On a proper definition of spin current

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P. Zhang, Shi, Xiao, and Niu (cond-mat 0503505)
P. Zhang and Niu (cond-mat/0406436)
Culcer, Sinova, Sintsyn, Jungwirth, MacDonald, and Niu
(PRL,93,046602,2004)
Spin current in spin-orbit coupled systems

- **Conventional definition**
  - Cannot be measured directly
    --- no conjugate force exists.
  - Can be finite even in Anderson insulators.

- **Connection to spin accumulation**

\[ \int S_z dx = \tau_s J^s \]

**But this is Wrong!**

\[ \vec{J}_s = \langle s_z \vec{r} \rangle \]
Proper spin current

- Focus on systems with no bulk spin generation.
- Then, we can introduce a new and measurable spin current, which
  - should be used to infer spin accumulation
  - Has a conjugate force and satisfies Onsager relation, and
  - has the desired property to vanish in simple insulators.
Outline

- Introduction
- A semiclassical picture
- The proper spin current
- Linear response and spin Hall effect
- Onsager relation and measurement
- Spin Hall in insulators
- Conclusions
A brighter future with semiconductor spintronics

• Can do what metals do:  
  GMR, spin transfer, ..., using ferromagnetic semiconductors

• Readily integrated with semiconductor devices:  
  possible way around impedance mismatch in spin injection.

• Tunable:  
  transport, magnetic and optical properties can be readily controlled by doping, gating, and pumping.

• Spin-orbit:  
  strong in semiconductors, may lead to novel effects such as electric generation and transport of spins
Semiclassical picture

- Spin-orbit built into the band structure: not a perturbation.
- Carrier of charge and spin: represented by wave packets.
- Effects of electric field: Drifting and band mixing.
- Impurity effects: scattering and relaxation.
Effect of electric field

**Mixing**

\[
|u_n\rangle \rightarrow |u_n\rangle + \sum_{n'} |u_{n'}\rangle \frac{\langle u_{n'}|i\partial u_n / \partial \vec{k}\rangle \cdot e\vec{E}}{\varepsilon_n - \varepsilon_{n'}}
\]

**Drifting**

\[
\hbar \vec{k}_c = -e\vec{E}
\]

\[
\hbar \vec{r}_c = \frac{\partial \varepsilon_n}{\partial \vec{k}_c} - \vec{k}_c \times \vec{\Omega}_n
\]

where

\[
\vec{\Omega}_n = i \left\langle \frac{\partial u_n}{\partial k} \times \frac{\partial u_n}{\partial k} \right\rangle
\]

Berry curvature
Spin-charge carrier

Charge \(-e\)  
Spin \(S_z\)

\[
S_z(\vec{r}, t) = \int_{}^{} \int_{}^{} d^3r_c d^3k_c f(\vec{r}_c, \vec{k}_c, t) \langle \hat{S}_z \delta(\vec{r} - \vec{r}_c) \rangle_c
\]
Semiclassical spin continuity equation

\[ \frac{\partial S_z}{\partial t} + \nabla \cdot \vec{J}^s = T_z + \int d^3k \frac{df}{dt} \langle \hat{S}_z \rangle \]

Torque density:

\[ T_z(\vec{r}, t) = \int d^3k f(\vec{r}, \vec{k}, t) \langle \hat{\tau}_z \rangle - \nabla \cdot \int d^3k f(\vec{r}, \vec{k}, t) \langle (\hat{\tau} - \vec{r})\hat{\tau}_z \rangle \]

Relaxation: \[ -\frac{S_z}{\tau} \]

Culcer et al (PRL,93,046602,2004)
Spin generation by electric field

Inside a homogeneous system:

\[
\frac{\partial S_z}{\partial t} = -e\vec{E} \cdot \int d^3k \ f(\vec{r}_c, \vec{k}, t) \ \frac{\partial}{\partial k} \langle \hat{s}_z \rangle - S_z / \tau
\]

Generally nonzero in inversion asymmetric crystals

Spin current and accumulation

Assume no spin-generation in the bulk
- Rashba (for spin $z$),
- 4-band Luttinger,
- Systems with inversion symmetry.

Spin continuity equation:

$$\frac{\partial S_z}{\partial t} + \nabla \cdot (\vec{J}^s + \vec{P}^\tau) = - \frac{S_z}{\tau}$$

Spin accumulation.

$$\int S_z \, dx = \tau (J^s + P^\tau)$$
General formulation

Continuity equation
\[ \frac{\partial S_z}{\partial t} + \nabla \cdot \vec{J}^s = T_z \]

Spin density
\[ S_z = \langle \Psi^+ (\vec{r}) s_z \Psi (\vec{r}) \rangle \equiv \langle s_z \rangle \]

Current density
\[ \vec{J}_s = \langle s_z \vec{r} \rangle \]

Torque density
\[ T_z = \langle \tau_z \rangle \]

where, \[ \tau_z = \dot{s}_z = [s_z, H] / i\hbar \]
New spin current

- Assume zero spin generation in the bulk
  \[ \frac{1}{V} \int d\mathbf{r}^3 T_z(\mathbf{r}) = 0 \]

- Torque dipole density
  \[ T_z(\mathbf{r}) = -\nabla \cdot \mathbf{P}_\tau(\mathbf{r}) \]

- Spin is conserved in the bulk
  \[ \frac{\partial S_z}{\partial t} + \nabla \cdot (\mathbf{J}_s + \mathbf{P}_\tau) = 0 \]

- New spin current
  \[ \mathbf{J}_{\text{eff}} = (\mathbf{J}_s + \mathbf{P}_\tau) \]
Torque dipole density

A material property

\[ \vec{P}_\tau (\vec{r}) = 0, \text{ outside sample} \]

Boundary torque

\[ \vec{n} \cdot \vec{P}_\tau \]
Displacement spin current

- On average over space

- Maxwell’s displacement current

- New spin current
Linear response

- On equilibrium
  \[ T_z(\vec{r}) = 0 \quad \text{everywhere} \]
  \[ \Rightarrow \quad P_\tau(\vec{r}) = 0 \quad \text{everywhere} \]

- Torque response to electric field
  \[ T_z(\vec{q}) = \chi_\beta(\vec{q}) E_\beta(\vec{q}) \approx \vec{q} \cdot \nabla_q \chi_\beta E_\beta(\vec{q}) \]

- Torque dipole density
  \[ \vec{P}_\tau = \text{Re} \left[ i \nabla_q \chi_\beta \right] E_\beta \]

- New spin current
  \[ J_\alpha^{\text{eff}} = (\sigma_{\alpha\beta} + \text{Re} \left[ i \partial_{q_\alpha} \chi_\beta \right]) E_\beta \]
Spin Hall effect: theory

**Extrinsic:**
- Dyakonov and Perel (71),
- J. E. Hirsch (99),
- S. Zhang (00)

**Intrinsic:**
- Murakami et al Science (03)
- Sinova et al PRL (04)
Spin Hall effect: experiments

- Rashba 2D holes
  - Wunderlich et al
  - PRL (05)

- n-type semiconductors
  - Kato et al
  - Science (04)
Spin Hall conductivity

Using conventional spin current
2d electrons (Rashba): \(e/8\pi\)
2d holes (cubic Rashba): \(-9e/8\pi\)
3d holes (Luttinger):

\[
\frac{e}{6\pi^2} (k_h - k_i) \frac{(\gamma_1 + 2\gamma_2)}{2\gamma_2}
\]

Using our new spin current
2d electrons (Rashba): \(-e/8\pi\)
2d holes (cubic Rashba): \(9e/8\pi\)
3d holes (Luttinger):

\[
\frac{e(\gamma_1 - \gamma_2)}{6\pi^2 \gamma_2} (k_h - k_i) + \frac{e}{6\pi^2} k_h
\]
Spin-charge conductivity tensor

\[
\begin{pmatrix}
J_s \\
J_c
\end{pmatrix}
= 
\begin{pmatrix}
\sigma^{ss} & \sigma^{sc} \\
\sigma^{cs} & \sigma^{cc}
\end{pmatrix}
\begin{pmatrix}
F_s \\
E
\end{pmatrix}
\]

\[
H = H_0 - E \cdot (-e\mathbf{r}) - F_s \cdot (s_z \mathbf{r})
\]

Spin force: Zeeman field gradient
\[g\] factor gradient + Zeeman field
Spin-dependent chemical potential gradient
Inverse spin Hall effect

- Transverse charge current induced by spin force:
  \[ J^y_c = \sigma^{yx}_{cs} F^s_x \]

- 2d electrons (Rashba):
  \[ \sigma^{yx}_{cs} = \frac{e}{8\pi} \]

- 2d holes (Cubic Rashba):
  \[ \sigma^{yx}_{cs} = -\frac{9e}{8\pi} \]
Onsager relation

\[ \sigma_{xy}^{yx} = -\sigma_{xy}^{sc} \]

- Violated if conventional spin current is used
- Saved if our new spin current is used:

\[ J_s^x = \langle \frac{d}{dt} xS_z \rangle = \langle x\dot{S}_z + x\ddot{S}_z \rangle \]

usual spin current  torque dipole
Onsager relation

three-line derivation

If

\[ H = H_0 - F_1 d_1 - F_2 d_2 \]

Then

\[ \langle \dot{d}_m \rangle = \sum_{\alpha'} f_{\alpha'} \langle \alpha' | \dot{d}_m | \alpha' \rangle \equiv \sum_n \sigma_{mn} F_n \]

\[ \sigma_{mn} = - \sum_{\alpha \neq \beta} \frac{\hbar \text{Im} [\langle \alpha | \dot{d}_m | \beta \rangle \langle \beta | \dot{d}_n | \alpha \rangle]}{(\epsilon_\alpha - \epsilon_\beta)^2} (f_\alpha - f_\beta) \]

Antisymmetric in m n
Measurement Methods

- Thermodynamic method:

\[
\frac{dQ}{dt} = J_s \cdot F_s
\]

\[
J_s = \frac{1}{F_s} \frac{dQ}{dt}
\]

- Electric method:

\[
J_s^y = \sigma_{sc}^{xy} E_y
\]

\[
\sigma_{sc}^{xy} = -\sigma_{cs}^{yx}
\]

\[
\sigma_{cs}^{yx} = J_c^y / F_x^s
\]
Spin Hall in insulators

Definition: Charge insulator with a spin Hall effect

-- Murakami, Nagaosa, Zhang

However, if we use conventional spin current, then essentially all insulators with spin-orbit coupling are spin Hall insulators

e.g., Yao and Fang found spin Hall conductivities of 0.001, 0.0015, and 0.0017 e/a for undoped GaAs, Si, and Ge.
No spin Hall in simple insulators based on our proper spin current

Kubo formula:

\[
\sigma_{xy}^{sc} = e \sum_{\alpha \neq \beta} \frac{\hbar \text{Im}[\langle \alpha | s_z \hat{x} + \hat{s}_z x | \beta \rangle \langle \beta | \hat{y} | \alpha \rangle]}{(\epsilon_\alpha - \epsilon_\beta)^2} (f_\alpha - f_\beta)
\]

For localized eigenstates, we can use

\[
< \alpha | \hat{x} s_z + \hat{s}_z x | \beta > = < \alpha | x s_z | \beta > (\epsilon_\alpha - \epsilon_\beta) / i\hbar
\]

\[
< \beta | \hat{y} | \alpha > = < \beta | y | \alpha > (\epsilon_\alpha - \epsilon_\beta) / i\hbar
\]

Then

\[
\sigma_{xy}^{sc} = \frac{e}{\hbar} \sum_\alpha f_\alpha < \alpha | [s_z x, y] | \alpha > \geq 0
\]

How about band insulators with localized Wannier orbitals?
Conclusions

- Spin transport in systems with no bulk generation
  - For all components if there is inversion symmetry
  - For some component ($S_z$) in many cases (2D electrons, holes)

- Spin ($S_z$) is conserved in the bulk
  - satisfies a sourceless continuity equation
  - new spin current = conventional spin current + torque dipole density
  -- Spin accumulation occurs at sample boundary due to balance between the new current and relaxation

- Linear response theory for the new current
  - Yields dramatically different spin Hall conductivity (sign reversal)

- Conjugate force exists
  - Measurement from heat generation
  - Onsager relation is satisfied and can also be used for measurement

- No spin Hall effect in simple insulators
Macroscopic densities

- **Spin density**
  \[
  S_z (\vec{r}, t) = \int d^3k \, f \left\langle \hat{s}_z \right\rangle - \nabla \cdot \int d^3k \, f \, \vec{p}^s
  \]

- **Torque density**
  \[
  T_z (\vec{r}, t) = \int d^3k \, f \left\langle \hat{\tau}_z \right\rangle - \nabla \cdot \int d^3k \, f \, \vec{p}^\tau
  \]
  \[
  \hat{\tau}_z = \frac{i}{\hbar} [\hat{H}, \hat{s}_z]
  \]

- **Spin current density**
  \[
  J^s (\vec{r}, t) = \int d^3k \, f \left\langle \dot{\hat{r}}\hat{s}_z \right\rangle - \nabla \cdot \int d^3k \, f \left\langle (\hat{r} - \vec{r}) \dot{\hat{r}}\hat{s}_z \right\rangle
  \]