On A Proper Definition of Spin Current

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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. Our theory predicts opposite signs of spin Hall coefficients for a few semiconductor models, urging critical tests of the concept by experiments and numerics.

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A central theme of spintronics research is on how to generate, control and manipulate the 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 of the currents of electrons in the two spin states. This concept has served well in early study of spin-dependent transport effects in metals. The ubiquitous presence of spin-orbit coupling inevitably makes the spin non-conserved, 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, 4, 5, 6, 7, 8, 9]. The question of how to define the spin current in the general situation therefore becomes unavoidable and 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 to this current is known to be possible, and there is strong evidence that it is not a proper representation of the physical spin current. Spin-accumulation measurements in recent experiments do not really determine it, one reason being that the spin accumulation has a contribution from the spin torque dipole density that is inseparable from the conventional spin current [10]. In addition, there does not exist a mechanical or thermodynamic force in conjugation with this current, so that it cannot be fitted into the standard near-equilibrium transport theory. As a result, the conventional spin current cannot be measured by linking to other transport phenomena. Finally, the conventional spin current can even be finite in insulators with localized states only, so it is disqualified as a true transport current [11].

In this Letter, we establish a proper definition of spin current which is measurable and free from the above difficulties [29]. Our new spin current is given by the time derivative of the spin displacement (product of spin and position vectors), which differs from the conventional definition by a term analogous to the torque dipole term found in semiclassical theory [10]. The new spin current is in conjugation with a mechanical force given by the gradient of the Zeeman field or spin-dependent chemical potential, and it also has the desirable property to vanish in Anderson insulators in which all orbitals are localized.

Our new concept of spin current thus fits well with standard near-equilibrium transport theory, which immediately suggests direct methods for its measurement. First, it can be measured in terms of energy dissipation by determining its conjugate force. Second, the Onsager relations can now be established, which provides a firm foundation for electrical measurement of the spin current as generated in the spin Hall effect through its reciprocal effect [4, 5, 12]. At the end, we will also discuss how our new spin current contributes to spin accumulation. We have re-calculated the spin Hall conductivity for a number of semiconductor models, and found the results to be dramatically different from previous values based on the conventional spin current. The fundamental change introduced by this new definition urges future experimental tests and theoretical investigations for its full implications.

Based on 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 state (spinor) $\psi(\mathbf{r})$ 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 $\hat{\tau} \equiv \mathrm{d}\hat{s}_z/\mathrm{d}t \equiv (1/i\hbar)[\hat{s}_z, \hat{H}]$, 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 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 a conserved quantity. A theory for the development of spin density must include a careful analysis of the torque in addition to the spin current.

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 lack the inversion symmetry. This is certainly true for the many models used for the study of spin Hall effect [6, 7, 13], and the experimental systems used to detect the effect so far also have this property [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. Therefore, in the bulk of systems where the average torque vanishes, the transport of spin S_z is governed by the spin current density:

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

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 $\boldsymbol{\mathcal{J}}_s = \mathrm{Re}\psi^*(\mathbf{r})\hat{\boldsymbol{\mathcal{J}}}_s\psi(\mathbf{r})$, where

$$\hat{\boldsymbol{\mathcal{J}}}_s \;=\; \frac{\mathrm{d}(\hat{\mathbf{r}}\hat{s}_z)}{\mathrm{d}t} \tag{5}$$

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

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:

$$\mathbf{P}_\tau \;=\; \mathrm{Re}[i\nabla_{\mathbf{q}}\boldsymbol{\chi}(\mathbf{q})]_{\mathbf{q}=0}\cdot\mathbf{E}\,. \tag{6}$$

Here we have utilized the condition $\boldsymbol{\chi}(0) = 0$, i.e., there is no bulk spin generation by the electric field. Combining Eq. (4) and (6), we can then determine the electric-spin transport coefficients for the new definition of spin current:

$$\sigma^s_{\mu\nu} \;=\; \sigma^{s0}_{\mu\nu} + \sigma^\tau_{\mu\nu}\,, \tag{7}$$

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

$$\sigma^\tau_{\mu\nu} = \mathrm{Re}[i\partial_{q_\mu}\chi_\nu(\mathbf{q})]_{\mathbf{q}=0}\,, \tag{8}$$

is the contribution from the spin torque dipole.

The correction introduced by the spin torque dipole turns out to be important. To see this, we evaluate the spin Hall coefficients based on the new definition of spin current Eqs. (4, 5). The linear response formalism outlined above should allow arbitrary disorder and interactions between the carriers. Here, mainly for the purpose of showing the consequence of redefining the spin current, we calculate the intrinsic contribution to the spin Hall conductivity in the clean limit for non-interacting systems. The Kubo formula for the conventional spin Hall coefficient reads [30]:

$$\sigma^{s0}_{\mu\nu} \;=\; -e\hbar\sum_{n\neq n',\mathbf{k}}[f(\epsilon_{n\mathbf{k}}) - f(\epsilon_{n'\mathbf{k}})]\times \frac{\mathrm{Im}\langle u_{n\mathbf{k}}|\frac{1}{2}\{\hat{v}_\mu,\,\hat{s}_z\}|u_{n'\mathbf{k}}\rangle\langle u_{n'\mathbf{k}}|\hat{v}_\nu|u_{n\mathbf{k}}\rangle}{(\epsilon_{n\mathbf{k}} - \epsilon_{n'\mathbf{k}})^2 + \eta^2} \tag{9}$$

where $\hat{\mathbf{v}}(\mathbf{k}) = \partial\hat{H}(\mathbf{k})/\hbar\partial\mathbf{k}$, $\hat{H}(\mathbf{k}) = \exp(-i\mathbf{k}\cdot\hat{\mathbf{r}})\hat{H}\exp(i\mathbf{k}\cdot\hat{\mathbf{r}})$, $|u_{n\mathbf{k}}\rangle$ is the periodic part of the electron Bloch wavefunction and $f(\epsilon)$ is the Fermi-Dirac distribution. The carrier charge is assumed to be $q = -e$. The spin torque response coefficient $\boldsymbol{\chi}(\mathbf{q})$ can be calculated in a similar manner:

$$\boldsymbol{\chi}(\mathbf{q}) \;=\; ie\hbar\sum_{n\neq n',\mathbf{k}}[f(\epsilon_{n\mathbf{k}}) - f(\epsilon_{n'\mathbf{k}+\mathbf{q}})]\times \frac{\langle u_{n\mathbf{k}}|\hat{\tau}(\mathbf{k},\mathbf{q})|u_{n'\mathbf{k}+\mathbf{q}}\rangle\langle u_{n'\mathbf{k}+\mathbf{q}}|\hat{\mathbf{v}}(\mathbf{k},\mathbf{q})|u_{n\mathbf{k}}\rangle}{(\epsilon_{n\mathbf{k}} - \epsilon_{n'\mathbf{k}+\mathbf{q}})^2 + \eta^2} \tag{10}$$

where $\hat{\tau}(\mathbf{k},\mathbf{q}) = \frac{1}{2}[\hat{\tau}(\mathbf{k}) + \hat{\tau}(\mathbf{k}+\mathbf{q})]$, $\hat{\mathbf{v}}(\mathbf{k},\mathbf{q}) = \frac{1}{2}[\hat{\mathbf{v}}(\mathbf{k}) + \hat{\mathbf{v}}(\mathbf{k}+\mathbf{q})]$ with $\hat{\tau}(\mathbf{k}) = (1/i\hbar)[\hat{s}_z,\,\hat{H}(\mathbf{k})]$. It is then straightforward to determine the spin Hall coefficient σ^s using Eqs. (7, 8). The limit of $\eta\to 0$ should be taken at the last step of calculation, and as a result, there is no intra-band ($n = n'$) contribution [13].

The intrinsic spin-Hall coefficients for a few semiconductor models are calculated and shown in Table I. The substantial corrections are evident. For both the k-linear [7] and k-cubed Rashba models [13], the correction from the spin torque dipole reverses the signs of the spin Hall coefficients. For the Luttinger model [6, 10], the spin Hall coefficient for the new spin current also

	Rashba	k^3 Rashba	Luttinger
σ_{xy}^{s0}	$-e/8\pi$	$9e/8\pi$	$\frac{e(\gamma_1+2\gamma_2)}{12\pi^2\gamma_2}(k_H-k_L)$
σ_{xy}^{τ}	$e/4\pi$	$-9e/4\pi$	$-\frac{3e\gamma_1}{12\pi^2\gamma_2}(k_H-k_L)+\frac{e}{6\pi^2}k_H$
σ_{xy}^{s}	$e/8\pi$	$-9e/8\pi$	$\frac{e(\gamma_2-\gamma_1)}{6\pi^2\gamma_2}(k_H-k_L)+\frac{e}{6\pi^2}k_H$

Table I: Intrinsic spin Hall coefficients for a few widely studied semiconductor models, including the Rashba model for 2D electrons [7], k-cubed Rashba model for 2D holes [13] and Luttinger model for 3D holes [6, 10]. For Rashba models, we only list the "universal" values for the case when both bands are occupied.

differs dramatically from the conventional one, and its sign is also reversed at the limit $\gamma_2 \to 0$. Further work is necessary to address the issue of disorder effects on our prediction. Recent studies have shown that the intrinsic spin Hall effect based on the conventional spin current is robust against weak disorder for the Luttinger model of 3D holes [14] and the k-cubed Rashba model of 2D holes [15], although it is apparently not so for the k-linear Rashba model of 2D electrons beyond the mesoscopic regime [16, 17, 18, 19, 20, 21].

To fully appreciate the validity and significance of the new definition of spin current, we turn our attention to the Onsager relations. As a demonstration, we establish the Onsager relation between the spin Hall effect and its inverse [22]. In the spin-Hall effect, an electric force drives a transverse spin current due to spin-orbit coupling. The inverse spin Hall effect is naturally expected as well, in which a spin force $\mathbf{F}^s$ induces a transverse charge current. In practice the spin force may be provided by the gradient of an inhomogeneous Zeeman field or that of a spin dependent chemical potential [23]. Such a spin force can be modeled as an external perturbation $V = -\mathbf{F}^s \cdot \mathbf{r} s_z$ [22].

In the presence of both electric and spin forces, the linear response of spin and charge currents may be written in the following manner,

$$\begin{pmatrix} \mathbf{J}_s \\ \mathbf{J}_c \end{pmatrix} = \begin{pmatrix} \sigma^{ss} & \sigma^{sc} \\ \sigma^{cs} & \sigma^{cc} \end{pmatrix} \begin{pmatrix} \mathbf{F}_s \\ \mathbf{E} \end{pmatrix}, \tag{11}$$

where $\mathbf{J}_s$ 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 (as in the spin Hall effect), and σ^{cs} denotes charge current response to a spin force (as in the inverse spin-Hall effect). The Onsager reciprocity dictates a general relation between the off-diagonal blocks (assuming time reversal symmetry):

$$\sigma^{sc}_{\alpha\beta} = -\sigma^{cs}_{\beta\alpha} \tag{12}$$

where the extra minus sign originates from the odd time-reversal parity of the spin displacement operator $\mathbf{r} s_z$ [24].

The Onsager relation Eq. (12) 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 electric driving, this displacement operator is $-e\mathbf{r}$, whose time derivative yields the charge current. 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 [25].

With the proper definition of spin current and its conjugate force $\mathbf{F}_s$, the energy dissipation rate for the spin transport can be written as $\mathrm{d}Q/\mathrm{d}t = \boldsymbol{\mathcal{J}}_s \cdot \mathbf{F}_s$. The new definition of spin current can then be fitted into the standard near-equilibrium transport theory. It immediately provides a thermodynamic way to determine the spin current by simultaneously measuring the Zeeman field gradient (spin force) and the heat generation.

Moreover, the existence of the Onsager relations makes the electric measurement of the spin current viable. 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, 12]. However, to do that, the spin Hall coefficient σ^{sc}_{xy} of the measuring device must be known in prior because the spin current is determined from $\mathcal{J}_{sx} = \sigma^{sc}_{xy} E_y$. With the Onsager relation, σ^{sc}_{xy} can be derived from the corresponding inverse spin Hall coefficient, and the later can be determined by a measurement of the charge current and the Zeeman field gradient.

In contrast, it is impossible to find a force in conjugation to the conventional spin current. As a result, all the benefits enjoyed by the new definition of spin current are not shared by the conventional one. This is responsible for the theoretical and experimental difficulties in finding a viable way to measure the conventional spin current.

To further illustrate the physical significance of the new definition of spin current, Eqs. (4, 5), we put it into a reality check: for simple insulators whose single particle eigenstates are localized (Anderson insulators), one expects their transport coefficients to vanish. Indeed, for spatially localized eigenstates, we can evaluate the spin transport coefficient as,

$$\begin{aligned} \sigma^s &= -e\hbar \sum_{\ell \neq \ell'} f_\ell \frac{\mathrm{Im}\langle \ell | \mathrm{d}(\hat{\mathbf{r}}\hat{s}_z)/\mathrm{d}t | \ell' \rangle \langle \ell' | \hat{\mathbf{v}} | \ell \rangle}{(\epsilon_\ell - \epsilon_{\ell'})^2} \\ &= -e\hbar \sum_{\ell} f_\ell \langle \ell | [\hat{\mathbf{r}}\hat{s}_z,\, \hat{\mathbf{r}}] | \ell \rangle = 0 \end{aligned} \tag{13}$$

where f_ℓ is the equilibrium occupation number in the ℓ-th state. Here, we have used $\langle \ell | \mathrm{d}(\hat{\mathbf{r}}\hat{s}_z)/\mathrm{d}t | \ell' \rangle = (-i/\hbar)(\epsilon_{\ell'} - \epsilon_\ell)\langle \ell | \hat{\mathbf{r}}\hat{s}_z | \ell' \rangle$ and $\langle \ell' | \hat{\mathbf{v}} | \ell \rangle = (-i/\hbar)(\epsilon_\ell - \epsilon_{\ell'})\langle \ell' | \hat{\mathbf{r}} | \ell \rangle$. The involved matrix elements are all well defined between spatially localized eigenstates.

Before ending, we discuss the connection between spin accumulation at a sample boundary and our spin current in the bulk. The spin accumulation $\bar{S}_z$ per unit area contributed by the bulk spin current can be determined by a balance between the spin current from the bulk $\mathcal{J}_s$ and spin relaxation $-\bar{S}_z/\tau_s$ at the boundary region, yielding $\bar{S}_z = \mathcal{J}_s\tau_s$ [10], where τ_s is the spin relaxation time. We emphasize that the torque dipole density and the conventional spin current enter here through $\mathcal{J}_s$ in a non-separable manner. We also note that in addition to this bulk contribution, the presence of the boundary could also introduce extra spin accumulation. It might be possible to discriminate these two kinds of contributions by exploiting their different length scales, because the bulk contribution has a length scale of the spin diffusion length $\ell_s = \sqrt{D\tau_s}$, which can be much larger than microscopic length scales that dictate the local boundary contribution. However, the complication from the boundary contribution and the necessity of determining the spin relaxation time suggests that spin accumulation measurement may not be an appropriate way to precisely determine the bulk spin current.

In summary, we have established a proper definition of spin current in the bulk of systems. The new definition resolves the fundamental difficulties suffered by the conventional one. This new definition has the desirable property to vanish in Anderson insulators so that it can be interpreted as a “transport current”. Onsager relations can now be established and for the first time spin transport can be fitted into the standard near-equilibrium transport theory. As a result, thermodynamic and electric measurement of the spin current are now possible. Spin Hall coefficients based on the new definition of spin current are found to be dramatically different from the conventional values.

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