconvenience is usually put off by focusing one's attention within the so-called spin relaxation time. In recent years, it has been found that one can make very good use of spin-orbit coupling, realizing electric control of spin generation and transport [3–9]. The question of how to define the spin current properly in the general situation therefore becomes urgent.

In most previous studies of bulk spin transport, it has been conventional to define the spin current simply as the expectation value of the product of spin and velocity observables. Unfortunately, no viable measurement is known to be possible for this spin current. The recent spin-accumulation experiments [8,9] do not directly determine it, and there is no deterministic relation between this spin current and the boundary spin accumulation, as demonstrated in Fig. 1.

In fact, the conventional definition of spin current suffers three critical flaws that prevent it from being relevant to spin transport. First, this spin current is not conserved. This issue alone has motivated a number of alternative definitions recently [10–12]. Second, this spin current can even be finite in insulators with localized eigenstates only, so it cannot really describe transport [13]. Finally, there does not exist a mechanical or thermodynamic force in conjugation with this current, so it cannot be fitted into the standard near-equilibrium transport theory. One consequence is that one cannot establish an Onsager relation linking the spin current with other transport phenomena.

In this Letter, we try to establish a proper definition of spin current free from all the above difficulties, which is found to be possible for systems where spin generation in the bulk is absent due to symmetry reasons. Our new spin current is given by the time derivative of the spin displacement (product of spin and position observables), which differs from the conventional definition by a torque dipole term. The torque dipole term is first found in a semiclassical theory [14], whose impact on spin transport has been further analyzed to assess the importance of the intrinsic spin-Hall effect [12]. In this Letter, we provide a quantum mechanical description of this term within the linear response theory for transport. Apart from showing its consequence in making the spin current conserved, we also reveal two additional properties: The new spin current vanishes identically in insulators with localized orbitals, and is in conjugation with a force given by the gradient of the Zeeman field or spin-dependent chemical potential. Together with conservation, these properties are crucial to establish the new spin current as the proper description for spin transport, and they also provide a firm foundation for various methods for its measurement.

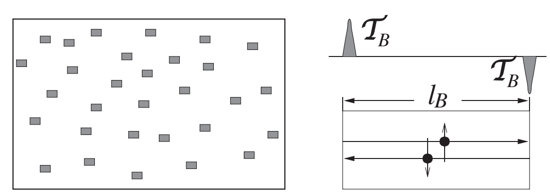

FIG. 1. An example demonstrating the irrelevance of the conventional spin current to spin transport. Left: A macroscopic system consisting of a uniform distribution of microscopic boxes (gray rectangles) in which an electron is confined. Right: The inside structure of the box, where the walls flips the spin of electron upon collision. When the system is driven to such a state schematized at the right, the macroscopic average of the conventional spin current is nonzero. However, because all electrons are localized, no spin transport or boundary spin accumulation can occur. $\mathcal{T}_B$ denotes the total boundary spin torque due to the spin-flip scattering. It is easy to show the corresponding spin torque dipole $P_\tau = -\mathcal{T}_B l_B$ exactly cancels the conventional spin current. As a result, the spin current $\mathcal{J}_s$ defined in Eq. (4) is zero.

Based on a general quantum mechanical principle, one can derive a continuity equation relating the spin, current, and torque densities as follows,

$$\frac{\partial S_z}{\partial t} + \nabla \cdot \mathbf{J}_s = \mathcal{T}_z. \tag{1}$$

The spin density for a particle in a (spinor) state $\psi(\mathbf{r})$ is defined by $S_z(\mathbf{r}) = \psi^\dagger(\mathbf{r})\hat{s}_z\psi(\mathbf{r})$, where $\hat{s}_z$ is the spin operator for a particular component (z here, to be specific). The spin current density here is given by the conventional definition $\mathbf{J}_s(\mathbf{r}) = \mathrm{Re}\psi^\dagger(\mathbf{r})\frac{1}{2}\{\hat{\mathbf{v}}, \hat{s}_z\}\psi(\mathbf{r})$, where $\hat{\mathbf{v}}$ is the velocity operator, and $\{,\}$ denotes the anticommutator. The right-hand side of the continuity equation is the torque density defined by $\mathcal{T}_z(\mathbf{r}) = \mathrm{Re}\psi^\dagger(\mathbf{r})\hat{\tau}\psi(\mathbf{r})$, where $\hat{\tau} \equiv d\hat{s}_z/dt \equiv (1/i\hbar)[\hat{s}_z, \hat{H}]$, and $\hat{H}$ is the Hamiltonian of the system. These definitions can be easily restated in a many-body language by regarding the wave functions as field operators and by taking the expectation value in the quantum state of the system. The presence of the torque density $\mathcal{T}_z$ reflects the fact that spin is not conserved microscopically in systems with spin-orbit coupling.

It often happens, due to symmetry reasons, that the average torque vanishes for the bulk of the system, i.e., $(1/V)\int dV \mathcal{T}_z(\mathbf{r}) = 0$. This is true to first order in the external electric field for any samples with inversion symmetry. Also, one is often interested in a particular component of the spin, and the corresponding torque component can vanish in the bulk on average even for samples without the inversion symmetry. This is certainly true for the many models used for the study of the spin-Hall effect [6,7,15], and for the experimental systems used to detect the effect so far [8,9]. For such systems, where the average spin torque density vanishes in the bulk, we can write the torque density as a divergence of a torque dipole density,

$$\mathcal{T}_z(\mathbf{r}) = -\nabla \cdot \mathbf{P}_\tau(\mathbf{r}). \tag{2}$$

Moving it to the left-hand side of (1), we have

$$\frac{\partial S_z}{\partial t} + \nabla \cdot (\mathbf{J}_s + \mathbf{P}_\tau) = 0, \tag{3}$$

which is in the form of the standard sourceless continuity equation. This shows that the spin in conserved on average in such systems, and the corresponding transport current is

$$\mathcal{J}_s = \mathbf{J}_s + \mathbf{P}_\tau. \tag{4}$$

We note that there is still an arbitrariness in defining the effective spin current because Eq. (2) does not uniquely determine the torque dipole density $\mathbf{P}_\tau$ from the corresponding torque density $\mathcal{T}_z$. We can eliminate this ambiguity by imposing the physical constraint that the torque dipole density is a material property that should vanish outside the sample. This implies, in particular, that $\int dV \mathbf{P}_\tau = -\int dV \mathbf{r} \nabla \cdot \mathbf{P}_\tau = \int dV \mathbf{r} \mathcal{T}_z(\mathbf{r})$. It then follows that, upon bulk average, the effective spin current density can be written in the form of $\mathcal{J}_s = \mathrm{Re}\psi^*(\mathbf{r})\hat{\mathcal{J}}_s\psi(\mathbf{r})$, where

$$\hat{\mathcal{J}}_s = \frac{d(\hat{\mathbf{r}}\hat{s}_z)}{dt} \tag{5}$$

is the effective spin current operator. Compared to the conventional spin current operator, it has an extra term $\hat{\mathbf{r}}(d\hat{s}_z/dt)$, which accounts the contribution from the spin torque.

Because the new spin current is given as a time derivative, it must vanish in an eigenenergy state in which the spin displacement operator is well defined, which is the case if the state is localized. Elementary perturbation theory shows that the spin current vanishes in such a system even in the presence of a weak electric field. Indeed, for spatially localized eigenstates, we can evaluate the spin-transport coefficient as,

$$\begin{aligned} \sigma^s &= -e\hbar \sum_{l \neq l'} f_l \frac{\mathrm{Im}\langle l | d(\hat{\mathbf{r}}\hat{s}_z)/dt | l' \rangle \langle l' | \hat{\mathbf{v}} | l \rangle}{(\epsilon_l - \epsilon_{l'})^2} \\ &= -e\hbar \sum_l f_l \langle l | [\hat{\mathbf{r}}\hat{s}_z, \hat{\mathbf{r}}] | l \rangle = 0 \end{aligned} \tag{6}$$

where f_l is the equilibrium occupation number in the lth state. Here, we have used $\langle l | d(\hat{\mathbf{r}}\hat{s}_z)/dt | l' \rangle = (-i/\hbar)(\epsilon_{l'} - \epsilon_l)\langle l | \hat{\mathbf{r}}\hat{s}_z | l' \rangle$ and $\langle l' | \hat{\mathbf{v}} | l \rangle = (-i/\hbar)(\epsilon_l - \epsilon_{l'})\langle l' | \hat{\mathbf{r}} | l \rangle$. The involved matrix elements are all well defined between spatially localized eigenstates.

Defined as a time derivative of the spin displacement operator $\hat{\mathbf{r}}\hat{s}_z$, the new spin current has a natural conjugate force $\mathbf{F}_s$, the gradient of the Zeeman field or of a spin-dependent chemical potential, which can be modeled as an external perturbation $V = -\mathbf{F}_s \cdot (\hat{\mathbf{r}}\hat{s}_z)$ [16]. The energy dissipation rate for the spin transport can be written as $dQ/dt = \mathcal{J}_s \cdot \mathbf{F}_s$. It immediately suggests a thermodynamic way to determine the spin current by simultaneously measuring the Zeeman field gradient (spin force) and the heat generation.

Moreover, Onsager relations can now be established. For example, in the presence of both electric and spin forces, the linear response of spin and charge currents may be written in the following manner,

$$\begin{pmatrix} \mathcal{J}_s \\ \mathbf{J}_c \end{pmatrix} = \begin{pmatrix} \sigma^{\mathrm{ss}} & \sigma^{\mathrm{sc}} \\ \sigma^{\mathrm{cs}} & \sigma^{\mathrm{cc}} \end{pmatrix} \begin{pmatrix} \mathbf{F}_s \\ E \end{pmatrix}, \tag{7}$$

where $\mathcal{J}_s$ is spin current and $\mathbf{J}_c$ denotes charge current. σ^{ss} and σ^{cc} are the spin-spin and charge-charge conductivity tensors, respectively. The off-diagonal block σ^{sc} denotes spin current response to an electric field (spin-Hall effect), and σ^{cs} denotes charge current response to a spin force (inverse spin-Hall effect) [17]. The Onsager reciprocity dictates a general relation between the off-diagonal blocks (assuming time-reversal symmetry):

$$\sigma^{\mathrm{sc}}_{\alpha\beta} = -\sigma^{\mathrm{cs}}_{\beta\alpha}, \tag{8}$$

where the extra minus sign originates from the odd time-reversal parity of the spin displacement operator $\mathbf{r}s_z$ [18]. We note that the Onsager relation Eq. (8) can only be established when the currents are defined in terms of the time derivative of displacement operators conjugate to the forces. In the case of spin force driving, we have the spin displacement operator $s_z\mathbf{r}$, whose time derivative corresponds to our new spin current Eq. (5), not the conventional spin current. This Onsager relation can also be directly verified using the linear response theory.

The existence of the Onsager relations makes the electric measurement of the spin current viable. A previous theoretical proposal had suggested that the spin current can be determined by measuring the transverse voltage generated by a spin current passing through a spin-Hall device [4,5,19]. However, to do that, the spin-Hall coefficient $\sigma_{xy}^{\mathrm{sc}}$ of the measuring device must be known in prior because the spin current is determined from $\mathcal{J}_{sx} = \sigma_{xy}^{\mathrm{sc}} E_y$. With the Onsager relation, $\sigma_{xy}^{\mathrm{sc}}$ can be derived from the corresponding inverse spin-Hall coefficient, and the latter can be determined by a measurement of the charge current and the Zeeman field gradient.

After these general considerations, we now show how to evaluate the spin-Hall conductivity based on the new definition of spin current. The torque dipole density can be determined unambiguously as a bulk property within the theoretical framework of linear response. Consider the torque response to an electric field at finite wave vector $\mathbf{q}$, $\mathcal{T}_z(\mathbf{q}) = \boldsymbol{\chi}(\mathbf{q}) \cdot \mathbf{E}(\mathbf{q})$. Based on Eq. (2) which implies $\mathcal{T}_z(\mathbf{q}) = -i\mathbf{q} \cdot \mathbf{P}_\tau(\mathbf{q})$, we can uniquely determine the dc response (i.e., $\mathbf{q} \to 0$) of the spin torque dipole:

$$\mathbf{P}_\tau = \mathrm{Re}\{i\nabla_{\mathbf{q}}[\boldsymbol{\chi}(\mathbf{q}) \cdot \mathbf{E}]\}_{\mathbf{q}=0}. \tag{9}$$

Here we have utilized the condition $\boldsymbol{\chi}(0) = 0$, i.e., there is no bulk spin generation by the electric field. Combining Eqs. (4) and (9), we can then determine the electric-spin-transport coefficients for the new definition of spin current:

$$\sigma_{\mu\nu}^{s} = \sigma_{\mu\nu}^{s0} + \sigma_{\mu\nu}^{\tau}, \tag{10}$$

where $\sigma_{\mu\nu}^{s0}$ is the conventional spin-transport coefficient that is the focus of most of previous studies, and

$$\sigma_{\mu\nu}^{\tau} = \mathrm{Re}[i\partial_{q_\mu}\chi_\nu(\mathbf{q})]_{\mathbf{q}=0} \tag{11}$$

is the contribution from the spin torque dipole. Standard Green function or many-body techniques can be used to evaluate this linear response for systems with arbitrary disorder and interactions between the carriers.

The spin-Hall coefficients for a few semiconductor models including effects of disorder are now considered by Sugimoto *et al.* based on our new definition of spin current [20]; they found results dramatically different from the conventional spin-Hall conductivities. For example, it is found that the spin-Hall conductivity depends explicitly on the scattering potentials for the two dimensional Rashba models with k-linear or k-cubic spin-orbit coupling. For the k-cubic model, the conventional spin-Hall conductivity is robust against disorder, but this is not so if the new spin current definition is adopted. It then implies that at smooth boundaries, spin accumulation in such systems is of extrinsic nature.

The conservation of our new spin current allows one to consider spin transport in the bulk without the need of laboring explicitly a spin torque (dipole density) which may be generated by the electric field. One can think of spin transport for systems with strong spin-orbit coupling in the "usual" sense established for systems with weak spin-orbit coupling. For example, it has been customary to link spin density and spin current through the following phenomenological equation of spin continuity,

$$\frac{\partial S_z}{\partial t} + \nabla \cdot \mathcal{J}_s = -\frac{S_z}{\tau_s}, \tag{12}$$

where τ_s is the spin relaxation time, and the spin current has the form $\mathcal{J}_s = \sigma E - D_s \nabla S_z$. This makes sense only if our new spin current is used in the calculation of spin-Hall conductivity σ, otherwise an extra term of field-generated spin torque must be added [21].

Equation (12) can serve as the basis to determine the spin accumulation at a sample boundary, which is of much current interest. Consider a system having a smooth boundary produced by a slowly varying confining potential. We assume that the length scale of variation is much larger than the mean free path, so that the above continuity equation may be applied locally. By integrating from the interior to the outside of the sample boundary, we obtain a spin accumulation per area with $\bar{S}_z = \mathcal{J}_s^{\mathrm{bulk}}\tau_s$ [14], where τ_s is the spin relaxation time. We emphasize that the transport spin current responsible for the boundary spin accumulation should be $\mathcal{J}_s$ instead of the conventional spin current $\boldsymbol{J}_s$.

For sharp boundaries, the spin continuity equation alone cannot yield a unique relationship between the spin current from the bulk and spin accumulation at the boundary. For a perfectly reflecting sharp wall in the case of strong spin-orbit coupling, the boundary spin accumulation seems to be determined by the conventional spin current from the bulk [22]. However, such a relationship is altered for other boundary conditions [23]. This calls for well-controlled experiments to explicitly eliminate the influence from the boundary condition. On the other hand, for the generic class of smooth boundaries discussed above, there is a unique relationship between spin accumulation and the spin current, provided one uses our new definition.

The real advantage of our new definition of spin current lies in the fact that it provides a satisfactory description of spin transport in the bulk. With our new spin current, one can now use the spin continuity Eq. (12) to discuss spin accumulation in the bulk, e.g., by generating a nonuniform electric field or spatially modulating the spin-Hall conductivity. Our new spin current vanishes in Anderson insulators either in equilibrium or in a weak electric field, which enables us to predict zero spin accumulation in such systems. More importantly, it posses a conjugate force (spin force), so that spin transport can be fitted into the standard formalism of near-equilibrium transport. The conventional spin current does not have a conjugate force, so it makes no sense even to talk about energy dissipation from that current. The existence of a conjugate force is crucial for the establishment of Onsager relations between spin transport and other transport phenomena, and its measurement will be important to thermodynamic and electric determination of the spin current.

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