Tunable Spin-charge Conversion in Topological Dirac Semimetals

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Based on arXiv: 2110.11823

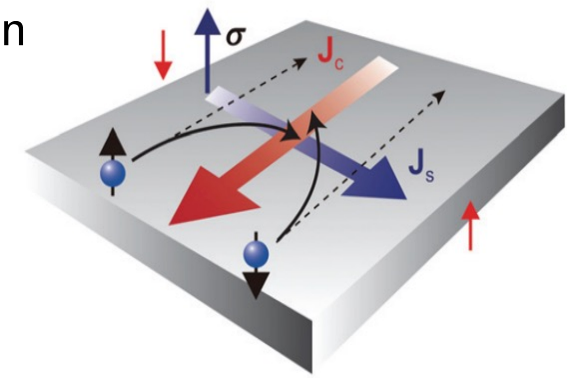
APS March Meeting 2022, Chicago, IL

03/16/2022

This presentation was made possible, in part, through financial support from the School of Graduate Studies at Case Western Reserve University.

Spin-charge conversion

- Spin Hall effect (SHE): charge-to-spin conversion
  - Intrinsic: related to the Berry curvature
  - Extrinsic: induced by disorder



Ando et al., J. Appl. Phys. **109**, 103913 (2011)

- SHE in topological Dirac semimetals (TDSMs): e.g.

  Taguchi et al., *PRB* **101**, 235201 (2020)

  Yen and Guo, *PRB* **101**, 064430 (2020)

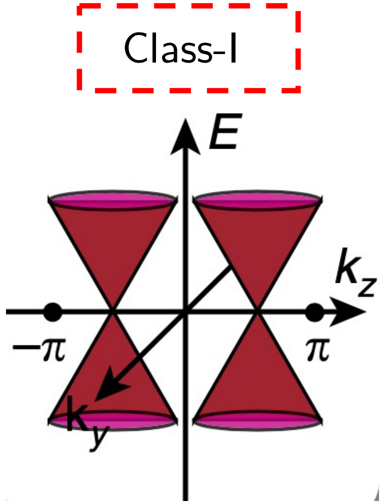
  Hou et al., *npj Comput. Mater.* **7**, 37 (2021)

- Our work: Tunable spin-charge conversion in TDSMs by external fields.

Topological Dirac semimetals (TDSMs)

- Host Dirac points (4-fold degenerate) protected by time-reversal + inversion + uniaxial rotation symmetries

Yang and Nagaosa, Nat. Commun. **5**, 4898 (2011)



A pair of Dirac points on the rotation axis

- Class-I TDSM materials: e.g., Cd_3As_2 (C_4 symm.), Na_3Bi (C_3 symm.)

Spin Hall effect in TDSMs

Low-energy Hamiltonian for a class-I TDSM:

Wang et al., PRB **85**, 195320 (2012);
Wang et al., PRB **88**, 125427 (2013)

spin-up

$$H_D(\mathbf{k}) = \begin{pmatrix} M(\mathbf{k}) & Ak_+ & 0 & 0 \\ Ak_- & -M(\mathbf{k}) & 0 & 0 \\ 0 & 0 & M(\mathbf{k}) & -Ak_- \\ 0 & 0 & -Ak_+ & -M(\mathbf{k}) \end{pmatrix} = H_W^{\uparrow} \oplus H_W^{\downarrow}$$

spin-down

spin polarization

spin Berry curvature

Spin Hall current: $$\mathbf{j}^z = \frac{e}{\hbar}\sum_{s,n} s \int \frac{d^3\mathbf{k}}{(2\pi)^3}\mathbf{E}\times\mathbf{\Omega}_n^s(\mathbf{k}) f_{n\mathbf{k}}^0 = \sigma_{\mathrm{SH}}^0(\mathbf{E}\times\hat{\mathbf{z}}) \qquad (s=\pm 1)$$

Anisotropic SHE

with spin Hall conductivity (SHC)

$$\boxed{\sigma_{\mathrm{SH}}^0 = \frac{ek_D}{\pi^2\hbar}} \qquad 2k_D = \text{separation of Dirac points}$$

Charge Hall current: $$\mathbf{j} = \frac{e}{\hbar}\sum_{s,n} \int \frac{d^3\mathbf{k}}{(2\pi)^3}\mathbf{E}\times\mathbf{\Omega}_n^s(\mathbf{k}) f_{n\mathbf{k}}^0 = 0$$

Pure spin current!

$\mathbf{B}$ in arbitrary directions

effective Landé g-factor ≈ 30

- Zeeman coupling: $H_Z = \tilde{g}\mu_B(\mathbf{L} + 2\mathbf{S}) \cdot \mathbf{B}$

$$= \tilde{g}\mu_B \begin{pmatrix} B_z & 0 & B_- & 0 \\ 0 & 2B_z & 0 & 0 \\ B_+ & 0 & -B_z & 0 \\ 0 & 0 & 0 & -2B_z \end{pmatrix}$$

z-component of spin is NOT conserved

$\implies$ unconventional SHC tensors $\sigma^x_{xy},\ \sigma^y_{xy} \neq 0$

- Kubo-Greenwood formula:

$$\sigma^i_{ab} = -e\hbar \int \frac{d^3\mathbf{k}}{(2\pi)^3} \sum_n f^0_{n\mathbf{k}} \sum_{n' \neq n} \frac{2\,\mathrm{Im}[\,\langle n\mathbf{k}|J^i_a|n'\mathbf{k}\rangle\ \langle n'\mathbf{k}|v_b|n\mathbf{k}\rangle]}{(\varepsilon_{n'\mathbf{k}} - \varepsilon_{n\mathbf{k}})^2 + \Gamma^2}$$

$$\sigma_{ab} = -e\hbar \int \frac{d^3\mathbf{k}}{(2\pi)^3} \sum_n f^0_{n\mathbf{k}} \sum_{n' \neq n} \frac{2\,\mathrm{Im}[\,\langle n\mathbf{k}|v_a|n'\mathbf{k}\rangle\ \langle n'\mathbf{k}|v_b|n\mathbf{k}\rangle]}{(\varepsilon_{n'\mathbf{k}} - \varepsilon_{n\mathbf{k}})^2 + \Gamma^2}$$

$J^i_a = \frac{1}{2}\{v_a, \sigma_i\}, \quad v_a = \frac{\partial \varepsilon(\mathbf{k})}{\hbar \partial k_a}$

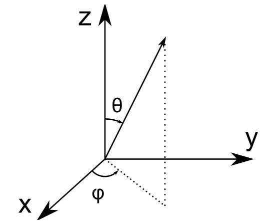
band broadening factor $\sim\ \hbar/\tau\ \approx$ 10 meV

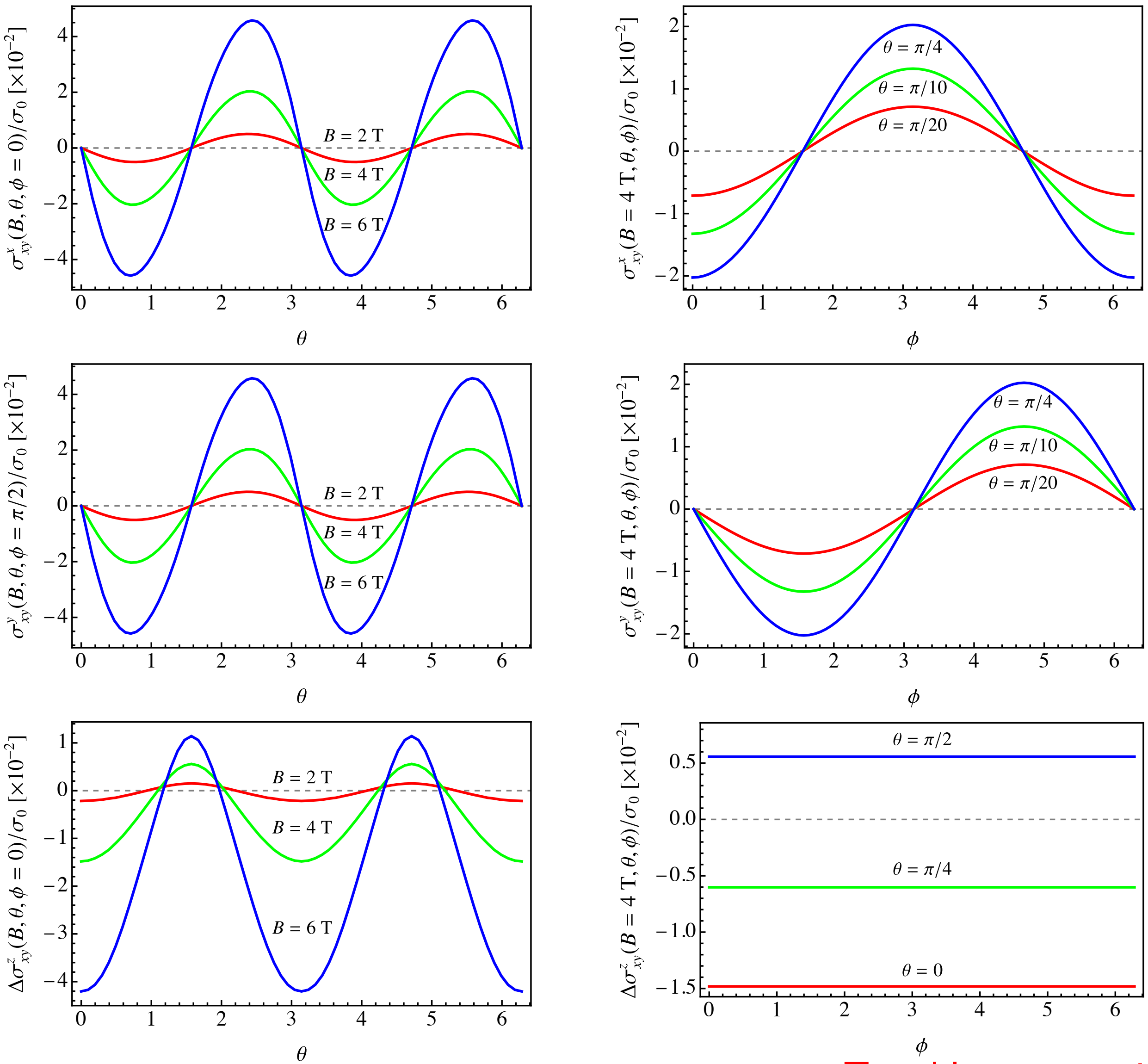
Spin/charge Hall currents

$$\boxed{\begin{aligned} &\mathbf{Q}^{x(y)} \approx \chi^{x(y)} B_z B_{x(y)} (\mathbf{E} \times \hat{\mathbf{z}}) \\ &\mathbf{Q}^{z} \approx \left[\sigma^0_{\mathrm{SH}} + \left(\chi^z_\perp B^2_\perp + \chi^z_\parallel B^2_z\right)\right] (\mathbf{E} \times \hat{\mathbf{z}}) \\ &\mathbf{j} \approx \kappa B_z (\mathbf{E} \times \hat{\mathbf{z}}) \end{aligned}}$$

- Electric tunability: band topology
- Magnetic tunability: symmetry breaking [also seen in spin currents in ferromagnets induced by magnetization; see Amin et al., PRB **99**, 220405 (2019)]

SHC **B**-dependence





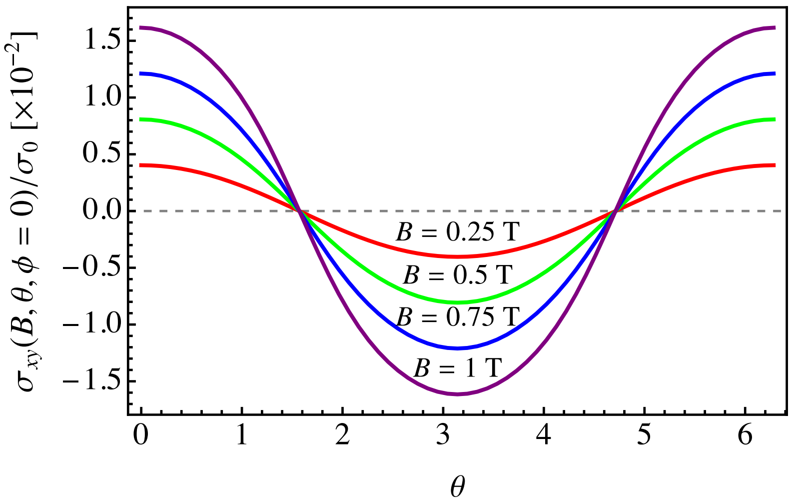
$$\sigma^x_{xy}(\mathbf{B}) \sim B_x B_z \sim B^2 \sin(2\theta)\cos\phi$$

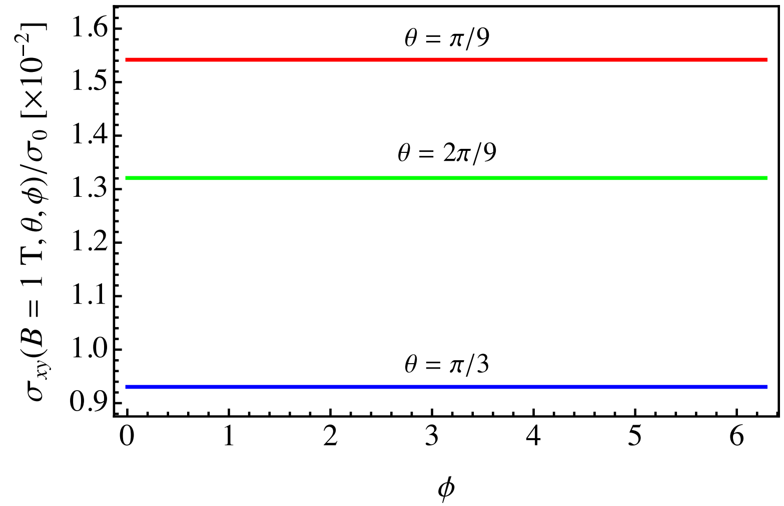
$$\sigma^y_{xy}(\mathbf{B}) \sim B_y B_z \sim B^2 \sin(2\theta)\sin\phi$$

$$\sigma^z_{xy}(\mathbf{B}) \sim \alpha(B_x^2 + B_y^2) + \beta B_z^2 \sim B^2\left(\alpha\sin^2\theta + \beta\cos^2\theta\right)$$

Tunable upon variation of magnetic field direction!

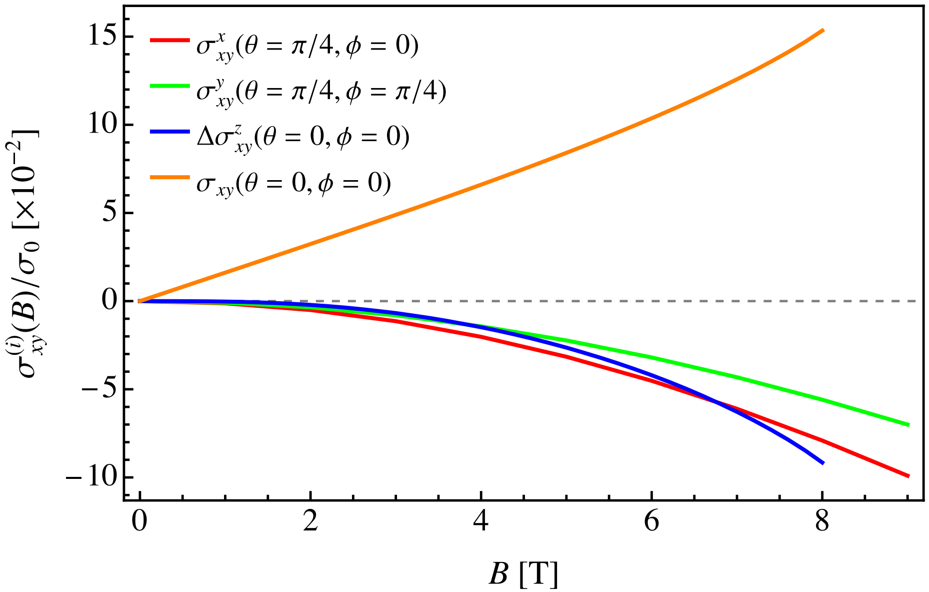
AHC **B**-dependence

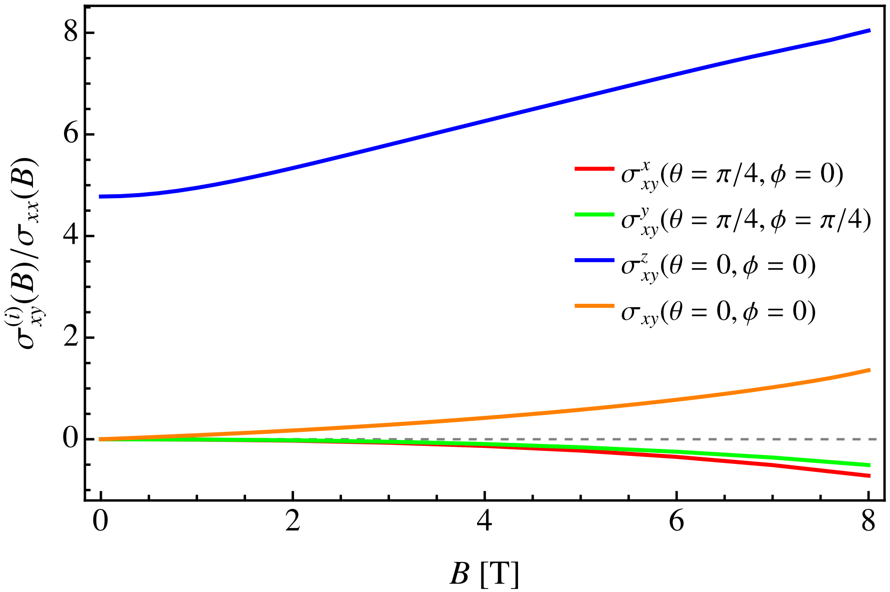




$$\sigma_{xy}(\mathbf{B}) \sim B_z \sim B \cos\theta$$

Spin-charge conversion efficiency





Summary & Outlook

- Take-home message:

  Topological Dirac semimetals can provide another platform for realizing electrically & magnetically tunable spin-charge conversion arisen from the interplay of unique band topology and symmetry breaking.

- No magnetic field: pure spin current;

  With external magnetic field: spin-to-charge conversion

- Spin-charge conversion efficiency can be enhanced by increasing the magnetic field strength.

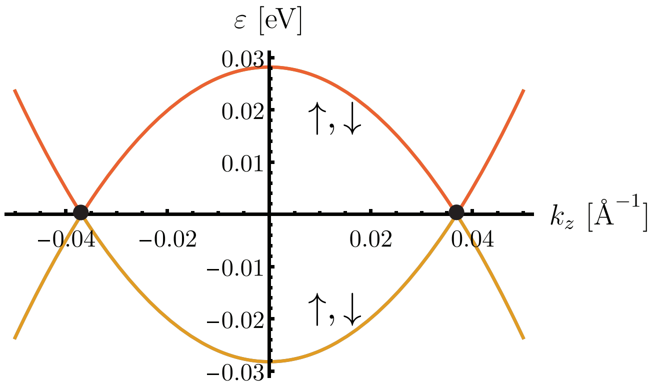
- Possible future directions: effects of tilting and energy displacement of the Dirac cones; orbital contribution of magnetic field; etc.

Back-up Slides

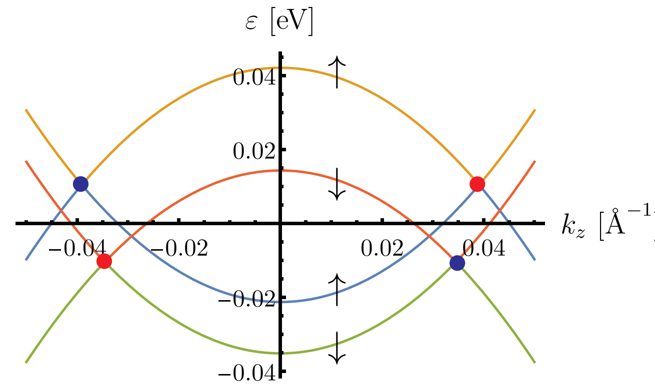
Tunability via external magnetic field

- Spin mixing
- Symmetry breaking

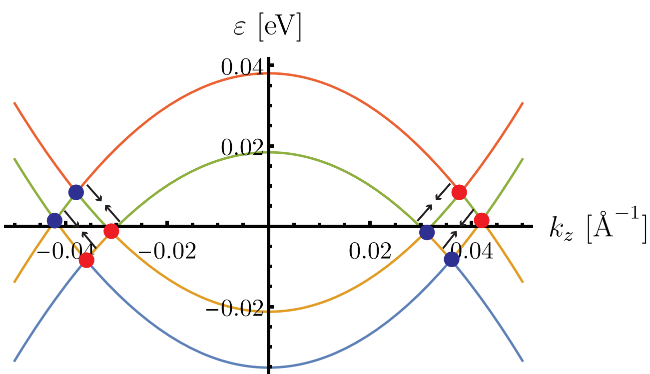
$\mathbf{B} = 0$



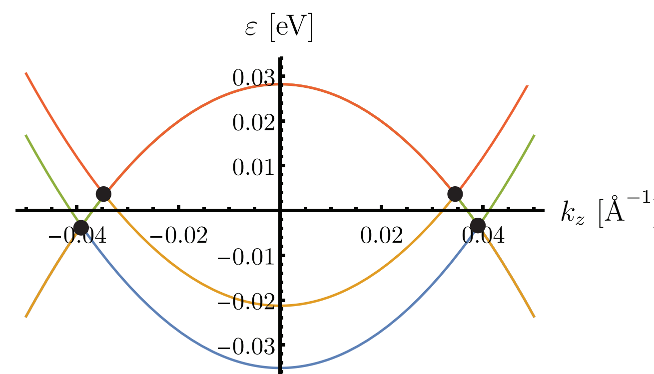
$\mathbf{B} = B(0,0,1)$



$\mathbf{B} = \frac{B}{\sqrt{2}}(1,0,1)$

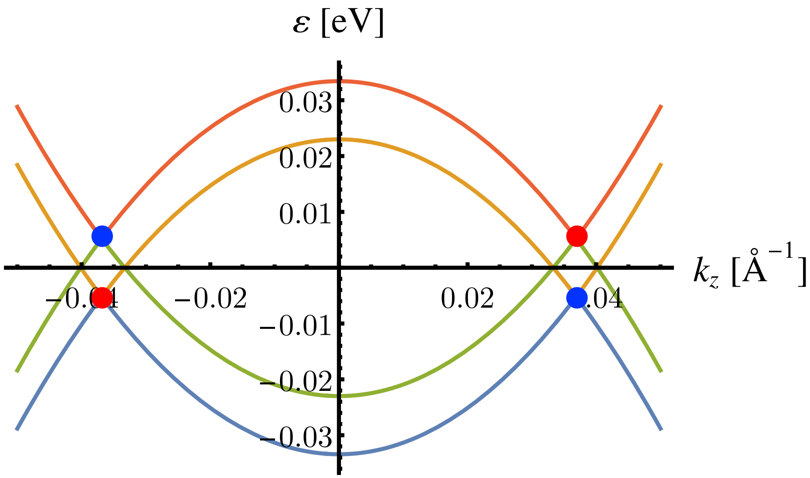


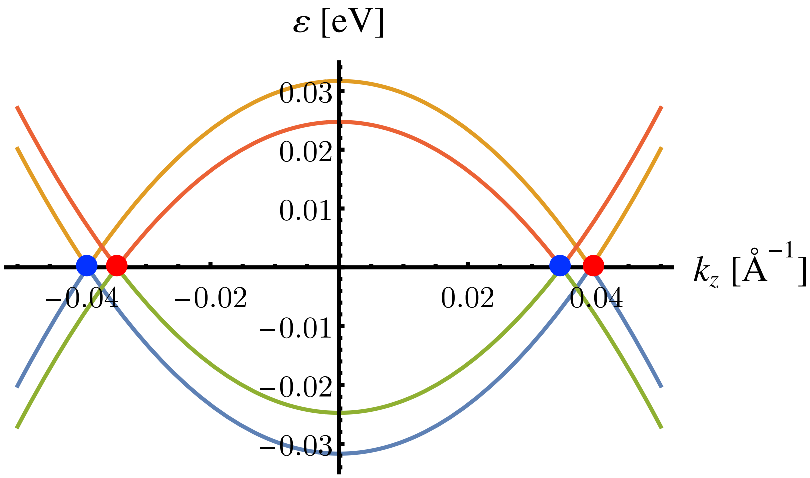
$\mathbf{B} = B(1,0,0)$



B along z-direction

Zeeman coupling: $H_Z = h_+ \sigma_z \tau_0 + h_- \sigma_z \tau_z$





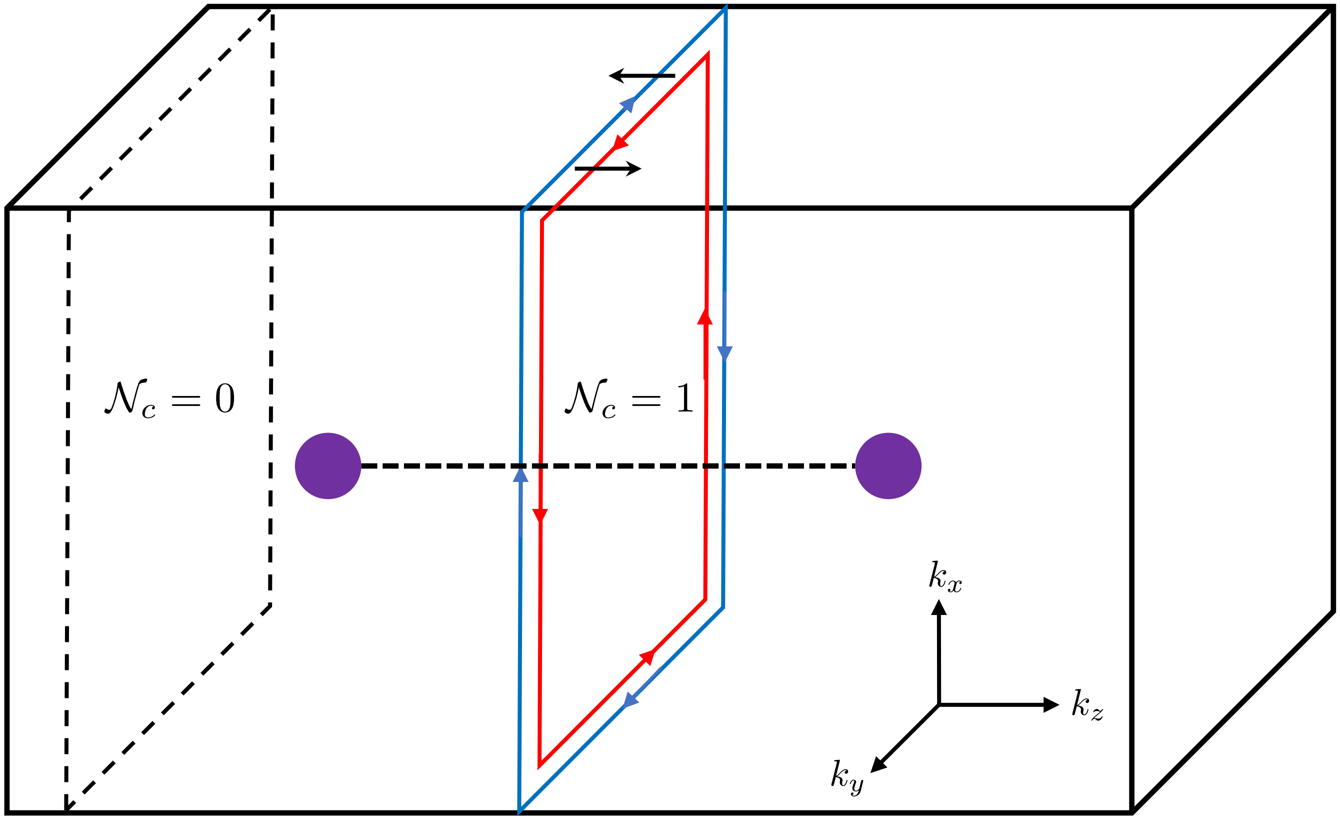
Orbital-symmetric: $$\sigma_{xy}^{z\ (+)} \simeq \left[1 - \left(\frac{1}{24M_0^2} + \frac{M_2}{3M_0A^2}\right) h_+^2\right] \sigma_{\mathrm{SH}}^0$$

Orbital-antisymmetric: $$\sigma_{xy}^{z\ (-)} \simeq \left(1 - \frac{h_-^2}{8M_0^2}\right) \sigma_{\mathrm{SH}}^0$$

$$\sigma_{xy}^{(-)} \simeq -\frac{h_-}{2|M_0|} \sigma_{\mathrm{SH}}^0$$

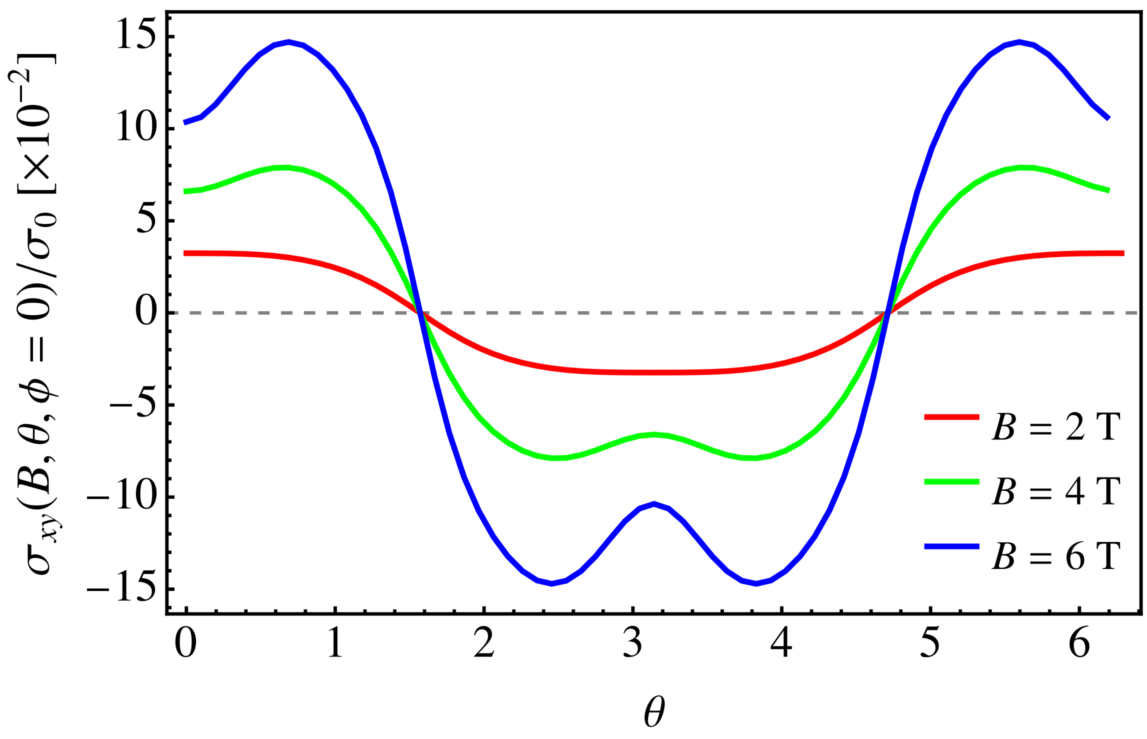
Spin-to-charge conversion!

SHC in TDSMs and Z_2 invariant



$$\mathcal{N}_c(k_z) \equiv \frac{1}{4\pi}\sum_s s \int dk_x dk_y \boldsymbol{\Omega}^s_{-,z}(\mathbf{k}) = \Theta\left(k_D^2 - k_z^2\right)$$

High-field behavior (AHC)



Magnitude dependence