# Spin currents in noncentrosymmetric crystals

**Kirill Samokhin**

Department of Physics
Brock University, Canada

**CAP 2026**

June 23, 2026

# Motivation

- Spin currents are fundamental for spintronics
- Most calculations use low-energy effective Hamiltonians: remote bands “integrated out”
- Question: how should observables be transformed when remote bands are eliminated?

KS, M. Sigrist, and M. H. Fischer, Phys. Rev. Res. **8**, 013216 (2026)

Brock University

ETH zürich

Universität Zürich UZH

NSERC CRSNG

Swiss National Science Foundation

# Conventional definition of spin current

PHYSICAL REVIEW B **68**, 241315(R) (2003)

**Spin currents in thermodynamic equilibrium: The challenge of discerning transport currents**

Emmanuel I. Rashba*
*Department of Physics, State University of New York at Buffalo, Buffalo, New York 14260, USA*
*and Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA*

use in what follows the standard and physically appealing definition of the SC tensor $\mathcal{J}_{ij}$:

$$\mathcal{J}_{ij}=\frac{1}{2}\sum_{\lambda}\int\frac{d^2k}{(2\pi)^2}\langle\sigma_i v_j+v_j\sigma_i\rangle_{\lambda\mathbf{k}}. \qquad (6)$$

Here $i,j=x,y$, with $i$ indicating the spin component and $j$ the transport direction. For $T=0$, the integration should be per-

VOLUME 92, NUMBER 12 PHYSICAL REVIEW LETTERS week ending 26 MARCH 2004

**Universal Intrinsic Spin Hall Effect**

Jairo Sinova,[1,2] Dimitrie Culcer,[2] Q. Niu,[2] N. A. Sinitsyn,[1] T. Jungwirth,[2,3] and A. H. MacDonald[2]
[1]*Department of Physics, Texas A&M University, College Station, Texas 77843-4242, USA*

where $n, n'$ are band indices, $\vec{j}^{z}_{\rm spin}=\frac{\hbar}{4}\{\sigma_z,\vec{v}\}$ is the spin-current operator, $\omega$ and $\eta$ are set to zero in the dc clean limit, and the velocity operators at each $\vec{n}$ are

PRL **93,** 226602 (2004) PHYSICAL REVIEW LETTERS week ending 26 NOVEMBER 2004

**Spin Current and Polarization in Impure Two-Dimensional Electron Systems with Spin-Orbit Coupling**

E. G. Mishchenko,[1,2] A. V. Shytov,[1,2] and B. I. Halperin[1]
[1]*Lyman Laboratory, Department of Physics, Harvard University, Massachusetts 02138, USA*

dimensional electron system (2DES) the spin current $\hat{j}^i_k=\frac{1}{4}\{\hat{\sigma}_i,\hat{v}_k\}$ develops a nonzero expectation value under an external electric field $\mathbf{E}$. (Here $\frac{1}{2}\hat{\boldsymbol{\sigma}}$ and $\hat{\mathbf{v}}$ are the operators

# Conventional definition of spin current

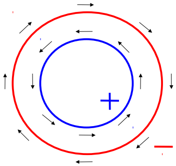
Noncentrosymmetric crystal $\rightarrow$ essential physics described by $\hat{H}_{\text{eff}}(\boldsymbol{k}) = \varepsilon(\boldsymbol{k})\hat{\sigma}_0 + \boldsymbol{\gamma}(\boldsymbol{k}) \cdot \hat{\boldsymbol{\sigma}}$

Spin current operator:

$$\hat{J}_{\mu,i} = \frac{1}{2\hbar}\left\{\frac{\partial \hat{H}_{\text{eff}}}{\partial k_i}, \hat{\sigma}_\mu\right\} = \frac{1}{2}\left\{\hat{v}_i(\boldsymbol{k}), \hat{\sigma}_\mu\right\}$$

Example: Rashba model

$\hat{H}_{\text{eff}} = \varepsilon(\boldsymbol{k}) + \alpha_R(k_y\hat{\sigma}_x - k_x\hat{\sigma}_y)$




in majority band: $v_y\langle\sigma_x\rangle \geq 0$

in minority band: $v_y\langle\sigma_x\rangle \leq 0$

No inversion $\rightarrow$ equilibrium spin current: $\langle j_{x,y}\rangle = -\langle j_{y,x}\rangle = J_S$

$J_s(T=0) \propto \alpha_R^3$ & concentration independent!

How to observe: mechanical torque near edges, bulk electric polarization

# Microscopic formalism

Microscopic Hamiltonian $\rightarrow$ EOM for spin density $\rightarrow$ averaging over fast variations

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix}\psi_\uparrow\\ \psi_\downarrow\end{pmatrix} = \hat{H}_{\rm micro}\begin{pmatrix}\psi_\uparrow\\ \psi_\downarrow\end{pmatrix} \quad \rightarrow \quad \frac{\partial s_\mu}{\partial t} = -\nabla_i j_{\mu,i} + \tau_\mu$$

"Exact" spin-current operator: $\hat{J}_{\mu,i}(\boldsymbol{k}) = \frac{1}{2\hbar}\left\{\frac{\partial \hat{H}}{\partial k_i}, \hat{S}_\mu\right\}$

"Exact" spin-torque operator: $\hat{T}_\mu(\boldsymbol{k}) = \frac{i}{\hbar}\left[\hat{H}, \hat{S}_\mu\right]$

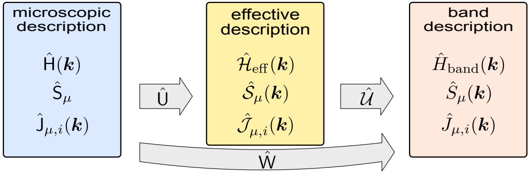
"Exact" spin operator: $\hat{S}_\mu = \begin{pmatrix}\hat{\sigma}_\mu & 0 & \cdots\\ 0 & \hat{\sigma}_\mu & \cdots\\ \vdots & \vdots & \ddots\end{pmatrix}$

expressed in terms of $\boldsymbol{k}\cdot\boldsymbol{p}$ Hamiltonian with SOC

$$\hat{H}(\boldsymbol{k}) = \begin{pmatrix}\hat{h}_1 & \hat{h}_{12} & \cdots\\ \hat{h}_{21} & \hat{h}_2 & \cdots\\ \vdots & \vdots & \ddots\end{pmatrix}$$

$2N \times 2N$ matrices ($\#$ of orbitals $N \rightarrow \infty$) are impractical for calculations

# Effective Hamiltonian formalism




Microscopic Hamiltonian $\rightarrow$ Effective Hamiltonian $\rightarrow$ Effective observables

"Downfolding" into the essential band subspace (Schrieffer–Wolff transformation):

$$\hat{H}(\boldsymbol{k}) = \begin{pmatrix} \hat{h}_1 & \hat{h}_{12} & \cdots \\ \hat{h}_{21} & \hat{h}_2 & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix} \rightarrow \hat{\mathcal{H}}_{\mathrm{eff}}(\boldsymbol{k}) = \hat{U}^{-1}\hat{H}\hat{U} = \begin{pmatrix} \hat{H}_{eff,1} & 0 & \cdots \\ 0 & \hat{H}_{eff,2} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}$$

Treat inter-orbital couplings $\hat{H}_{\mathrm{inter}}$ as a perturbation $\rightarrow$ find $\hat{U}(\boldsymbol{k})$ to any desired order in $\hat{H}_{\mathrm{inter}}$

# Main result

Observables must be transformed consistently: $\hat{O}_{\text{eff}}(\boldsymbol{k}) = \hat{U}^{-1}(\boldsymbol{k})\hat{O}(\boldsymbol{k})\hat{U}(\boldsymbol{k})$

Spin-current operator in the essential band subspace:

$$\hat{J}_{\mu,i} = \frac{1}{2\hbar}\left\{\frac{\partial \hat{H}_{\text{eff}}}{\partial k_i}, \hat{\sigma}_\mu\right\} + \delta\hat{J}_{\mu,i}$$

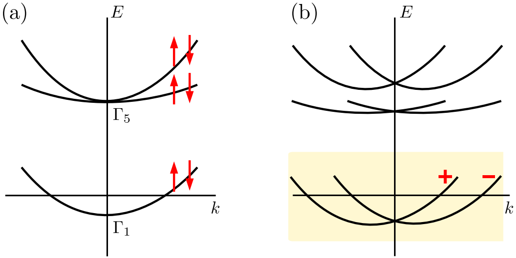
- first term: conventional contribution
- $\delta\hat{J}_{\mu,i}$: generated by eliminating remote bands
- cannot be reconstructed from $\hat{H}_{\text{eff}}$ alone

# Example: $C_{4v}$ crystal

Quasi-2D noncentrosymmetric tetragonal crystal: rotation $C_{4z}$ + reflection $\sigma_y$, $\boldsymbol{k} = (k_x, k_y)$

Include two orbitals: 1D orbital + 2D orbital (oxide interfaces, 2D chalcogenides, ...)

- lower $\Gamma_1$ orbital ($p_z$, $s$) or $\Gamma_4$ orbital ($d_{xy}$)
- upper $\Gamma_5$ orbital ($p_{x,y}$ or $d_{xz,yz}$)
- inter-orbital hybridization + SOC




no SOC

with SOC

# Emergent Rashba SOC

Microscopic $\boldsymbol{k}\cdot\boldsymbol{p}$ Hamiltonian:

$$\hat{H}(\boldsymbol{k})=\begin{pmatrix}\varepsilon_1(\boldsymbol{k})\hat{\sigma}_0 & -i\tilde{a}k_x\hat{\sigma}_0-i\tilde{b}\hat{\sigma}_y & -i\tilde{a}k_y\hat{\sigma}_0+i\tilde{b}\hat{\sigma}_x\\ i\tilde{a}k_x\hat{\sigma}_0+i\tilde{b}\hat{\sigma}_y & \varepsilon_2(\boldsymbol{k})\hat{\sigma}_0 & -ib\hat{\sigma}_z\\ i\tilde{a}k_y\hat{\sigma}_0-i\tilde{b}\hat{\sigma}_x & ib\hat{\sigma}_z & \varepsilon_2(\boldsymbol{k})\hat{\sigma}_0\end{pmatrix}$$

Schrieffer–Wolff transformation $\rightarrow$ effective Rashba SOC in the lower band subspace:

$$\hat{H}_{\mathrm{eff}}=\varepsilon(\boldsymbol{k})\hat{\sigma}_0+\boldsymbol{\gamma}(\boldsymbol{k})\cdot\hat{\boldsymbol{\sigma}}$$

$$\boldsymbol{\gamma}(\boldsymbol{k})=\alpha_R(k_y,-k_x,0),\qquad \alpha_R=\frac{2\tilde{a}\tilde{b}}{E_{\mathrm{gap}}}$$

Rashba SOC emerges from inter-orbital hybridization, at 2nd order in $\hat{H}_{\mathrm{inter}}$

# Effective spin current operator

Spin-current operator in the essential band subspace:

$$\hat{J}_{\mu,i}(\boldsymbol{k}) = \hat{J}^{\mathrm{conv}}_{\mu,i}(\boldsymbol{k}) + \delta\hat{J}_{\mu,i}(\boldsymbol{k})$$

- Conventional contribution recovered:

$$\hat{J}^{\mathrm{conv}}_{x,i} = \frac{\hbar k_i}{m^*}\hat{\sigma}_x + \frac{\alpha_R}{\hbar}\delta_{iy}\hat{\sigma}_0$$

- Additional terms appear at the same perturbative order as the effective SOC:

$$\delta\hat{J}_{\mu,i} = -\frac{2\tilde{b}^2}{E_{\mathrm{gap}}^2}\frac{\hbar k_i}{m}\hat{\sigma}_x - \frac{2b\tilde{a}^2}{\hbar E_{\mathrm{gap}}^2}(\delta_{ix}k_y - \delta_{iy}k_x)\hat{\sigma}_y + \frac{2b\alpha_R}{E_{\mathrm{gap}}^2}\frac{\hbar k_i k_y}{m}\hat{\sigma}_0$$

- These terms are essential for consistency

# Equilibrium spin current

Average spin current in uniform equilibrium: $\langle j_{x,y}\rangle = -\langle j_{y,x}\rangle = J_s$

At $T = 0$: $J_s = \left(\frac{E_F}{E_{\rm gap}}\right)^2 \frac{mb}{\pi\hbar^3}\alpha_R$ – scales linearly with $\alpha_R$, depends on concentration

Non-conventional terms produce dominant effect: $\frac{J_s^{\rm ours}}{J_s^{\rm conv}} \propto \frac{E_F}{E_{\rm SOC}} \gg 1$

Next steps: modified spin-current operator $\hat{J}_{\mu,i} = \hat{J}^{\rm conv}_{\mu,i} + \delta\hat{J}_{\mu,i}$ $\rightarrow$ correlators (spin Hall effect, etc)

boundary effects, spin current conversion/injection

# Summary

| | Conventional | This work |
|---|---|---|
| Spin-current operator | $\{v_i, \sigma_\mu\}/2$ | $\{v_i, \sigma_\mu\}/2 + \delta J_{i,\mu}$ |
| ESC scaling with SOC | $\alpha_R^3$ | $\alpha_R$ |
| ESC depends on electron concentration | no | yes |
| Interband effects | not included | included |

- Spin transport is intrinsically multiband
- Virtual transitions survive in effective observables
- The conventional definition of the spin-current operator is generally incomplete
- Effective Hamiltonians alone are insufficient
- Interband corrections dominate the equilibrium spin current