Numerical study of the intrinsic spin Hall effect in finite size systems

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Motivation and topics of this study

**Naive motivation**

- Charge transport and spin transport in a system with the spin-orbit interaction (SOI) are very different from each other.
- Spin Hall current/conductivity → spin accumulation?
- Visual understanding of the peculiar feature of spin transport in systems with SOI.

**Topics in this study**

**Two types of intrinsic spin Hall effect (SHE)**
- Do any physical consequences come from the difference between these mechanisms?
- It is emphasized that the intrinsic spin Hall effect is dissipationless in nature.
  → What is the role of relaxation?

**Spin Hall insulator (SHI), Quantum spin Hall system (QSHS)**
- What is happening in the spin Hall effect of the spin Hall insulator?
- What are the essential differences between them?
### Peculiar feature of spin transport

**Charge**

\[
\frac{\partial \rho(\vec{r}, t)}{\partial t} + \vec{\nabla} \cdot \vec{J}(\vec{r}, t) = 0
\]

\[
\rho(\vec{r}) = ec^+ (\vec{r})c(\vec{r}) : \text{charge density}
\]

\[
\vec{J}(\vec{r}) = ec^+ (\vec{r}) \hat{v}c(\vec{r}) : \text{current density}
\]

**Spin**

\[
\frac{\partial S^\mu(\vec{r}, t)}{\partial t} + \vec{\nabla} \cdot \vec{J}^{S^\mu}(\vec{r}, t) = T^\mu(\vec{r}, t)
\]

\[
S^\mu(\vec{r}) = c^+ (\vec{r}) S^\mu c(\vec{r}) : \text{spin density}
\]

\[
\vec{J}^{S^\mu}(\vec{r}) = \frac{1}{2} c^+ (\vec{r}) \left[ S^\mu, \vec{\nabla} \right] c(\vec{r}) : \text{spin current density}
\]

\[
T^\mu(\vec{r}) = ic^+ (\vec{r}) \left[ \vec{H}, S^\mu \right] c(\vec{r}) : \text{torque density}
\]

- No net charge current in equilibrium nor in the direction of open boundary
- Finite net spin current in equilibrium and in the direction of open boundary.
  

- Charge Hall current → Charge accumulation (Linear response + Poisson equation)
- Spin Hall current + Torque density + Balancing with relaxation → Spin accumulation

D. Culcer *et al.*, PRL 93, 046602 (2004); P. Zhang, cond-mat/0503505
SHE in $p$-type GaAs (Luttinger model)

\[ j_y^{\text{S}} = \frac{eE_x}{12\pi^2\hbar} (3k_F^H - k_F^L) = \frac{1}{2e} \sigma_x E_x \]

x: electric field
y: spin current
z: spin direction

**SU(2) analog of the QHE**
- topological origin
- dissipationless
- All occupied states in the valence band contribute.

External electric field does not break time-reversal symmetry. Spin current is allowed in this system with time-reversal symmetry

Berry curvature $\sim$ Magnetic field in $k$-space

\[
\frac{d\vec{r}}{dt} = \frac{\partial \varepsilon_n (\vec{k})}{\partial \vec{k}} + \frac{d\vec{k}}{dt} \times \tilde{\Omega}_n (\vec{k})
\]

Anomalous velocity $\rightarrow$ Intrinsic Hall Effect

\[
\frac{d\vec{k}}{dt} = -\frac{\partial V (\vec{r})}{\partial \vec{r}} + \frac{d\vec{r}}{dt} \times e\vec{B} (\vec{r})
\]

Lorentz force $\rightarrow$ Classical Hall Effect

M.-C. Chang and Q. Niu, PRL 75, 1348 (1995); PRB 53, 7010 (1996)

SU(2) Berry curvature
$\rightarrow$ Spin-dependent anomalous velocity
$\rightarrow$ SHE
SHE in $n$-type GaAs (Rashba model)

\[ H = \frac{p^2}{2m} - \frac{\lambda}{\hbar} \hat{\sigma} \cdot (\hat{z} \times \vec{p}) \]

J. Sinova et al., PRL 92, 126603 (2004)
Two types of intrinsic SHE

**Luttinger model (4-band, double degeneracy)**
- Spin-dependent anomalous velocity $\rightarrow$ spin current
- SU(2) Berry curvature (plus torque effect)

**Rashba model (2-band, no degeneracy)**
- Momentum-dependent torque $\rightarrow$ spin current
- Berry curvature is zero $\rightarrow$ no anomalous velocity
- J. Sinova et al., PRL 92, 126603 (2004)

D. Culcer et al., PRL 93, 046602 (2004).
Spin current due to anomalous velocity (\textit{p}-type Luttinger model)

Spin current due to torque (\textit{n}-type Rashba model)
**Real space Keldysh formalism**

**Steady state**

\( G^{<}_{\vec{r}\vec{r}',\sigma\sigma',t-t'} = i \left\langle c_{\vec{r}\sigma}'(t')c_{\vec{r}\sigma}(t) \right\rangle \)

\( G^{<}(E) = G^{R}(E)\Sigma^{<}(E)G^{A}(E) \)

\( G(E) \): matrix with the index \( \vec{r}\sigma \)

\( O_{\vec{r}\vec{r}} \): physical observable

\[ \langle O_{\vec{r}\vec{r}} \rangle = -i \int dE \text{Tr}^{(\sigma)}[O_{\vec{r}\vec{r}} G^{<}_{\vec{r}\vec{r}}(E)] \]

\( \Sigma^{R}(E) \): retarded selfenergy

\[ \Sigma^{R}(E) = \Sigma^{R,\text{contact}}(E) + \Sigma^{R,\text{system}}(E) \]

\[ \Sigma^{R,\text{system}}(E) = \frac{-i}{2\tau_{\vec{r}}(E)} \delta_{\vec{r}\vec{r}'}\delta_{\sigma\sigma'} \propto \gamma N_{\vec{r}}(E) \delta_{\vec{r}\vec{r}'}\delta_{\sigma\sigma'} \]

\( N_{\vec{r}}(E) \): local density of states

\( G^{R}(E) \) is determined selfconsistently.

\( \Sigma^{<}(E) \): selfenergy of \( G^{<}(E) \)

\[ n_{\vec{r}}(E) = -i \text{Tr} G^{<}_{\vec{r}\vec{r}}(E) = f_{\vec{r}}(E) N_{\vec{r}}(E) \]

\( \text{Im} \Sigma^{<}(E) = 2 f_{\vec{r}}(E) \text{Im} \Sigma^{R}(E) \)

\( f_{\vec{r}}(E) \): local distribution function

\[ f_{\vec{r}}(E) = \frac{1}{1 + e^{\beta(E-\mu_{L,R})}} \]

\( f_{\vec{r}}(E) \) is determined selfconsistently.

\( L_{x} \times L_{y} \): system size

Electrodes at \( x = -\frac{L_{x}}{2} \) and \( x = \frac{L_{x}}{2} \).

Open boundary condition in the y direction.

This formalism is recently applied to the ballistic Rashba system in a different approximation.

Lattice Rashba model (Ando model)

\[ H = \sum_{\tilde{r}} \left[ c_{\tilde{r}+\tilde{x}}^+ \left( -t_0 + it_1 \sigma_y \right) c_{\tilde{r}} + c_{\tilde{r}+\tilde{y}}^+ \left( -t_0 - it_1 \sigma_x \right) c_{\tilde{r}} + \text{H.c.} \right] \]

\[ t_0^2 + t_1^2 = 1, \quad t_0 \cdot t_1 = 1 : S \]

\[ \Gamma \text{ point, } \frac{1}{2m} t_0 a^2, \quad \lambda = t_1 a \]

\[ \sim \sum_{\vec{k}} \left[ \frac{k^2}{2m} + \lambda (\vec{e}_z \times \vec{k}) \cdot \vec{\sigma} \right] c_{\vec{k}} + O(k^3) \]

\[ \dot{\vec{r}}_c = \nabla_{\vec{k}_c} E_{\vec{n}_c} + \vec{k}_c \times \vec{\Omega}_{\vec{k}_c} \]

\[ \dot{k}_c = e \vec{E} \]

\[ \vec{\Omega}_{\vec{k}_c} = 0 \rightarrow \text{anomalous velocity} = 0 \]

**Characteristics of the model**
- Time-reversal symmetry
- Universal spin Hall conductivity
- No anomalous velocity

Vertex correction -> SHE = 0 ?


R. Raimondi and P. Schwab, PRB 71, 033311 (2005)

K. Nomura *et al.*, PRB 71, 041304 (2005)

O. Chalaev and D. Loss, PRB 71, 245318 (2005)

K. Nomura *et al.*, cond-mat/0506189
2D version of lattice Luttinger model

\[ H = \sum_r c_r^+ [\Delta (\Gamma_1 + \Gamma_2) + M \Gamma_5] c_r + \sum_r \sqrt{1-S^2} t [c_{r+\hat{x}}^+ c_r + c_{r+\hat{y}}^+ c_r + \text{H.c.}] \]

\[ -St \sum_r \left[ c_{r+\hat{x}}^+ \sqrt{3\Gamma_4 + \Gamma_5} c_r + c_{r+\hat{y}}^+ \sqrt{-3\Gamma_4 + \Gamma_5} c_r + \text{H.c.} \right] \]

\[ +St \sum_r \left[ c_{r+\hat{x}+\hat{y}}^+ \left( -\frac{\sqrt{3}}{2} \Gamma_3 + \Gamma_5 \right) c_r + c_{r+\hat{x}-\hat{y}}^+ \left( \frac{\sqrt{3}}{2} \Gamma_3 + \Gamma_5 \right) c_r + \text{H.c.} \right] \]

\[ \Gamma \text{ point, } \gamma_1 : \gamma_2 = \sqrt{1-S^2} : S \]

\[ \sim \sum_k c_k^+ \left[ -\frac{1}{2m} \left( \gamma_1 + \frac{5}{2} \gamma_2 \right) k^2 + \frac{\gamma_2}{m} \left( S_x k_x + S_y k_y \right)^2 + M \left( S_z^2 - \frac{5}{4} \right) + \frac{\Delta}{\sqrt{3}} \left\{ S_x + S_y, S_z \right\} \right] c_k \]

**2D version of the model introduced by Murakami et al.**


**Characteristics of the model**

Time-reversal symmetry, double degeneracy
SU(2) Berry curvature \( \rightarrow \) spin-dependent anomalous velocity
Thin film \( \rightarrow M \propto k_z^2 > 0, \Delta \sim 0 \). No vertex correction
B. A. Bernevig and S.-C. Zhang, PRL 95, 016801 (2005)
\( |\varepsilon_F| \sim 0.5t, \frac{1}{\tau} \sim 0.3t \)

\( |\varepsilon_F| \sim 2.0t, \frac{1}{\tau} \sim 0.25t \)

\( |\varepsilon_F| \sim 2.0t, \frac{1}{\tau} \sim 1.25t \)
Spin accumulation
Rashba: $1/\tau \sim 0.3t$

Luttinger: $1/\tau \sim 0.25t$ (solid lines), $1.25t$ (dashed lines)

Spin accumulation at the edges due to $\text{div}J_s$ and torque balancing with the spin relaxation.

Spin accumulation in the bulk predicted by

Equation of expectation value
\[ \frac{\partial \langle S^\mu (\vec{r}) \rangle}{\partial t} + \vec{\nabla} \cdot \langle \vec{J}^S (\vec{r}) \rangle = \langle T^\mu (\vec{r}) \rangle - \frac{\langle S^\mu (\vec{r}) \rangle}{\tau_s} \]

\( \langle S^\mu (\vec{r}) \rangle \): spin density
\( \langle \vec{J}^S (\vec{r}) \rangle \): spin current density
\( \langle T^\mu (\vec{r}) \rangle \): torque density
\( \tau_s \): spin relaxation time

\textit{k - linear Rashba model}
\[ \langle T^x (\vec{r}) \rangle = 2m\lambda \langle J^z_x (\vec{r}) \rangle \]
\[ \langle T^y (\vec{r}) \rangle = 2m\lambda \langle J^z_y (\vec{r}) \rangle \]
\[ \langle T^z (\vec{r}) \rangle = -2m\lambda \left[ \langle J^z_x (\vec{r}) \rangle + \langle J^z_y (\vec{r}) \rangle \right] \]

\( \tau_s \): spin relaxation time

\textit{Steady state (k - linear Rashba)}

\textit{Bulk}:
\[ \langle S^y (\vec{r}) \rangle \approx 2m\lambda \tau_s \langle J^z_y (\vec{r}) \rangle \]

\textit{Edge}:
\[ \langle S^z (\vec{r}) \rangle = -\tau_s \left[ \vec{\nabla} \cdot \langle \vec{J}^S (\vec{r}) \rangle + 2m\lambda \left( \langle J^z_x (\vec{r}) \rangle + \langle J^z_y (\vec{r}) \rangle \right) \right] \]
Reversal of the pattern of the spin accumulation

Luttinger $S=0.29$
Rashba $S=0.10$
Rashba $S=0.05$
Rashba $S=0.02$
Rashba $S=0.01$

Remaining problem in Rashba system
Finite size effect ?
$k^n$-term ($n>3$) ?
For finite $\tau$, no exact cancellation ?
(Raimodi and Schwab)

$1/\tau$ dependence of $dS_z$ at $x \sim 0$, $|y| \sim L_y/2$

Nitta et al. (PRL97) InGaAs/InAlAs

\[ n_{3D} = 4 \times 10^{18} \text{cm}^{-3} \ (1.9 \times 10^{12} \text{cm}^{-2}) \]
\[ \varepsilon_F \sim 50 \text{meV}, \ \Gamma \sim 2 \text{meV}, \ \Delta_R \sim 5 \text{meV} \]

Kato et al. (Science04) AlGaAs, InGaAs

\[ n_{3D} = 3 \times 10^{16} \text{cm}^{-3} \]
\[ \varepsilon_F \sim 1 \text{meV}, \ \Gamma \sim 1 \text{meV}, \ \Delta_R \sim 10^{-3} \text{meV} \? \]

Wunderlich et al. (PRL05) (Al,Ga)As/GaAs

\[ n_{2D} = 2 \times 10^{12} \text{cm}^{-2} \]
\[ \varepsilon_F \sim 20 \text{meV}, \ \Gamma \sim 1.2 \text{meV}, \ \Delta_{\text{HH-LH}} \sim 40 \text{meV} \]

Present calculation Rashba model

\[ n_{3D} = 3 \times 10^{16} \text{cm}^{-3} \]
\[ \varepsilon_F \sim 2 \text{meV}, \ \Gamma \sim 1.2 \text{meV}, \ \Delta_R \sim 0.06 \text{meV} \]

Present calculation Luttinger model

\[ n_{2D} = 1.6 \times 10^{12} \text{cm}^{-2} \]
\[ \varepsilon_F \sim 20 \text{meV}, \ \Gamma \sim 2.5 \text{meV}, \ \Delta_{\text{HH-LH}} \sim 40 \text{meV} \]

\[ E \sim 10 \text{mV} \mu \text{m}^{-1} \]
\[ j_c \sim 25 \mu \text{A} \mu \text{m}^{-2}, j_s \sim 5 \text{nA} \mu \text{m}^{-2} \]
\[ n_{\text{spin}} \sim 10 \mu \text{m}^{-3} \]

\[ I \sim 100 \mu \text{A} \]
\[ \text{p-channel of 1.5} \mu \text{m width} \]
\[ n_{\text{spin}} \sim ?, \ \text{CP} \sim 1\% \]

\[ E \sim 10 \text{mV} \mu \text{m}^{-1} \]
\[ j_c \sim 70 \mu \text{A} \mu \text{m}^{-2}, j_s \sim 35 \text{nA} \mu \text{m}^{-2} \]
\[ n_{\text{spin}} \sim 2.6 \mu \text{m}^{-3} \]

\[ E \sim 200 \text{mV} \mu \text{m}^{-1} \]
\[ 5 \text{nm depth} \]
\[ n_{\text{spin}} \sim 300 \mu \text{m}^{-2}, P_{\text{spin}} \sim 2\% \]
Spin Hall insulator (SHI)

Zero gap semiconductors

HgTe, HgSe, HgS, alpha-Sn

Rocksalt structure: PbTe, PbSe, PbS

Quantum spin Hall system and spin Hall insulator

Quantum spin Hall system (QSHS)
Zero charge conductivity in bulk
Finite spin Hall conductivity
Finite spin accumulation

Spin Hall insulator (SHI)
Zero charge conductivity
Finite spin Hall conductivity
No spin accumulation

What is the difference between the QSHS and the SHI?
What does mean the SHE of SHI in the finite size system?
### Observables and their symmetry

<table>
<thead>
<tr>
<th>Time reversal</th>
<th>Even</th>
<th>Odd</th>
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</thead>
<tbody>
<tr>
<td>Inversion</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Even</td>
<td>$\rho$ charge</td>
<td>$\vec{S}$ spin</td>
</tr>
<tr>
<td>Odd</td>
<td>$\vec{j}_s$, $\vec{P}$ spin current, polarization</td>
<td>$\vec{j}$, $\vec{T}$ current, toroidal moment</td>
</tr>
</tbody>
</table>
Lattice model for spin Hall insulator

\[ H = \sum_{\vec{r}} c_{\vec{r}}^+ [\Delta(\Gamma_1 + \Gamma_2) + MT_5] c_{\vec{r}} \]

\[ -\frac{t}{\sqrt{6}} \sum_{\vec{r}} [c_{\vec{r}+\vec{x}}^+ \left[ \sqrt{3}\Gamma_4 + \Gamma_5 \right] c_{\vec{r}} + c_{\vec{r}+\vec{y}}^+ \left[ -\sqrt{3}\Gamma_4 + \Gamma_5 \right] c_{\vec{r}} + \text{H.c.}] \]

\[ +\frac{t}{\sqrt{6}} \sum_{\vec{r}} \left[ c_{\vec{r}+\vec{x}+\vec{y}}^+ \left[ -\frac{\sqrt{3}}{2} \Gamma_3 + \Gamma_5 \right] c_{\vec{r}} + c_{\vec{r}+\vec{x}-\vec{y}}^+ \left[ \frac{\sqrt{3}}{2} \Gamma_3 + \Gamma_5 \right] c_{\vec{r}} + \text{H.c.} \right] \]

\( \Gamma \) point

\[ \sim \sum_{\vec{k}} c_\vec{k}^+ \left[ \frac{1}{2m} \left[ -\frac{5}{2} k^2 + 2(S_x k_x + S_y k_y)^2 \right] + M(S_z^2 - \frac{5}{4}) + \frac{\Delta}{\sqrt{3}} \left\{ S_x + S_y, S_z \right\} \right] c_{\vec{k}} \]

Characteristics of the model

Time-reversal symmetry, double degeneracy, SU(2) Berry curvature

\( \Delta = 0, M < 0 \rightarrow \) two of independent QHS’s \( \sim \) quantum spin Hall system (QSHS)

Any component of spin is not conserved.

\( \rightarrow \) different from the QSHS in C. L. Kane and E. J. Mele, cond-mat/0411737

The same with the QSHS in X.-L. Qi, Y.-S. Wu, S.-C. Zhang, cond-mat/0505308
Spin Hall conductivity for QSHS and SHI

NOTE: $M>0, \Delta=0$ is essentially the same with the above case, i.e., SHI
- Charge current (not shown) flows along the edges in QSHS
- Spin current flows along the edges in QSHS, only at the contacts in SHI
- Source and drain at the edges in QSHS, at the contacts in SHI
- Spin accumulation at the edges in QSHS, no accumulation in SHI
NOTE: the curves are shifted in $x$ or $y$ direction.
Low energy cost in undoped QSHS and SHI

(about 45 % of doped systems)
(a) QHS
(b) QSHS
(c) SHI
(d) SHI
Summary

- **Two types of intrinsic spin Hall effect**
  - 4-band system (anomalous velocity)
    - The spin current flows both in the bulk and along the edge
    - The sign of spin accumulation is the same with that expected from the spin Hall conductivity when the bulk contribution is dominant.
  - 2-band system (torque)
    - The spin current flows mainly in the bulk
    - The sign of spin accumulation is the same with that expected from the spin Hall conductivity.
  - The spin current can flow in the direction of open boundary due to its source and sink.
  - The spin accumulation in the 4-band system is an order larger than in the 2-band system.

- **Edge state and spin current in SHI**
  - No edge state → No spin accumulation. The spin current flows at the contact.

- **Spin accumulation in the heterostructure of SHI and conductors without SOI**
  - Artificial channel of charge current → spin accumulation
  - Time-reversal symmetry breaking due to leakage charge current

- Although the relaxation is necessary in any case, the dissipationless nature of the intrinsic spin Hall effect does not lose its meaning in order to suppress the energy cost.