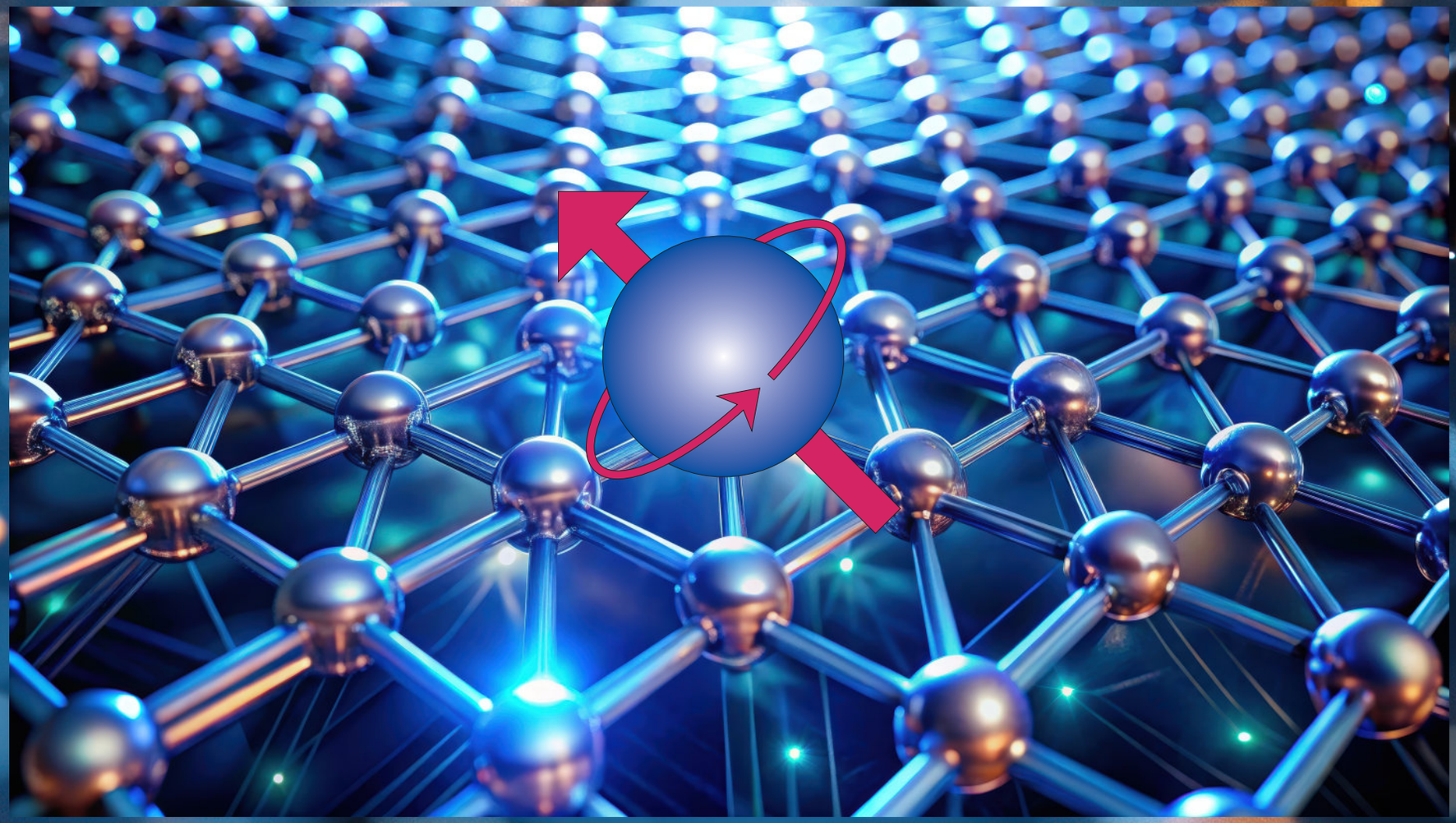
Spin-Orbitronics

Aires Ferreira

UNIVERSITY of York

YORK CENTRE FOR QUANTUM TECHNOLOGIES



European School of Magnetism 2025, Liège, Belgium - 30 Jun to 11 July

Spintronics

“Spintronics” is believed to soon become a mainstream alternative
to conventional (charge-based) electronics

Overarching aim is two fold:

(i) to understand spin-dependent phenomena in condensed matter

(ii) to exploit the spin degree of freedom (DOF) of electrons for new computing paradigms

Žutić, RMP 76 (2004) **I** Lenk, Phys. Rep. 507 (2011) **I** Sinova, RMP 87 (2015) **I** Soumyanarayanan, Nature 539 (2016) **I** Baltz, RMP 90 (2018) …

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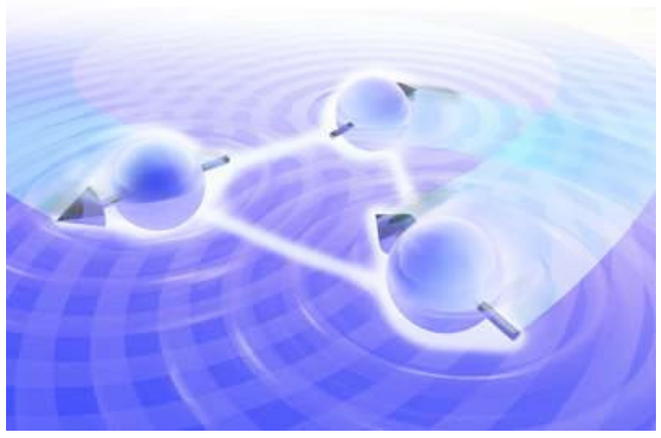

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(a) real-space **spin textures** in magnetic systems

(b) creation of **spin-polarised carriers** in non-magnetic materials

(c) **topologically-protected spin transport** channels

(d) **magnetisation dynamics**

(e) spin and orbital moment **relaxation**

(f) **spin/orbital Hall** & related **galvanic** effects

…

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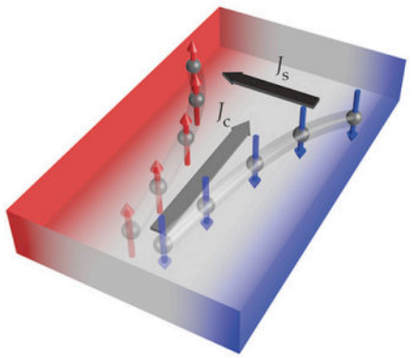
Timeline



Spin Hall effect (Prediction)

70s

Spin current

Spin-polarised currents (FM/SC junctions)

80s

GMR

90s

CPP-GMR

00s

SHE, SGE QSHE

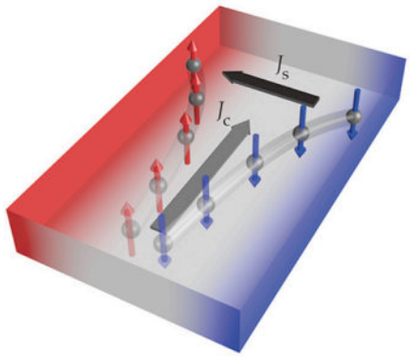
10s

SOT, AFs

20s

On-going

Timeline



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Lateral spin valves (LSVs): Electrical spin injection & detection

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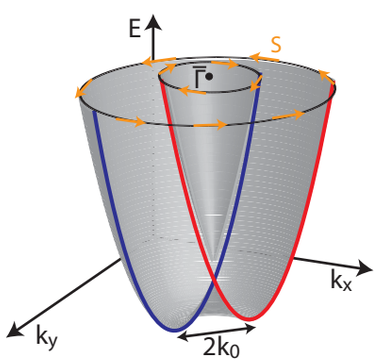
Broken symmetry & spin galvanic effects (SGEs)



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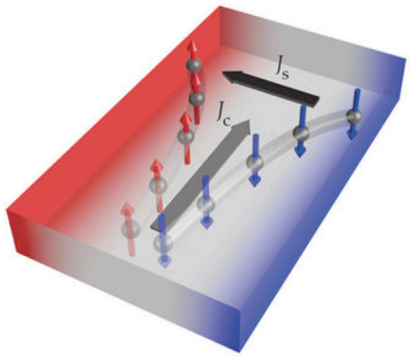

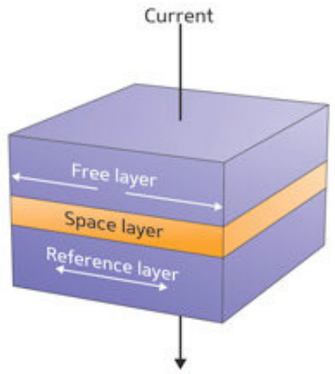

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Optical spin injection & detection in Semiconductors (SCs)

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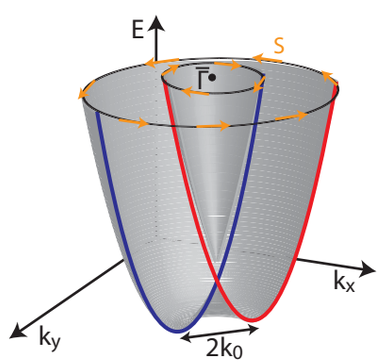

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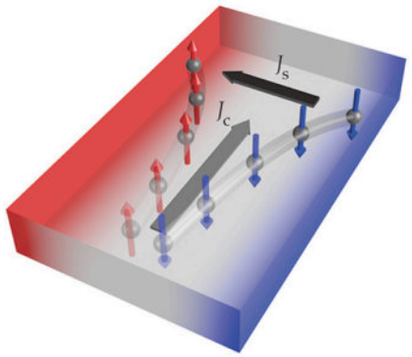

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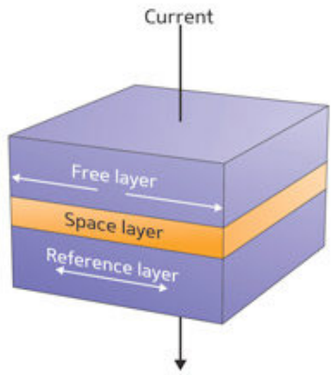

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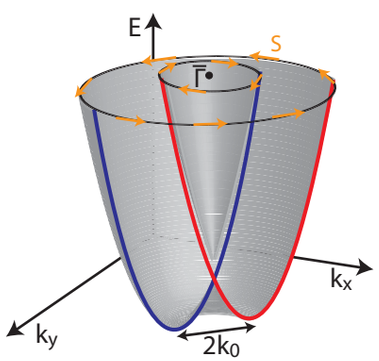


STT-MRAM

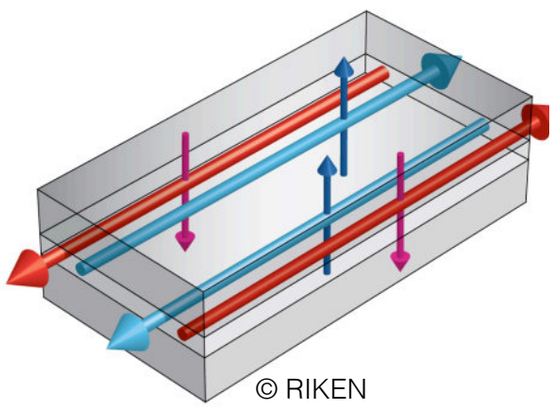
magnonics

00s

SHE, SGE QSHE

Observation of direct/inverse SHE and SGEs in metals and SCs

QSHE prediction & observation in quantum wells



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SOT, AFs

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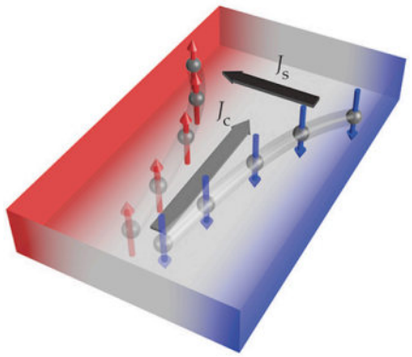
On-going

Timeline



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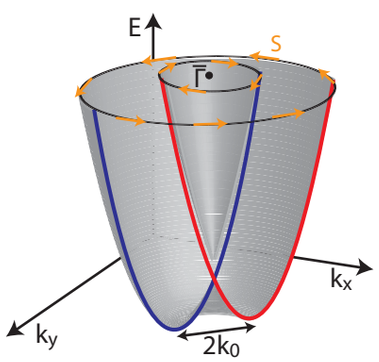

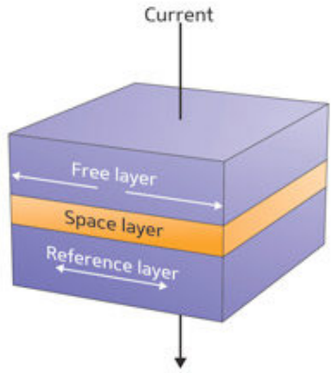

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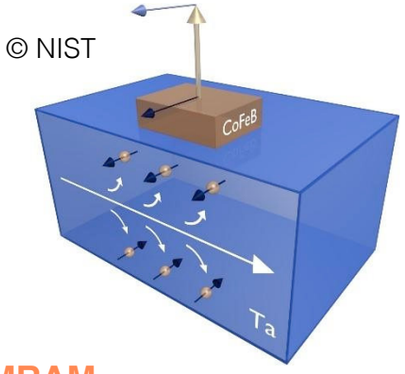

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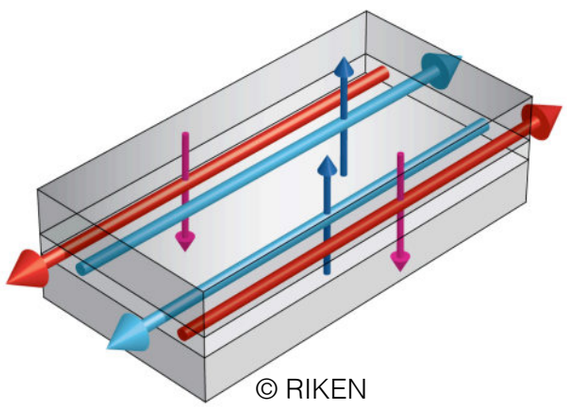

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10s

SOT, AFs

Antiferromagnetic (AF) metal spintronics

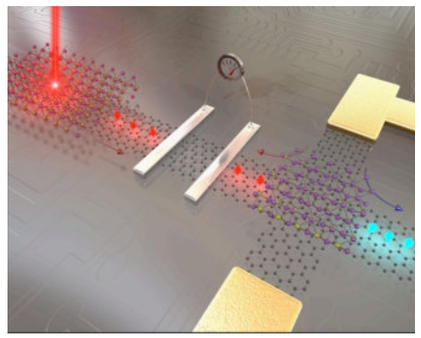
Spin-orbit torque (SOT)

20s

On-going

Orbitronics

Altermagnets



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2D spintronics

Outline

Today's focus: Some fundamentals of spintronics, spin-orbitronics and orbitronics

1. Spin currents & orbital currents in solids

2. Spin-orbit coupling in **k**-space & broken symmetries

3. Relaxation & out-of-equilibrium spin-orbital (transport) processes

Notation/conventions for this lecture

- ***bold*** *symbols for vector/pseudo-vector quantities*

- *acronyms:* ***SO*** *= spin-orbit;* ***SOC*** *= spin-orbit coupling;* ***OAM*** *= orbital angular momentum*

  NM *= normal metal;* ***FS*** *= Fermi surface;* ***TI*** *= Topological Insulator*

- *Natural units with* $\hbar = 1$

Notation/conventions for this lecture

Spin operator *definition:*

$$\hat{\mathbf{s}} = (\hat{s}_x, \hat{s}_y, \hat{s}_z) \equiv (\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z)$$

vector of Pauli matrices

$$\hat{\boldsymbol{\mu}}_s = -\mu_B \hat{\mathbf{s}} \qquad (g_s = 2)$$

Expectation values*:*

$$O(t) \equiv \langle \hat{O} \rangle_t = \langle \Psi(t) | \, \hat{O} \, | \Psi(t) \rangle$$

$$O(t) \equiv \mathrm{Tr}[\hat{O}\, \hat{\rho}(t)] \qquad \textbf{[mixed states]}$$

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- ***symmetries***

$$|\Psi\rangle \to \hat{U}_S |\Psi\rangle$$
$$\hat{O} \to \hat{U}_S^\dagger \, \hat{O} \, \hat{U}_S$$

Wigner's theorem:

$\hat{U}_S$ *: unitary/anti-unitary*

Anti-unitary symmetry *example:*

Time reversal:

$$\hat{U}_{\mathcal{T}}^\dagger \{\hat{\mathbf{r}}, \hat{\mathbf{p}}, \hat{\mathbf{L}}, \hat{\mathbf{s}}\} \hat{U}_{\mathcal{T}} \to \{\hat{\mathbf{r}}, -\hat{\mathbf{p}}, -\hat{\mathbf{L}}, -\hat{\mathbf{s}}\}$$

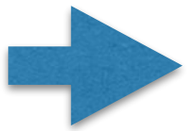
Unitary symmetry *example:*

Mirror reflection about the yz-plane

$$\hat{U}_x^\dagger \, \hat{\mathbf{p}} \, \hat{U}_x = (-\hat{p}_x, \hat{p}_y, \hat{p}_z) \qquad \hat{U}_x^\dagger \, \hat{\mathbf{s}} \, \hat{U}_x = (\hat{s}_x, -\hat{s}_y, -\hat{s}_z)$$

1a. Spin and orbital currents

- ***Intuitive definition***

charge current $I_c = \sum_{\sigma=\uparrow,\downarrow} I_\sigma = I_\uparrow + I_\downarrow$  **spin current** $I_s = \sum_{\sigma=\uparrow,\downarrow} s_\sigma I_\sigma = I_\uparrow - I_\downarrow$

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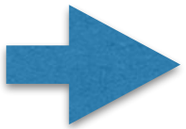

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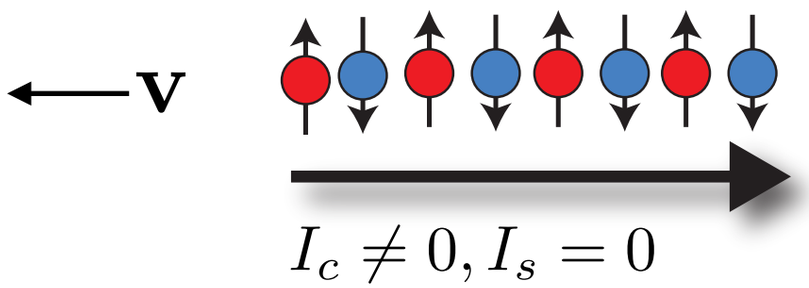
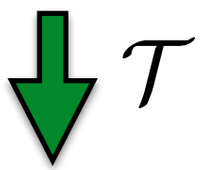
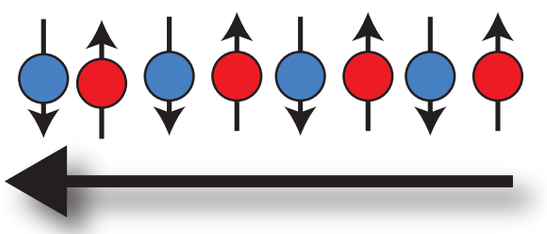


$I_c \neq 0, I_s = 0$

Pure charge current





$I_c \to -I_c$

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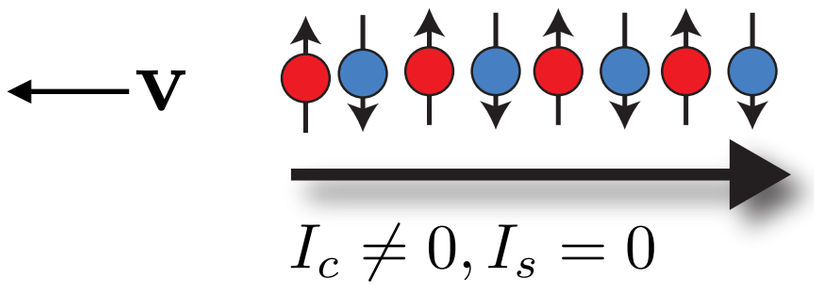

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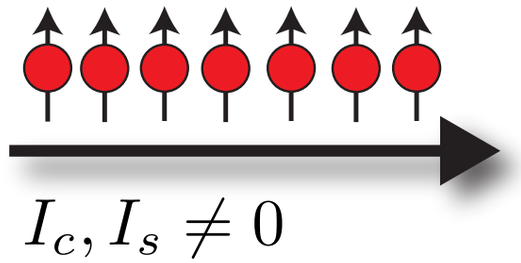

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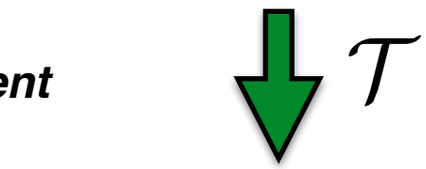

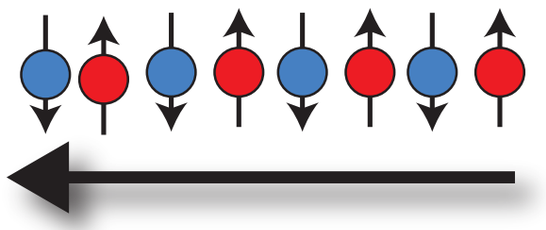

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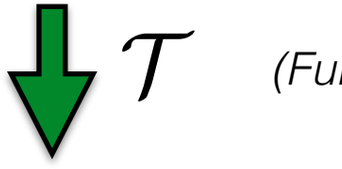
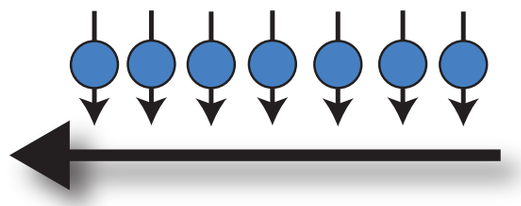


(Fully) ***spin-polarised current***



$\{I_c, I_s\} \to \{-I_c, -I_s\}$

1a. Spin and orbital currents

Can we have $I_s \neq 0$ with $I_c = 0$?

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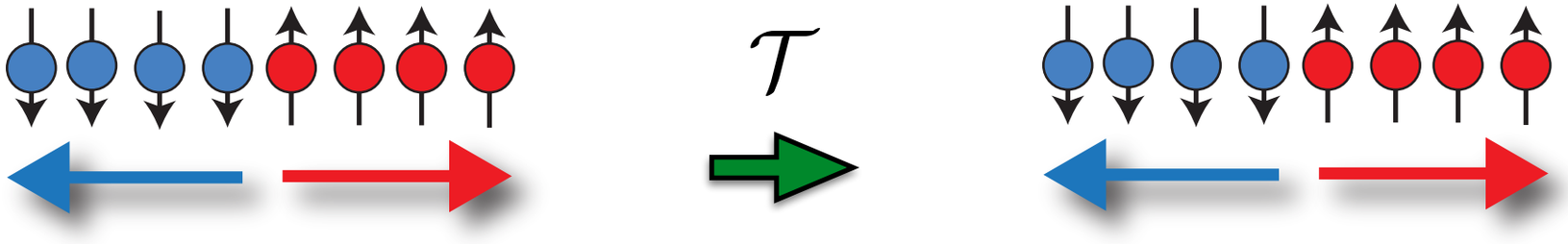
Pure spin currents:



Invariant under $\mathcal{T}$
(non-dissipative)

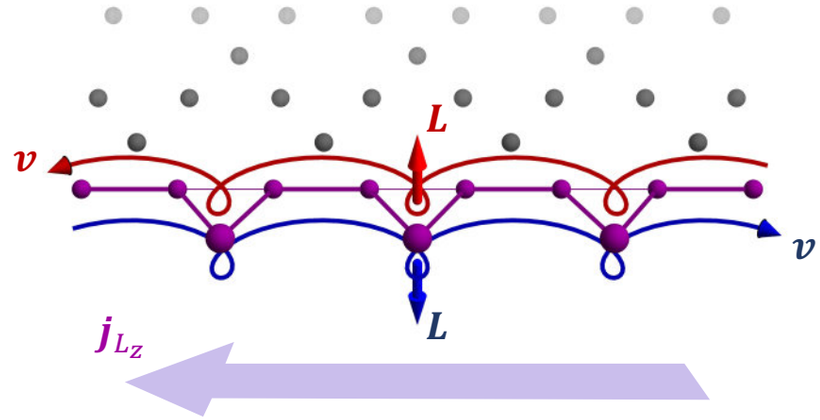
- May manifest in equilibrium (i.e. as ‘color’ diamagnetic currents induced by internal SO fields)
- Detectable (transport) spin currents can be induced electrically (see later)

Tokatly, PRL 101, 106601(2008)
Rashba, PRB 68, 241315(R) (2003)

1a. Spin and orbital currents

Pure orbital currents:

- OAM version of a spin current



Bush, PRR 5, 043052 (2023)

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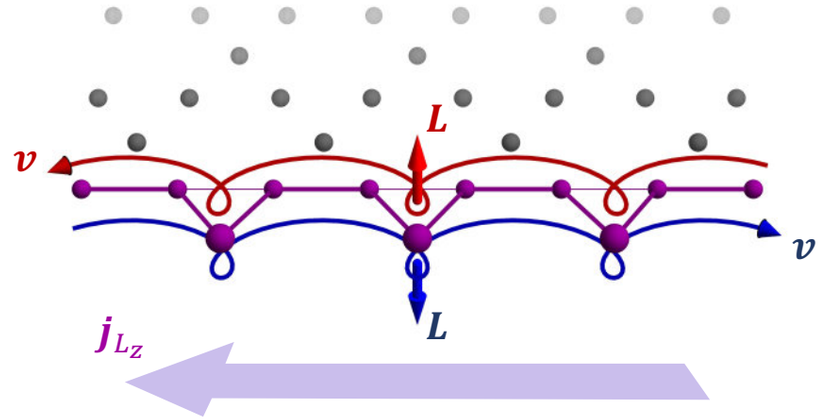
Pure orbital currents:

- OAM version of a spin current
- May exist even for s-electrons (modern description)



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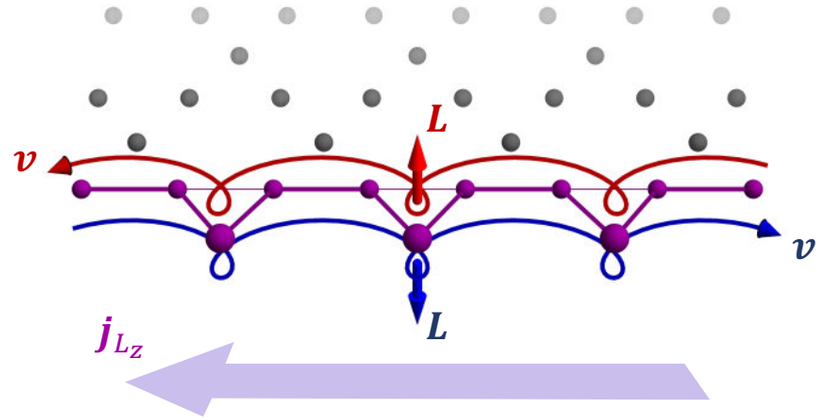

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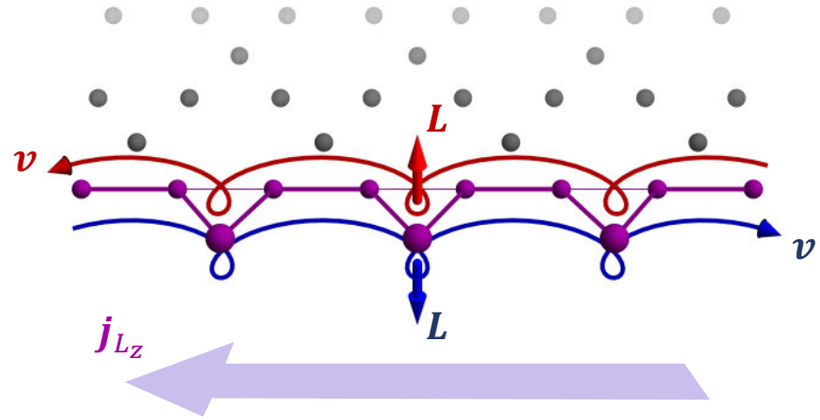

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SOC entangles spin and orbital degrees of freedom [$\hat{H}_{\mathrm{SO}} = \beta_{\mathrm{SO}} \hat{\mathbf{L}} \cdot \hat{\mathbf{s}}$] and thus allows for interconversion between spin and orbital currents, which is key for spintronic devices.

Tanaka, PRB 77, 165117 (2008); Jo, PRB 98, 214405 (2018)

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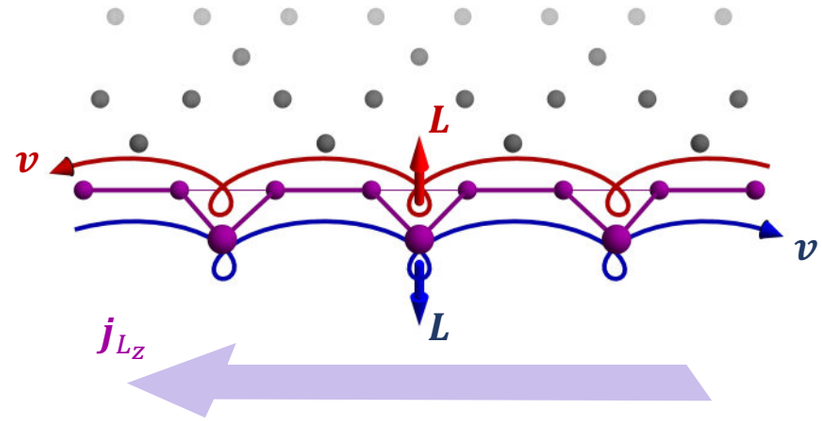

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➡ The description of non-equilibrium OAM presents interesting challenges and is currently an active topic of research

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Spin current operator

Conventional form: $$\hat{\mathbf{j}}_s^a = \frac{\hbar}{2}\,\hat{\mathbf{v}}\,\hat{s}^a$$

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Sanity check:

$$\mathcal{T}^{-1}\,\hat{\mathbf{j}}^a\,\mathcal{T} = \frac{\hbar}{2}\,(-\hat{\mathbf{v}})\,(-\hat{s}^a) = \hat{\mathbf{j}}^a$$

1a. Spin and orbital currents

Spin current operator

Conventional form: $\hat{\mathbf{j}}_s^a = \frac{\hbar}{2}\,\hat{\mathbf{v}}\,\hat{s}^a$

Sanity check:

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Note that in general $\hat{\mathbf{v}}\,\hat{s}^a \neq \hat{s}^a\,\hat{\mathbf{v}}$.

Solution: symmetrise $\hat{\mathbf{j}}_s^a$ according to $\hat{\mathbf{j}}_s^a = \frac{\hbar}{4}\,\{\hat{\mathbf{v}}, \hat{s}^a\}$ ⋯⋯▶ *anti-commutator*

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Orbital current operator

A simple, *intra-atomic* orbital current operator can be defined in an analogous fashion with $\hat{s}^a \to \hat{L}^a$, but there is another definition (modern description) as we will see later.

1a. Spin and orbital currents

Spin current operator

$\hat{\mathbf{j}}_s^a$ does not obey a continuity equation (spin is generally not conserved):

$$\frac{\partial s^a}{\partial t} + \nabla \cdot \mathbf{j}_s^a = \mathcal{T}^a$$

⇢ ***spin sink/source*** *term*
or 'torque density' usually due to SOC

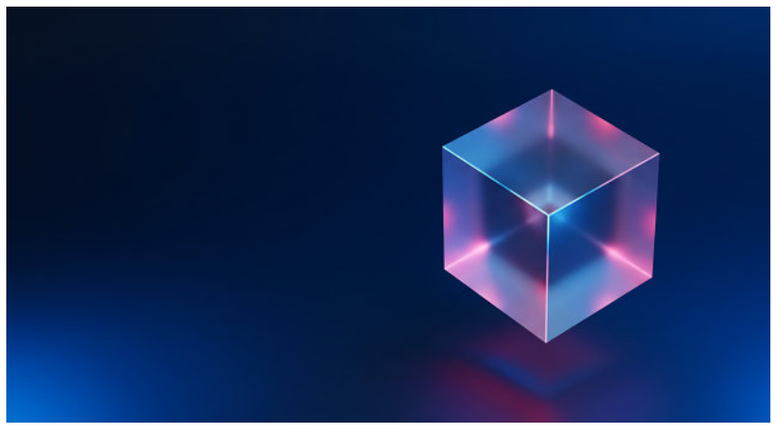
A conserving spin current can be defined, with some caveats [see Shi, PRL 96, 076604 (2006)]

Further reading: Rashba, PRB 68, 241315(R) (2003) | Tokatly, PRL 101, 106601(2008) | Droghetti PRB 105, 024409 (2022)

1b. Spin and orbital currents: role of symmetries

Which kinds of non-equilibrium effects can be realised in a crystal?

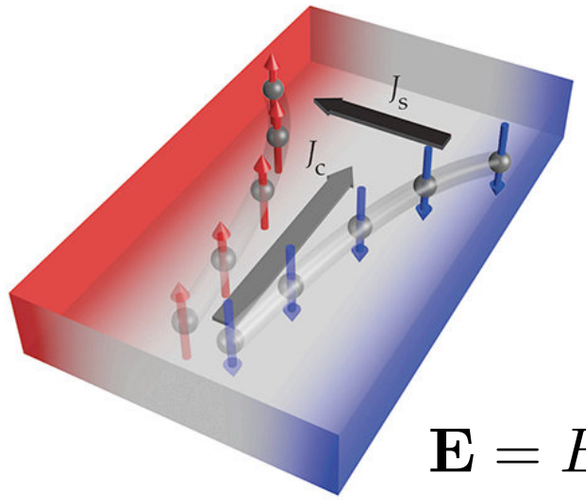
Use symmetries as a guiding principle!



(Recall lecture on symmetries.)

1b. **Spin current and spin density**: role of symmetries

Spin Hall effect (SHE)



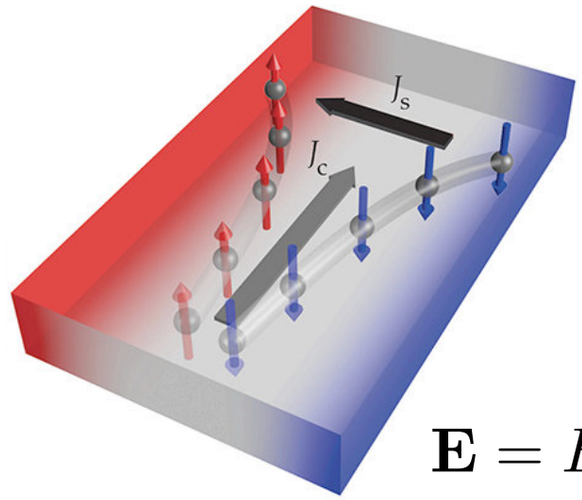
$$\mathbf{E} = E_x \mathbf{e}_x$$

1b. Spin current and spin density: role of symmetries

Spin Hall effect (SHE)

Consider a crystalline system with 3 perpendicular mirror planes

$$j^a_{s,j} = \sigma^a_{jx}\, E_x$$



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Under $x \to -x$, we have $E_x \to -E_x$. What about $\mathbf{j}^a_s$?

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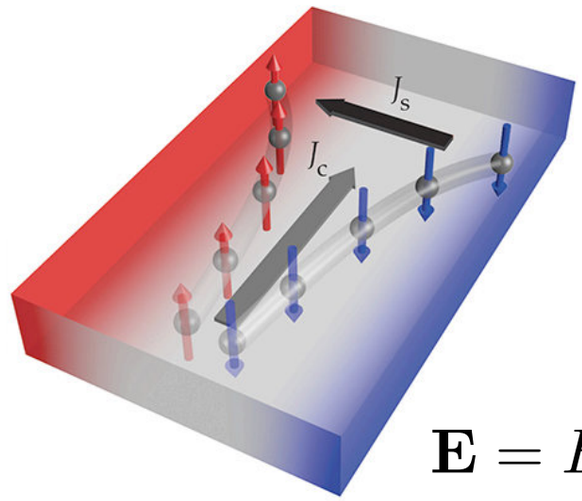

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Under $x \to -x$, we have $E_x \to -E_x$. What about $\mathbf{j}^a_s$?

Start with $\hat{j}^z_{s,x} \propto \hat{v}_x\, \hat{s}_z$

$$\hat{U}_x^{-1}\, \hat{s}_z\, \hat{U}_x = -\hat{s}_z \quad \text{and} \quad \hat{U}_x^{-1}\, \hat{v}_x\, \hat{U}_x = -\hat{v}_x \quad \Rightarrow \quad \hat{U}_x^{-1}\, \hat{j}^z_{s,x}\, \hat{U}_x = +\hat{j}^z_{s,x}$$

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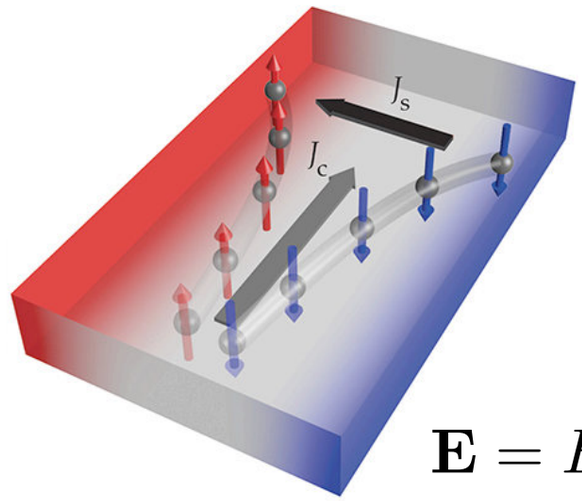

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$$j^z_{s,x} \to +\, j^z_{s,x}$$

$$E_x \to -\, E_x$$

1b. Spin current and spin density: role of symmetries

Spin Hall effect (SHE)

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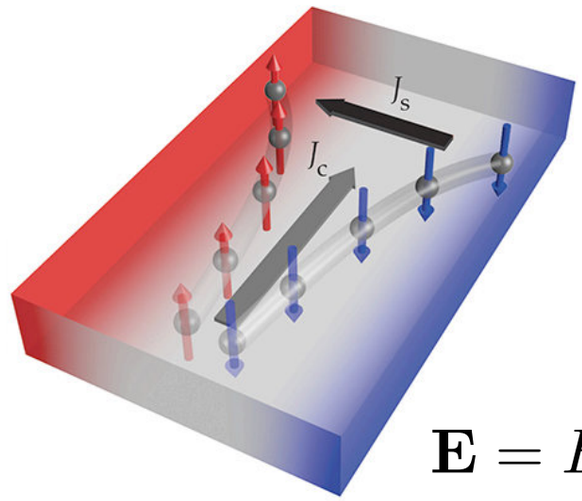

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$$j^z_{s,x} \to +j^z_{s,x}$$

$$E_x \to -E_x$$

$$j^z_{s,x} = \sigma^z_{xx}\, E_x$$

$$\downarrow \hat{U}_x$$

$$j^z_{s,x} = -\sigma^z_{xx}\, E_x$$

$$\sigma^z_{xx} = 0$$

xx-response is symmetry forbidden

1b. Spin current and spin density: role of symmetries

Symmetry ⇓ Op.⟹	$j^x_{s,x}$	$j^x_{s,y}$	$j^x_{s,z}$	$j^y_{s,x}$	$j^y_{s,y}$	$j^y_{s,z}$	$j^z_{s,x}$	$j^z_{s,y}$	$j^z_{s,z}$
$x \to -x$							$-$		
$y \to -y$							$-$		
$z \to -z$							$+$		
Allowed responses ⟹							✗		

$\pm$ = same (opposite) parity w.r.t E_x

1b. Spin current and spin density: role of symmetries

Symmetry ⇓ Op.⟹	$j^x_{s,x}$	$j^x_{s,y}$	$j^x_{s,z}$	$j^y_{s,x}$	$j^y_{s,y}$	$j^y_{s,z}$	$j^z_{s,x}$	$j^z_{s,y}$	$j^z_{s,z}$
$x \to -x$							$-$	$+$	
$y \to -y$							$-$	$+$	
$z \to -z$							$+$	$+$	
Allowed responses ⟹							✗	✓	

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1b. Spin current and spin density: role of symmetries

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$x \to -x$							$-$	$+$	$+$
$y \to -y$							$-$	$+$	$-$
$z \to -z$							$+$	$+$	$-$
Allowed responses ⟹							✗	✓	✗

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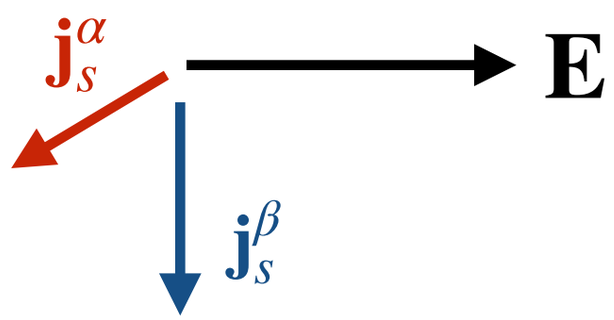
Symmetry ⇓ Op.⟹	$j^x_{s,x}$	$j^x_{s,y}$	$j^x_{s,z}$	$j^y_{s,x}$	$j^y_{s,y}$	$j^y_{s,z}$	$j^z_{s,x}$	$j^z_{s,y}$	$j^z_{s,z}$
$x \to -x$	$+$	$-$	$-$	$-$	$+$	$+$	$-$	$+$	$+$
$y \to -y$	$-$	$+$	$-$	$+$	$-$	$+$	$-$	$+$	$-$
$z \to -z$	$-$	$-$	$+$	$-$	$-$	$+$	$+$	$+$	$-$
Allowed responses ⟹	✗	✗	✗	✗	✗	✓	✗	✓	✗

$\pm$ = same (opposite) parity w.r.t E_x

$$j^a_{s,b} = \sigma_{\mathrm{sH}}\, \varepsilon_{abc}\, E_c\,, \qquad \sigma_{\mathrm{sH}} \equiv \sigma^z_{xy}$$

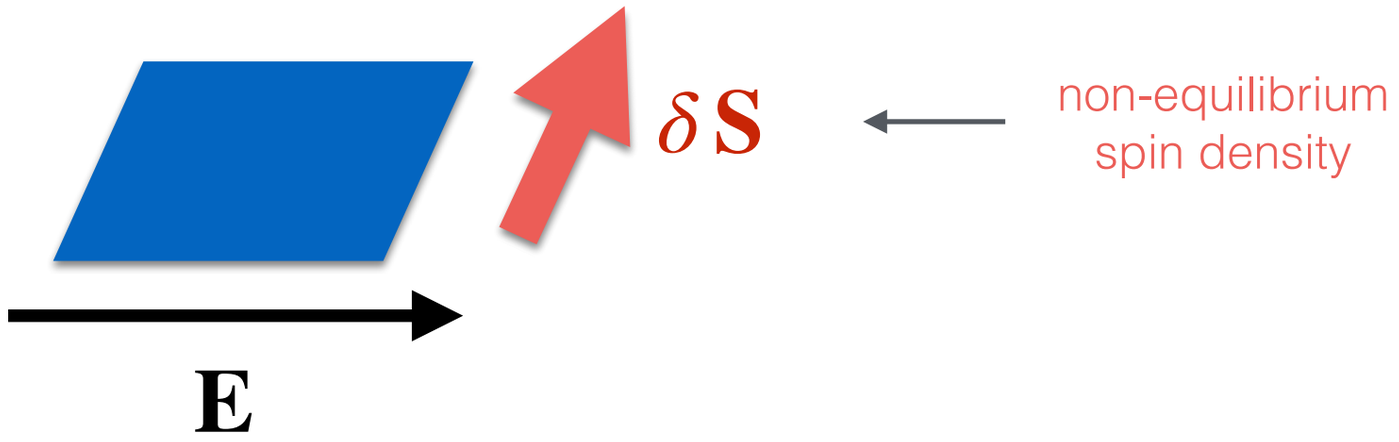


1b. Spin current and spin density: role of symmetries

Non-equilibrium spin polarisation

Inverse spin Galvanic effect (ISGE) also known as Edelstein effect

Broken spatial symmetries allow for the possibility that
an applied current may magnetise a non-magnetic material!



Let's see how this comes about!

1b. Spin current and spin density: role of symmetries

Non-equilibrium spin polarisation

Inverse spin Galvanic effect (ISGE)

Linear response: $S_i = K_{ij} E_j$

1b. Spin current and spin density: role of symmetries

Non-equilibrium spin polarisation

Inverse spin Galvanic effect (ISGE)

Linear response: $S_i = K_{ij} E_j$ First show that 3 mirror planes **=** no charge-spin response

$x \to -x$

$E_x \to -E_x$

Assume $\mathbf{E} = E\hat{\mathbf{x}}$

1b. Spin current and spin density: role of symmetries

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$x \to -x$ $\quad S_x \to S_x$ ✗

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1b. Spin current and spin density: role of symmetries

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$x \to -x$	$S_x \to S_x$	✗
$E_x \to -E_x$	$S_y \to -S_y$	$K_{xx} = 0$
	$S_z \to -S_z$	

1b. Spin current and spin density: role of symmetries

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$x \to -x$	$S_x \to S_x$ ✗	$K_{xx} = 0$
$E_x \to -E_x$	$S_y \to -S_y$	
	$S_z \to -S_z$	
$y \to -y$	$S_y \to S_y$	$K_{zx} = 0$
$E_x \to +E_x$	$S_z \to -S_z$ ✗	

1b. Spin current and spin density: role of symmetries

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Assume $\mathbf{E} = E\hat{\mathbf{x}}$

$x \to -x$ $E_x \to -E_x$	$S_x \to S_x$ ✗ $S_y \to -S_y$ $S_z \to -S_z$	$K_{xx} = 0$
$y \to -y$ $E_x \to +E_x$	$S_y \to S_y$ $S_z \to -S_z$ ✗	$K_{zx} = 0$
$z \to -z$ $E_x \to +E_x$	$S_y \to -S_y$ ✗	$K_{yx} = 0$

1b. Spin current and spin density: role of symmetries

Non-equilibrium spin polarisation

Inverse spin Galvanic effect (ISGE)

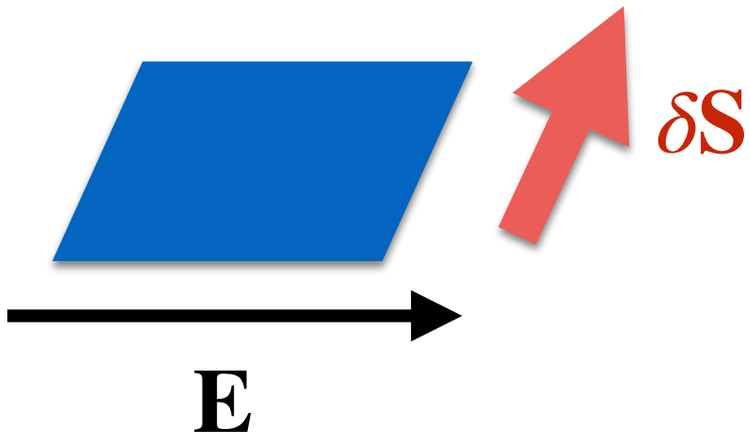
Linear response: $S_i = K_{ij} E_j$

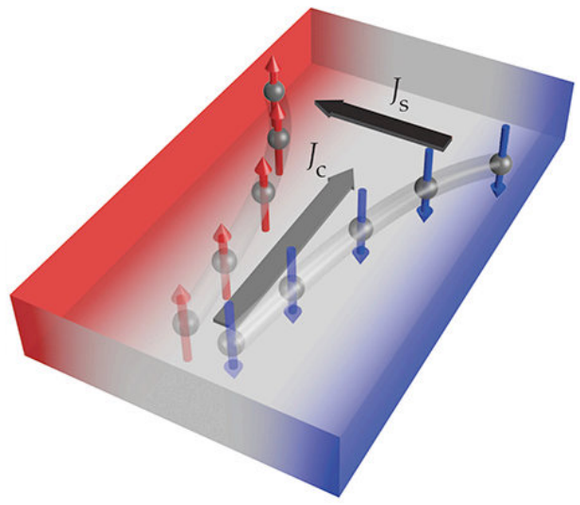
Assume $\mathbf{E} = E\hat{\mathbf{x}}$

$x \to -x$	$S_x \to S_x$ ✗	
$E_x \to -E_x$	$S_y \to -S_y$	$K_{xx} = 0$
	$S_z \to -S_z$	
$y \to -y$	$S_y \to S_y$	
$E_x \to +E_x$	$S_z \to -S_z$ ✗	$K_{zx} = 0$

If one mirror plane is broken, e.g. $z \to -z$,
a response, $S_y = K_{yx} E_x$, is now symmetry allowed!

1b. Spin current and spin density: role of symmetries





The two phenomena coexist when the symmetry is sufficiently low

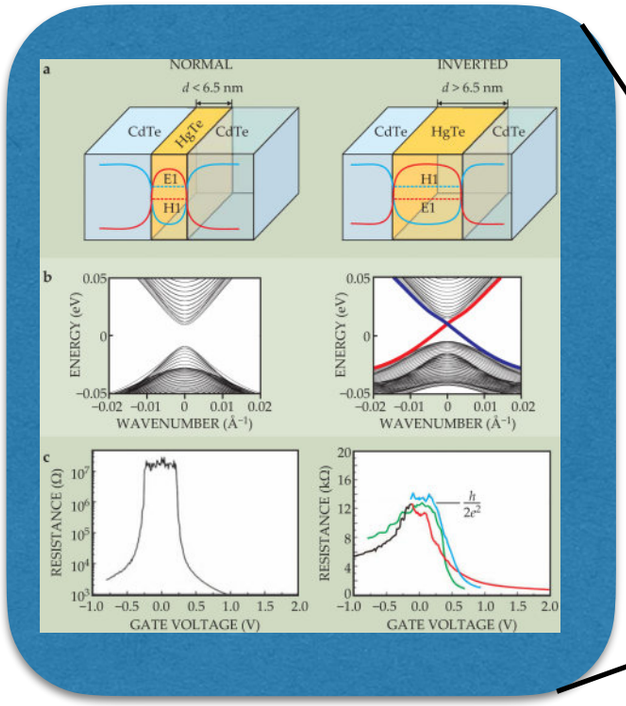
Microscopic mechanisms for both **SHE** and **ISGE** rely on **spin-orbit coupling**

2. Spin-orbit coupling & broken symmetries

$$V_{\mathrm{SO}} = \mathcal{B}(\mathbf{p}) \cdot \mathbf{s}$$

2. Spin-orbit coupling & broken symmetries

Z2 Topological Insulator



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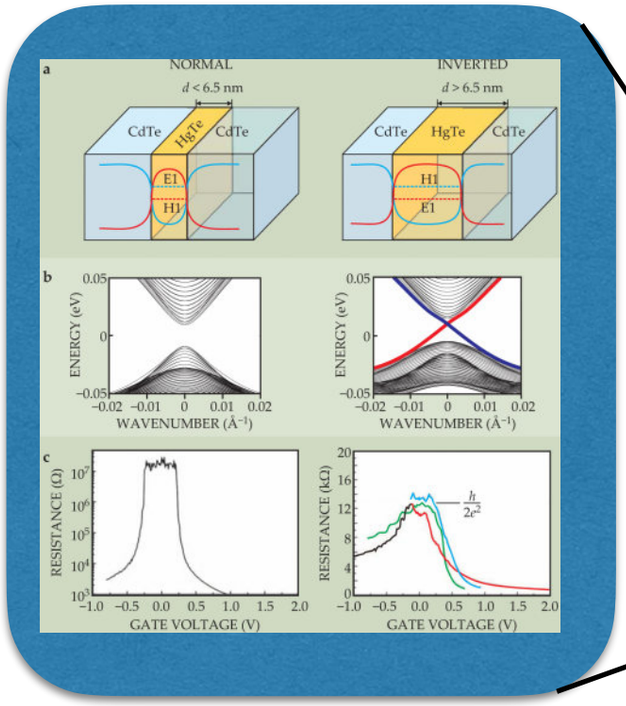
X.-L. Qi & S.-C. Zhang,
Phys. Today, 63, 33 (2010)

2. Spin-orbit coupling & broken symmetries

Z2 Topological Insulator



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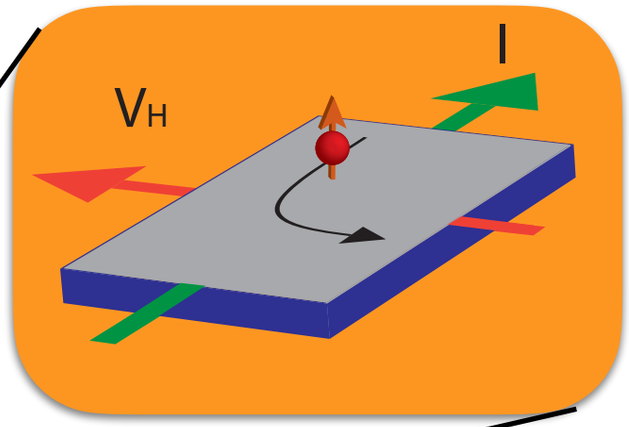
Spin/Anomalous Hall effects



J. Sinova *et al.*,
Rev. Mod. Phys. 87, 1213 (2015)

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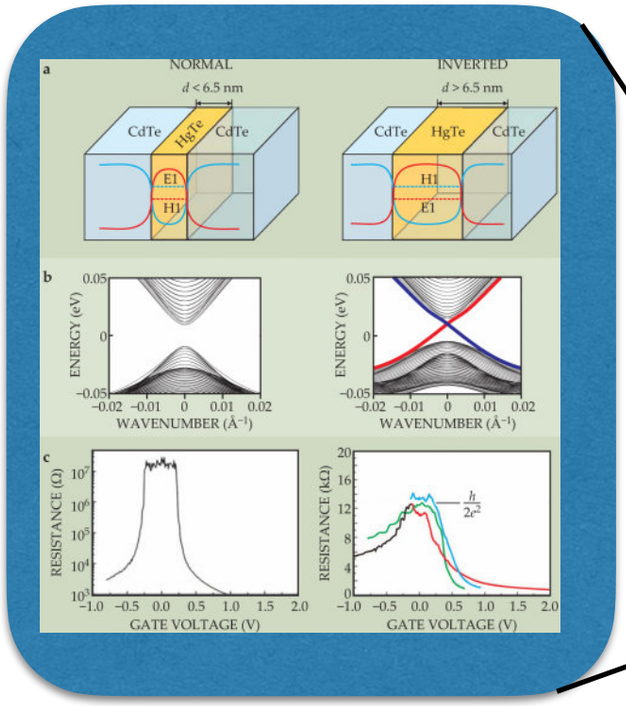

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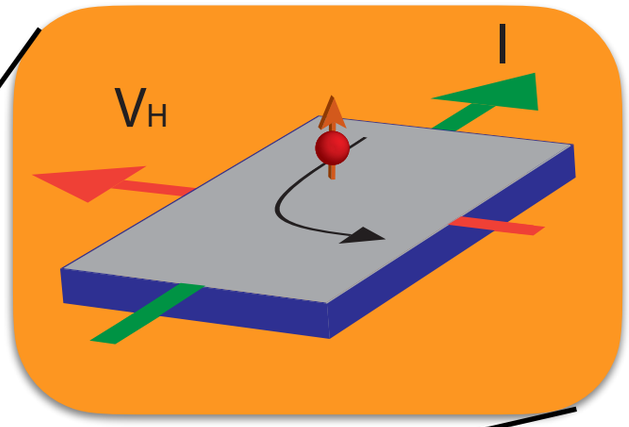
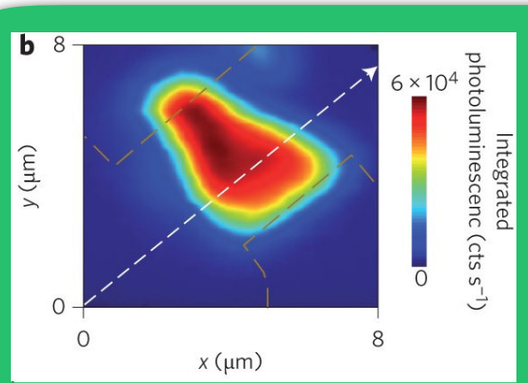
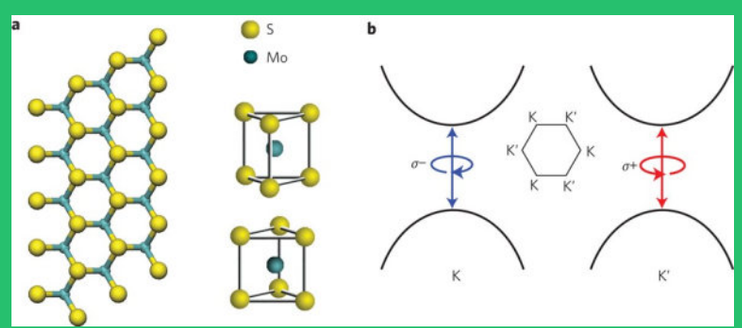
Spin/Anomalous Hall effects



J. Sinova *et al.*,
Rev. Mod. Phys. 87, 1213 (2015)

spin-valley effects in 2D semiconductors



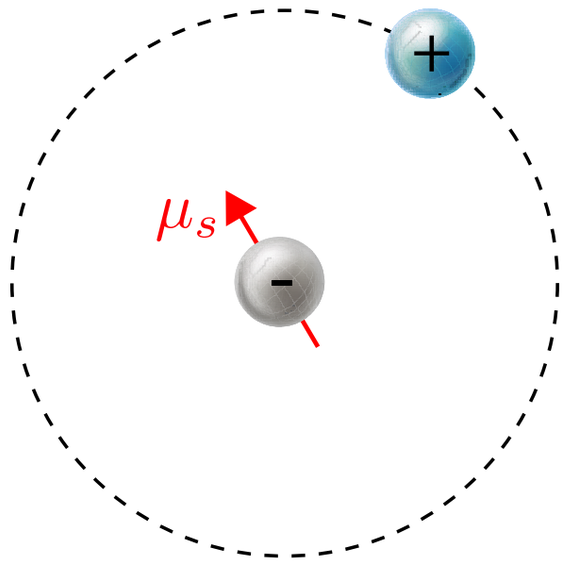


G. Wang *et al.*,
Rev. Mod. Phys. 90, 021001 (2018)

2. Spin-orbit coupling & broken symmetries

Revisiting atomic physics

➡ **Electron experiences a magnetic field in its rest frame**



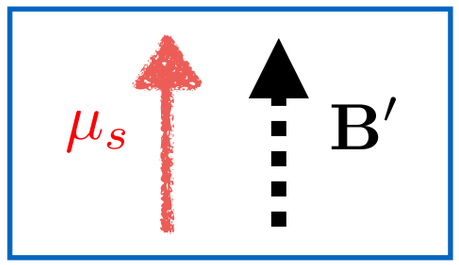
$$\mathbf{B}' \simeq -\frac{1}{c^2}\mathbf{v} \times \mathbf{E}$$

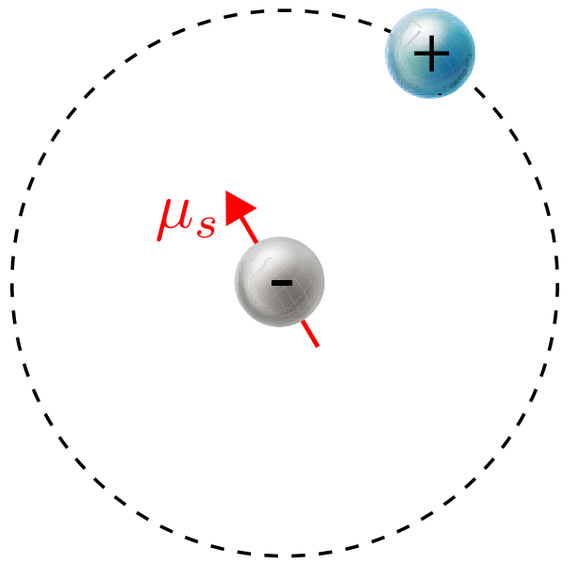
2. Spin-orbit coupling & broken symmetries

Revisiting atomic physics

➡ **Electron experiences a magnetic field in its rest frame**

$$H_{\mathrm{SO}} = -\boldsymbol{\mu}_s \cdot \mathbf{B}'$$





$$\mathbf{B}' \simeq -\frac{1}{c^2}\mathbf{v} \times \mathbf{E}$$

2. Spin-orbit coupling & broken symmetries

Revisiting atomic physics

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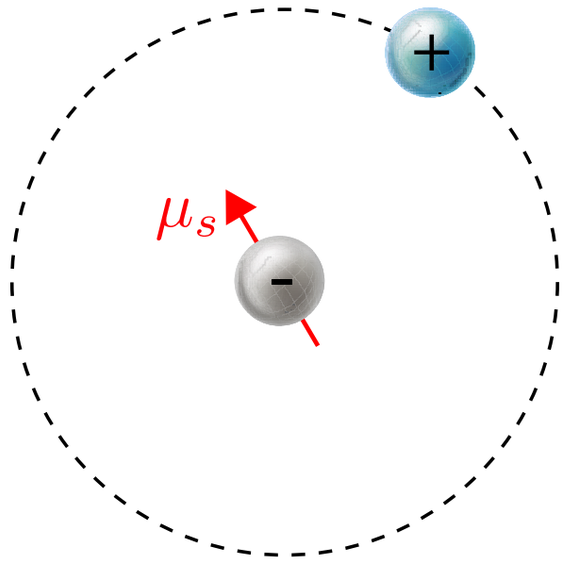
$$V_{\mathrm{SO}} = \frac{1}{2m^2c^2}(\nabla V \times \mathbf{p}) \cdot \mathbf{s}$$



- Even a H atom is affected by SOC (fine structure)
- SOC strength grows as $Z^\alpha\,, \quad 2 \lesssim \alpha \lesssim 4$

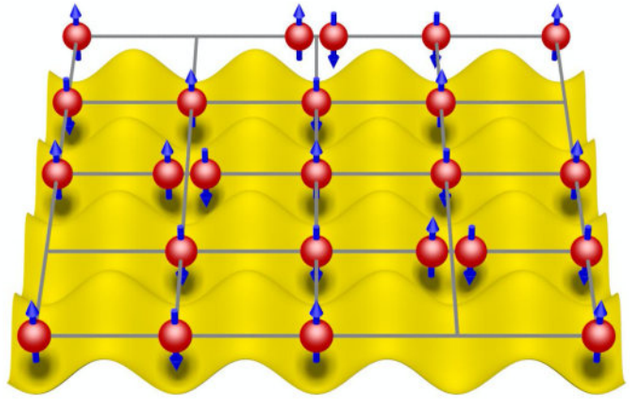
2. Spin-orbit coupling & broken symmetries

SOC in a crystal lattice

➡ **Symmetry-independent SOC**

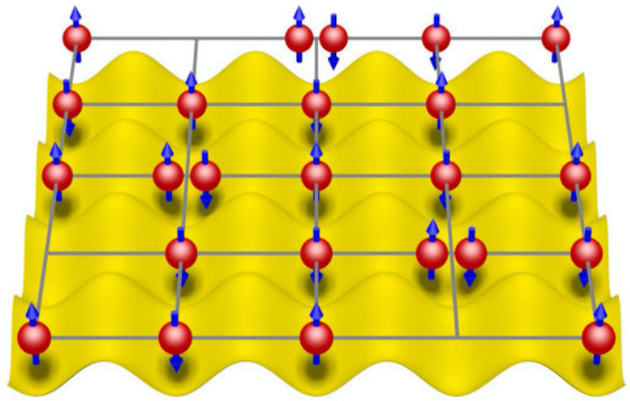
✳ **Exists in every crystal structure**

(stems from atomic SOC)



2. Spin-orbit coupling & broken symmetries

SOC in a crystal lattice



➡ **Symmetry-independent SOC**

✳ **Exists in every crystal structure**

(stems from atomic SOC)

$$H = \frac{p^2}{2m} + V(\mathbf{r}) + \frac{1}{2m^2c^2}\left(\boldsymbol{\nabla} V \times \mathbf{p}\right) \cdot \mathbf{s}$$

✳ **Bloch's theorem** $\psi_{n\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}\hat{u}_{n\mathbf{k}}(\mathbf{r})$

band index — plane wave — Bloch spinor

2. Spin-orbit coupling & broken symmetries

✳ **inversion symmetry**

$$E_{n,\uparrow}(\mathbf{k}) = E_{n,\uparrow}(-\mathbf{k})$$

✳ **time-reversal symmetry**

$$E_{n,\uparrow}(\mathbf{k}) = E_{n,\downarrow}(-\mathbf{k})$$

$$E_{n,\uparrow}(\mathbf{k}) = E_{n,\downarrow}(\mathbf{k})$$

Kramers degeneracy

2. Spin-orbit coupling & broken symmetries

✳ **inversion symmetry**

$$E_{n,\uparrow}(\mathbf{k}) = E_{n,\uparrow}(-\mathbf{k})$$

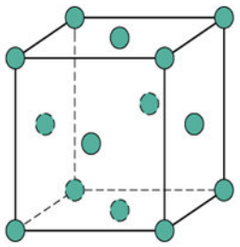
✳ **time-reversal symmetry**

$$E_{n,\uparrow}(\mathbf{k}) = E_{n,\downarrow}(-\mathbf{k})$$

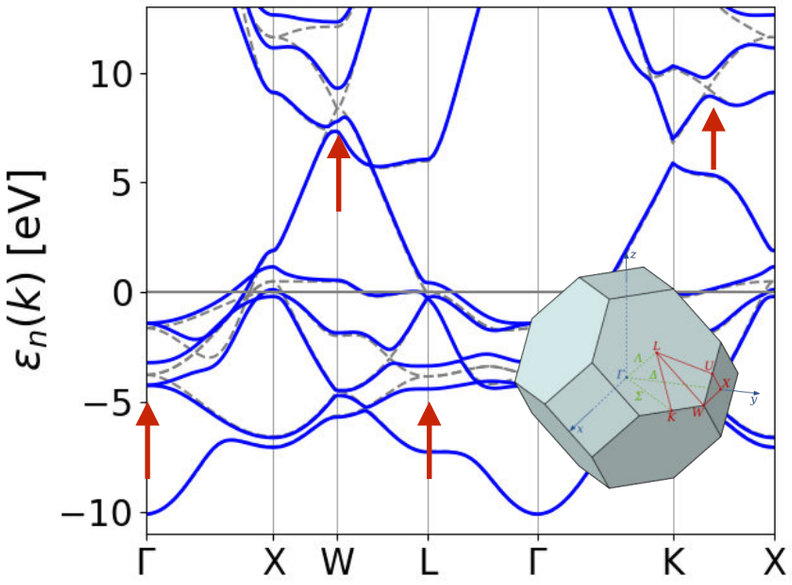
$$E_{n,\uparrow}(\mathbf{k}) = E_{n,\downarrow}(\mathbf{k})$$

Kramers degeneracy

- SOC lifts band degeneracies (orbital splitting)



Pt



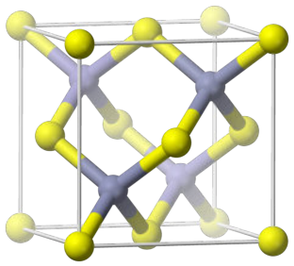
2. Spin-orbit coupling & broken symmetries

SOC in a crystal lattice

➡ **Symmetry-dependent SOC** $E_{n,\uparrow}(\mathbf{k}) \neq E_{n,\downarrow}(\mathbf{k})$

✳ Dresselhaus interaction (bulk inversion asymmetry)

G. Dresselhaus. ‘55



✳ Bychkov-Rashba interaction (structural inversion asymmetry @ surface/interface)

Y. A. Bychkov, E. I. Rashba, ‘84

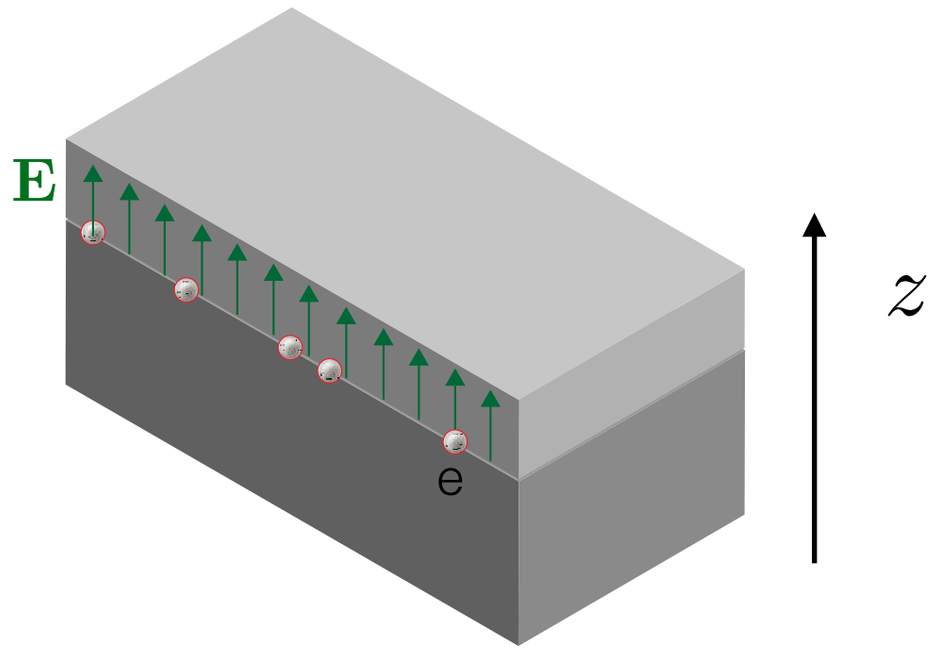
2. Spin-orbit coupling & broken symmetries

Symmetry breaking by an interface

➡ **The Rashba effect**

Non-relativistic band dispersion of a 2D electron gas:

$$\varepsilon_{\mathbf{k}} = \frac{\hbar^2 k^2}{2m^*}$$



2. Spin-orbit coupling & broken symmetries

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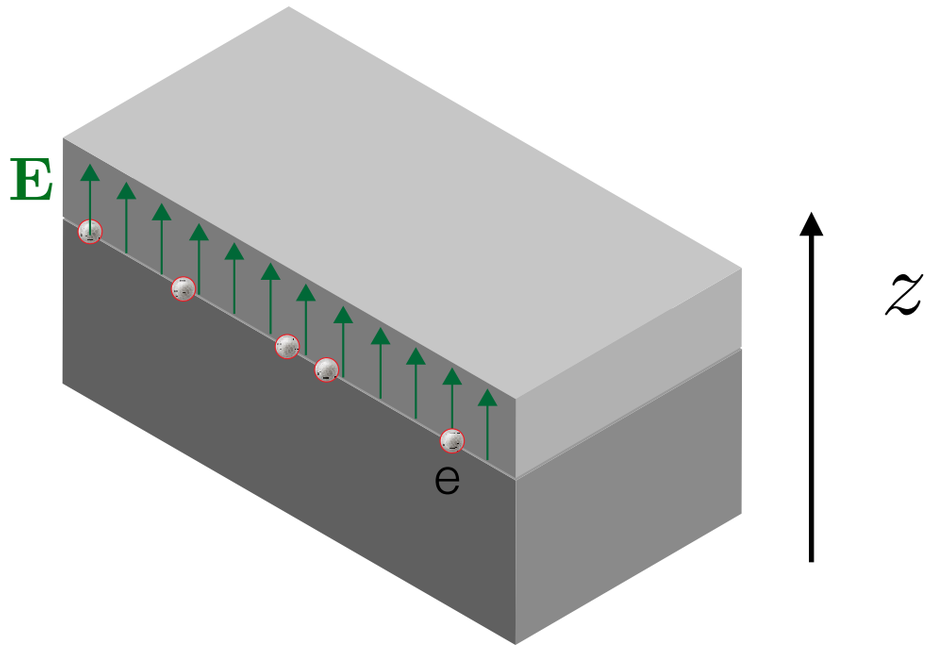
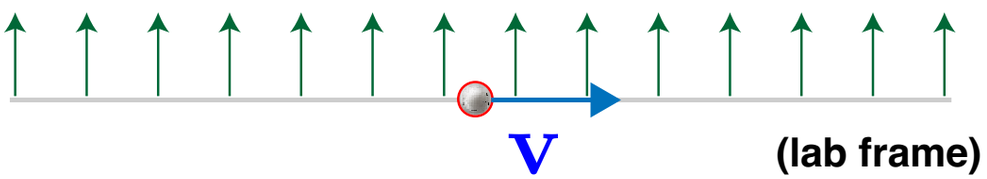
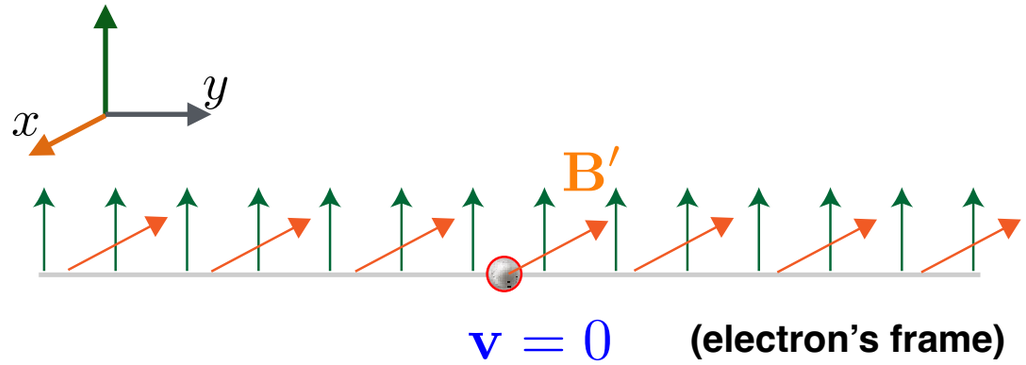


Relativist frame change:





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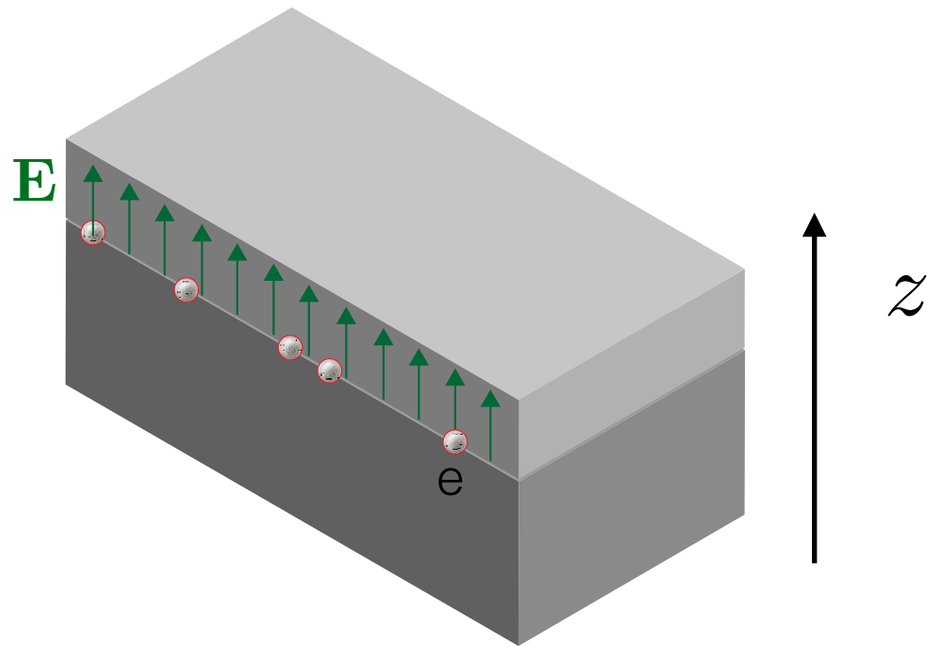

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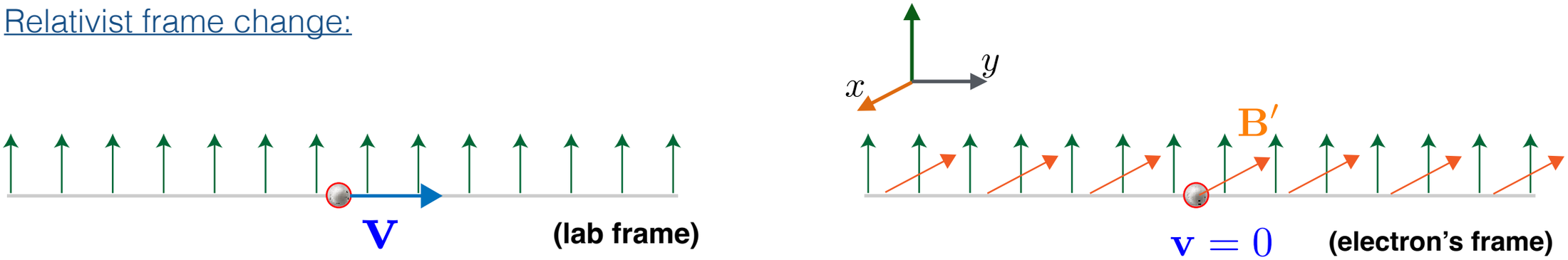

$$\mathbf{B}' \simeq -\frac{1}{c^2}\underbrace{(\hbar\,\mathbf{k}/m^*)}_{v_{\mathbf{k}}} \times (E_0\hat{\mathbf{z}}) \equiv v_{\mathrm{SO}}(-k_y, k_x, 0)$$

in-plane effective SO field

2. Spin-orbit coupling & broken symmetries

Symmetry breaking by an interface

➡ **The Rashba effect**

$$V_{\mathrm{SO}} = \Omega_{\mathrm{so}}(\mathbf{k}) \cdot \mathbf{s}$$

✳ **BR spin-orbit field**

$$\Omega_{\mathrm{BR}}(\mathbf{k}) = v_{\mathrm{SO}} \left(-k_y, k_x, 0\right)^T \perp \mathbf{k}$$

2. Spin-orbit coupling & broken symmetries

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2×2 matrix

$[H_{0\mathbf{k}}, V_{so}(\mathbf{k})] = 0$

Eigenvalues of V_{so}

$$\varepsilon_\alpha(\mathbf{k}) = \frac{\hbar^2 \mathbf{k}^2}{2m^*} + \varepsilon_{\mathrm{SO},\alpha}(\mathbf{k})$$

spin helicity quantum number, $\alpha = \pm$

2. Spin-orbit coupling & broken symmetries

Symmetry breaking by an interface

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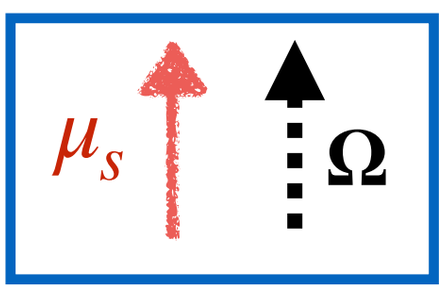

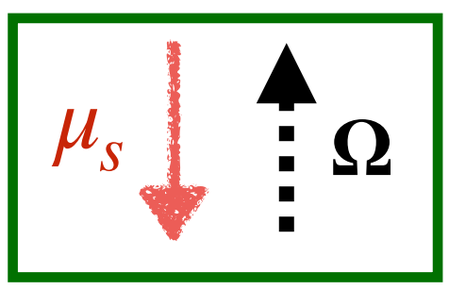

$$\varepsilon_{\mathrm{SO},-}(\mathbf{k}) = -|\boldsymbol{\Omega}_{\mathrm{SO}}(\mathbf{k})|$$

$$\varepsilon_{\mathrm{SO},+}(\mathbf{k}) = +|\boldsymbol{\Omega}_{\mathrm{SO}}(\mathbf{k})|$$

2. Spin-orbit coupling & broken symmetries

Symmetry breaking by an interface

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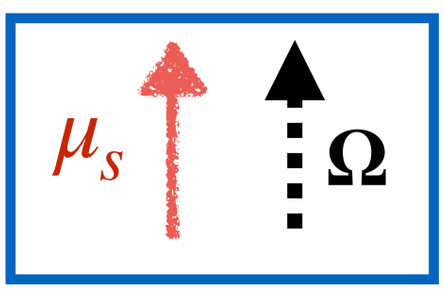

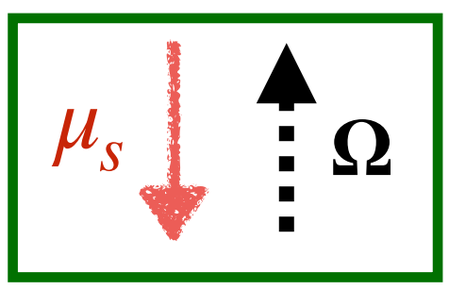

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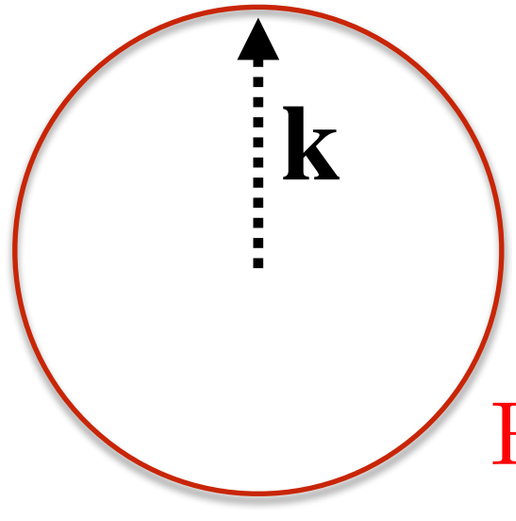

$\boldsymbol{\Omega}(\mathbf{k}) \perp \mathbf{k}$

2. Spin-orbit coupling & broken symmetries

Symmetry breaking by an interface

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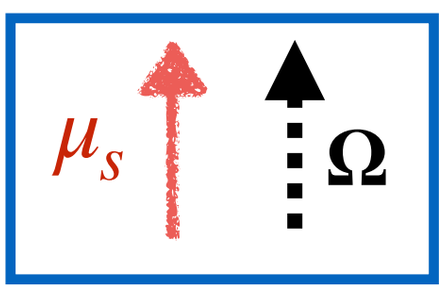

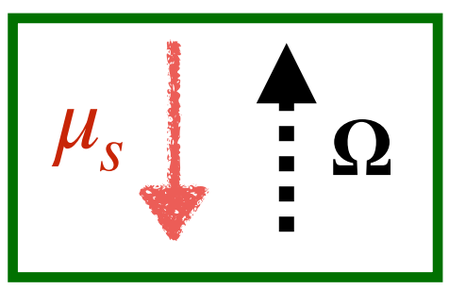

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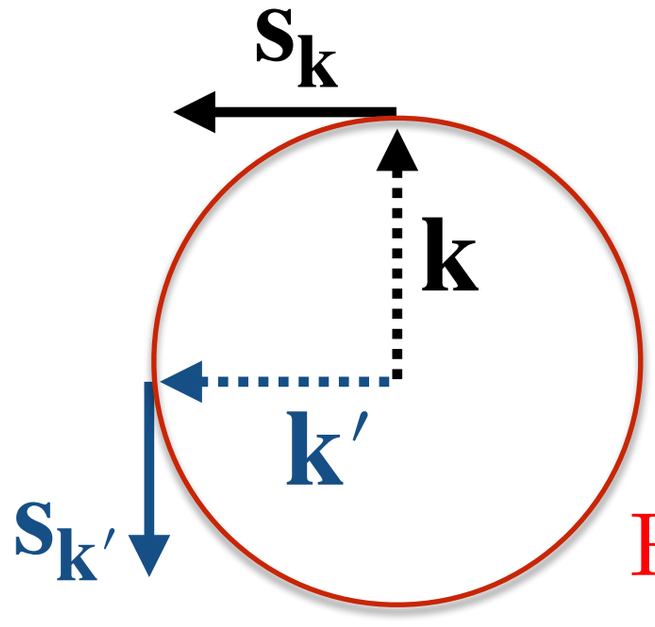

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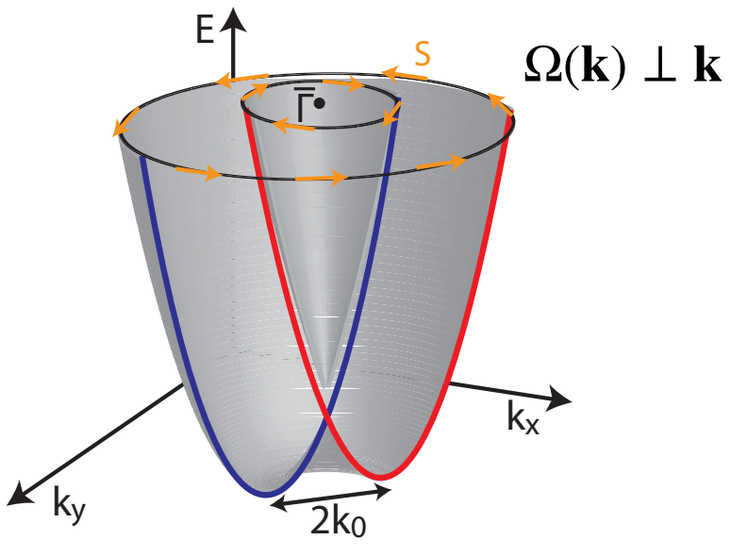

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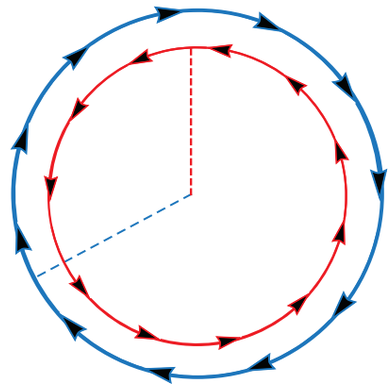


***k*-space spin texture**

$$\mathbf{s}_\alpha(\mathbf{k}) = \langle u_{\alpha\mathbf{k}} | \, \hat{\mathbf{s}} \, | u_{\alpha\mathbf{k}} \rangle$$

$\alpha = \pm$

spin-orbit entangled Fermi surface

2. Spin-orbit coupling & broken symmetries

Time reversal symmetry

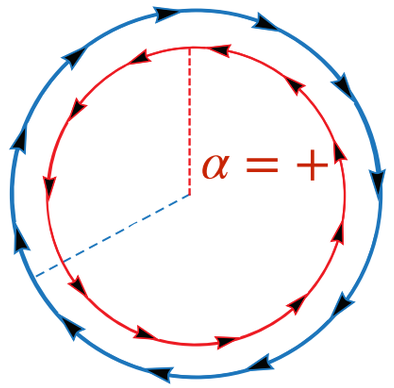
➡ **Anti-unitary symmetries**

Fermi-Dirac distribution function

$$\mathbf{S}_{\mathrm{e.q.}} = \mathrm{Tr}\left[\hat{\mathbf{s}}\,\hat{\rho}_{\mathrm{eq}}\right] = \sum_{\alpha,\mathbf{k}} f_{\alpha}(\mathbf{k})\,\mathbf{s}_{\alpha}(\mathbf{k}) = 0$$

single-electron picture

k-space Rashba spin texture



$$\mathbf{s}_{\alpha}(\mathbf{k}) = -\mathbf{s}_{\alpha}(-\mathbf{k})$$

2. Spin-orbit coupling & broken symmetries

Time reversal symmetry

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Fermi-Dirac distribution function

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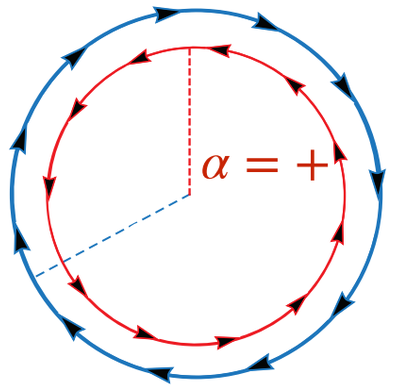


$$\mathbf{s}_\alpha(\mathbf{k}) = -\mathbf{s}_\alpha(-\mathbf{k})$$

This holds in general for a TR-invariant system:

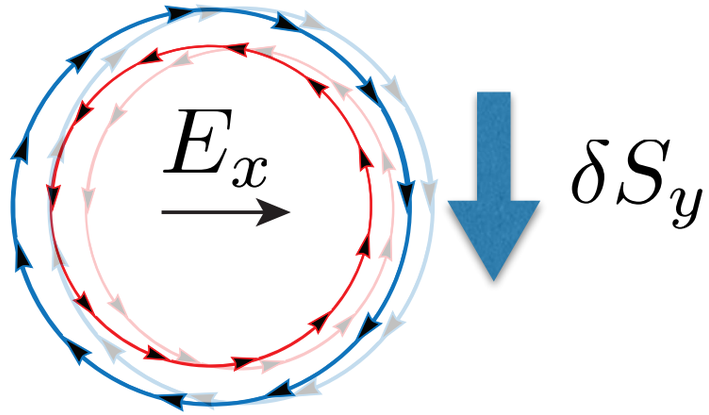
$$\mathcal{T}^{-1}\hat{\mathbf{s}}\,\mathcal{T} = -\hat{\mathbf{s}} \quad \Rightarrow \quad \mathbf{S}_{\mathrm{e.q.}} = 0$$

2. Spin-orbit coupling & broken symmetries

Out-of-equilibrium physics are different!

Under an applied current, $\mathscr{T}$ is effectively broken:

$$\delta\mathbf{S} = \mathrm{Tr}\left[\hat{\mathbf{s}}\,\hat{\rho}_{\mathrm{ne}}\right] \neq 0$$



2. Spin-orbit coupling & broken symmetries

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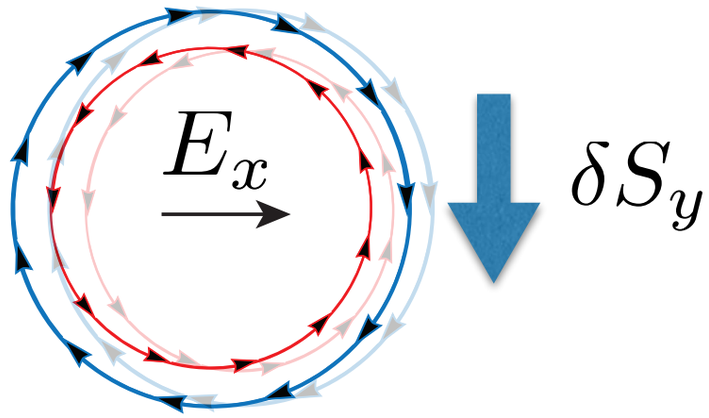


We saw earlier that the transverse spin-charge response is symmetry allowed,
but what about the underlying microscopic mechanism?

Broken $z \to -z$ symmetry

$$\delta S_y = K_{yx}\, E_x$$

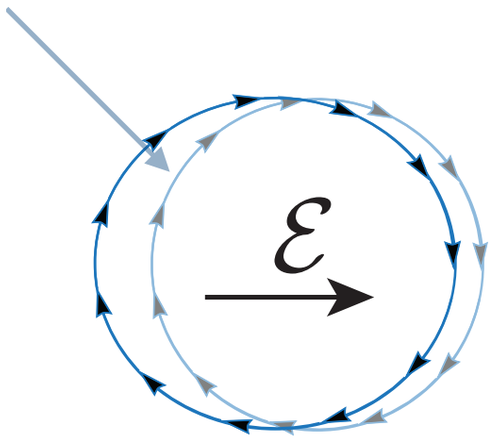
Inverse spin-galvanic effect (ISGE)

2. Spin-orbit coupling & broken symmetries

ISGE: *microscopic mechanism picture*

Simple semiclassical analysis: $\delta f_{\mathbf{k}} \sim \cos(\theta_{\mathbf{k}})\tau_{||}$

Isolated one sub-band
(i.e. ignore inter-band processes)



2. Spin-orbit coupling & broken symmetries

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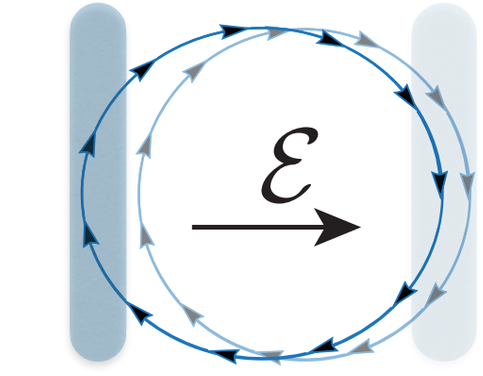

$\delta f > 0$ $\delta f < 0$

$\mathbf{J}$

2. Spin-orbit coupling & broken symmetries

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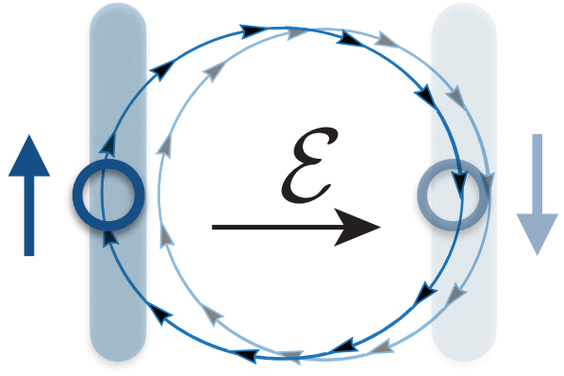

$\delta f > 0$ $\delta f < 0$

$\mathbf{J}$

$$\delta\mathbf{S} = \sum_{\alpha,\mathbf{k}} \delta f_{\alpha\mathbf{k}} \langle \mathbf{s} \rangle_{\alpha\mathbf{k}} \neq 0 \quad (*)$$

S_y component:

$\{\mathbf{k}, -\mathbf{k}\}$ contributions no longer cancel out!

(*) The two sub-bands give opposite-in-sign contributions with $|\delta\mathbf{S}_+| > |\delta\mathbf{S}_-|$ due to $k_{F+} > k_{F-}$.

2. Spin-orbit coupling & broken symmetries

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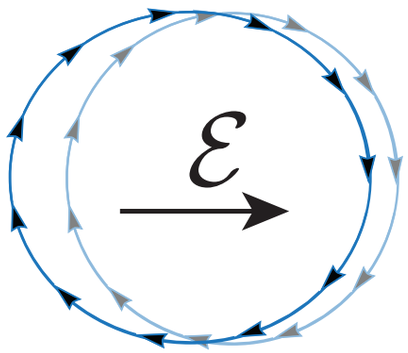


spin-momentum locking

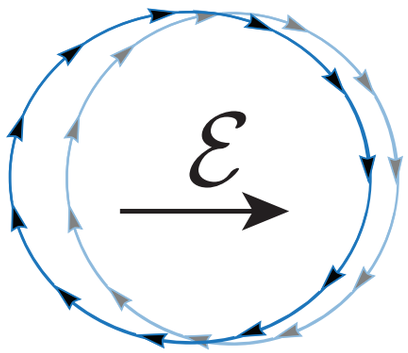
$$\mathbf{k} \perp \mathbf{s}(\mathbf{k}) \Rightarrow \mathbf{J} \perp \mathbf{S}$$

$$\langle S_y \rangle_{\mathcal{E}} \neq 0$$

2. Spin-orbit coupling & broken symmetries

ISGE: *microscopic mechanism picture*

Simple semiclassical analysis: $\delta f_{\mathbf{k}} \sim \cos(\theta_{\mathbf{k}})\tau_{\|}$



spin-momentum locking

$$\mathbf{k} \perp \mathbf{s}(\mathbf{k}) \Rightarrow \mathbf{J} \perp \mathbf{S}$$

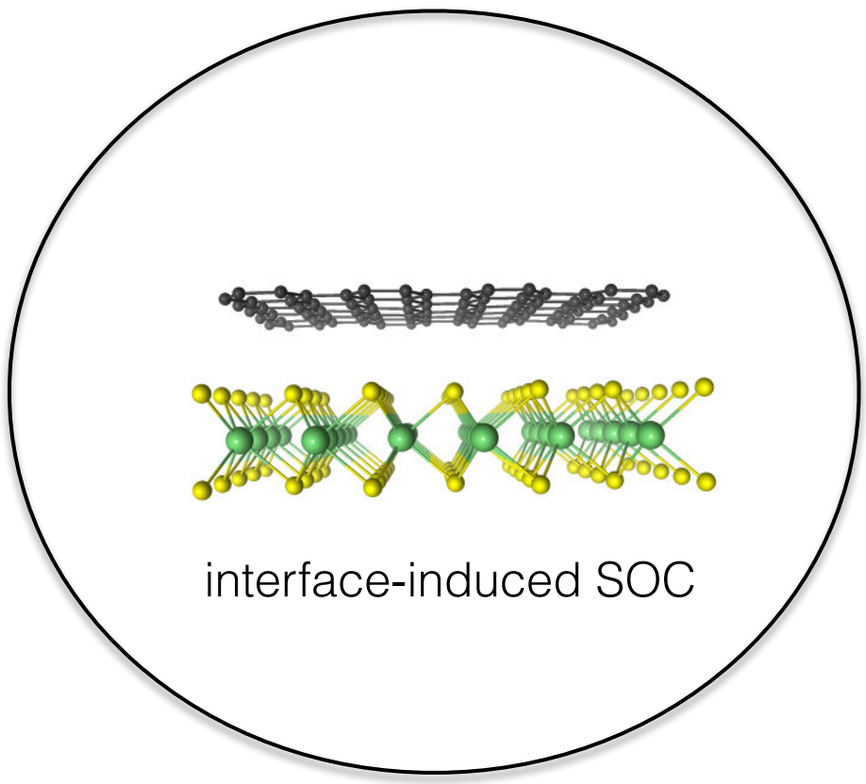
$$\langle S_y \rangle_{\mathcal{E}} \neq 0$$

Efficiency of the charge-to-spin conversion process is sensitive to band structure details…
Choice of correct materials is paramount!

2. Spin-orbit coupling & broken symmetries

ISGE in 2D van der Waals materials

$\bar{\lambda}_{\mathrm{SO}} \sim 5 - 15$ meV



interface-induced SOC

broken $z \rightarrow -z$ symmetry

C_{3v} point group
for aligned layers

Avsar et al. Nat. Comm. 5, 4875 (2014)

Gmitra & Fabian. PRB 92, 155403 (2015)

Island et al. Nature 571, 85 (2019)

Benitez et al. Nat. Mat. 19, 170 (2020)

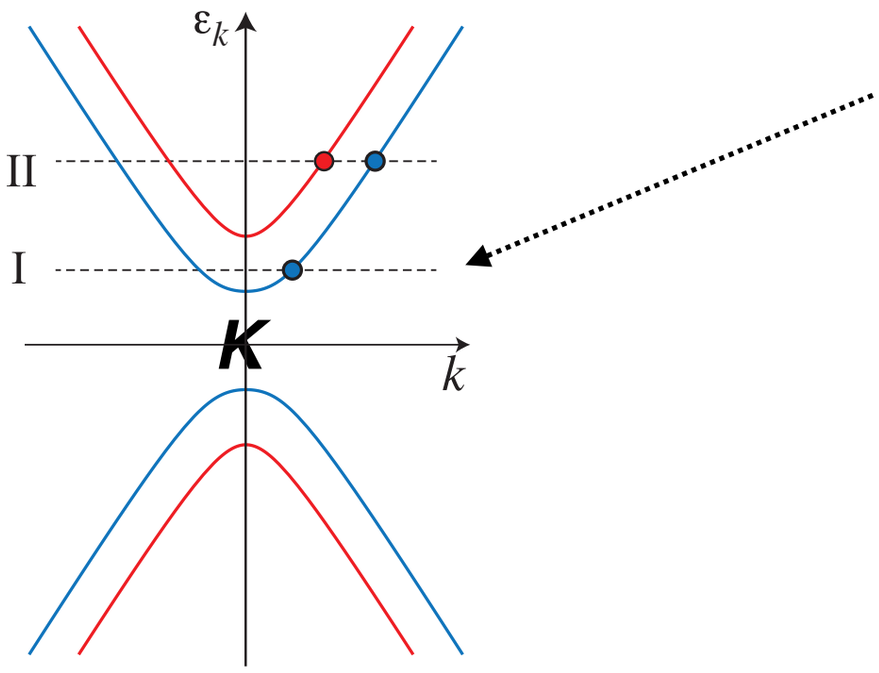
Sun et al. Nat. Comm. 14, 3771 (2023)

Rao et al. Nat. Comm. 14, 6124 (2023)

2. Spin-orbit coupling & broken symmetries

ISGE in 2D van der Waals materials

spin-split Dirac states with tilted Rashba spin textures



At sufficiently low Fermi energies,
only spins with $\alpha = +1$ *contribute to the ISGE*

$$\delta\mathbf{S} = \sum_{\mathbf{k}} f_+(\mathbf{k})\,\mathbf{s}_+(\mathbf{k})$$

Offidani *et al*. Phys. Rev. Lett. 119, 196801 (2017)

Milletari *et al*. Phys. Rev. Lett. 119, 246801 (2017)

2. Spin-orbit coupling & broken symmetries

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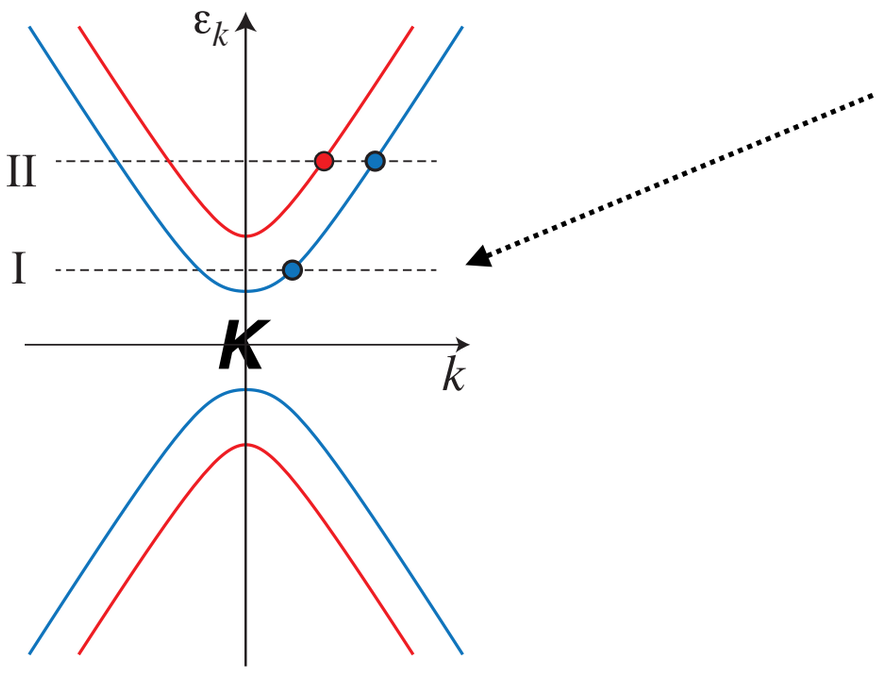

Offidani *et al.* Phys. Rev. Lett. 119, 196801 (2017)

Milletari *et al.* Phys. Rev. Lett. 119, 246801 (2017)

At sufficiently low Fermi energies,
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$$\delta\mathbf{S} = \sum_{\mathbf{k}} f_+(\mathbf{k})\, \mathbf{s}_+(\mathbf{k})$$

Maximum charge-to-spin conversion efficiency

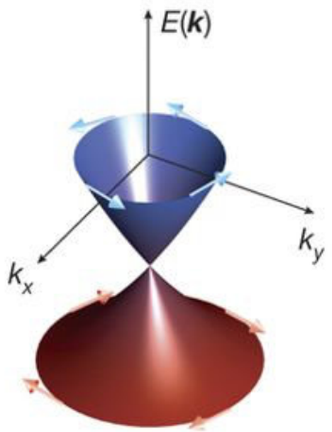
$$\langle S_y \rangle_{\mathcal{E}} = \pm \frac{1}{2v} \langle J_x \rangle_{\mathcal{E}}$$

Regime I: **full spin-charge locking**

2. Spin-orbit coupling & broken symmetries

Spin-helical fermions: TIs *vs* van der Waals

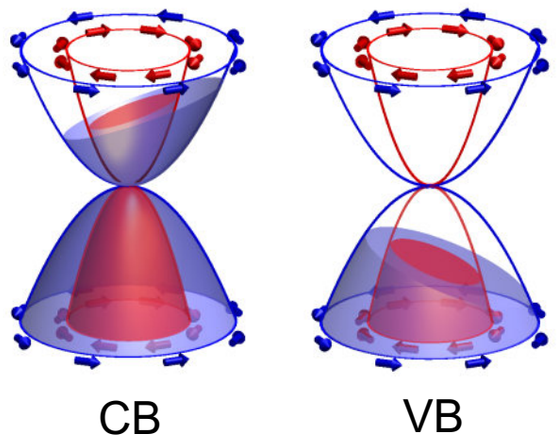
A.S. *et al.* Nature 539, 509 (2016) K. Kondou *et al,* Nat. Phys. 12 (2016)



Helical 2D fermions
(surface of a 3D TI)

- ✳ **Fermi level fixed**
- ✳ **SGE has fixed sign for e/h carriers**

Offidani *et al.* PRL 119, 196801 (2017) Benitez *et al.* Nat. Mat. (19, 170, 2020)



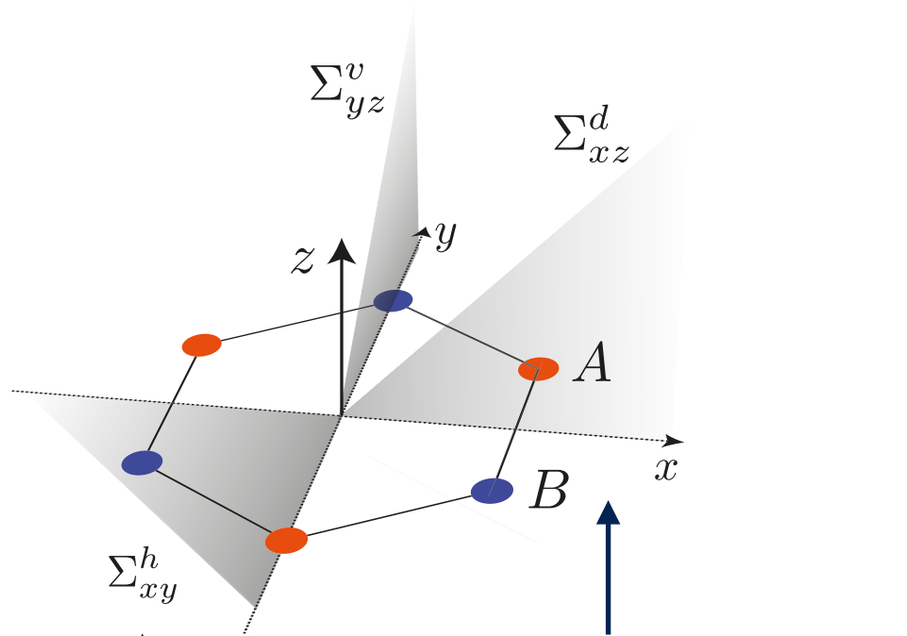
Helical 2D fermions
(vDW heterostructures)

- ✳ **Fermi level can be tuned**
- ✳ **spin ambipolar effect**

2. Spin-orbit coupling & broken symmetries

Breaking the last mirror plane: *twisting spin textures*

Consider a honeycomb layer (2D hexagonal system):



$y \to -y$ (broken)

$z \to -z$ (broken)

proximity effect

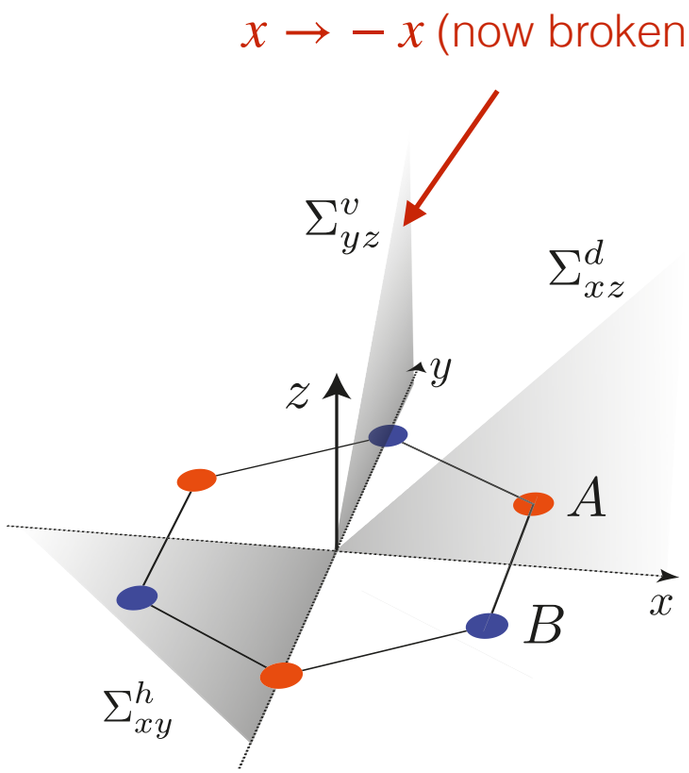
graphene/TMD bilayer

Perkins & Ferreira. Encyclopedia of CMP, 2nd Ed. (2024)

2. Spin-orbit coupling & broken symmetries

Breaking the last mirror plane: *twisting spin textures*

Consider a honeycomb layer (2D hexagonal system):



C_{6v}

↓ *Broken A/B sublattice symmetry*

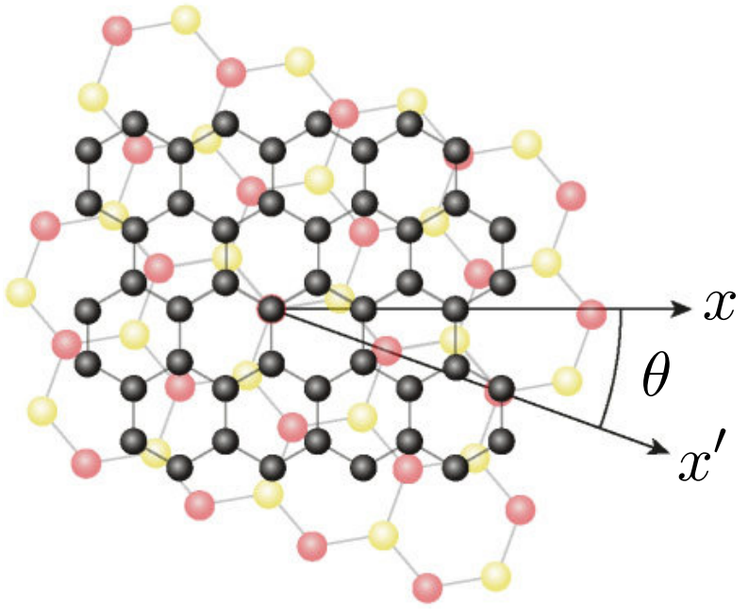
$C_{3v} \to C_3$

Broken $x \to -x$ reflection

Perkins & Ferreira. Encyclopedia of CMP, 2nd Ed. (2024)

2. Spin-orbit coupling & broken symmetries

Breaking the last mirror plane: ***twisting spin textures***



Perkins & Ferreira. Encyclopedia of CMP, 2nd Ed. (2024)

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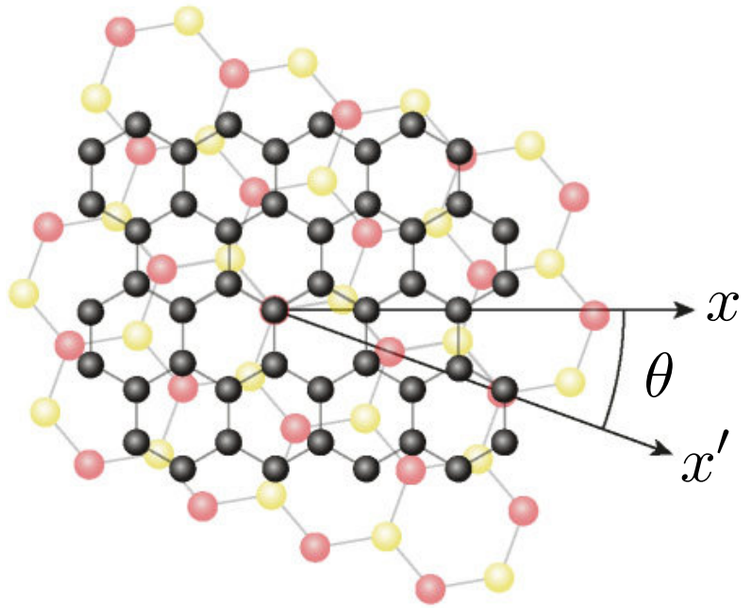


$$S_x = K^{\mathrm{sc}}_{xx}\, E_x$$

mirror reflection Σ^v_{yz}: $x \to -x$

$$K^{\mathrm{sc}}_{xx}\big|_{C_{3v}} = 0$$

Σ^v_{yz}

twisting

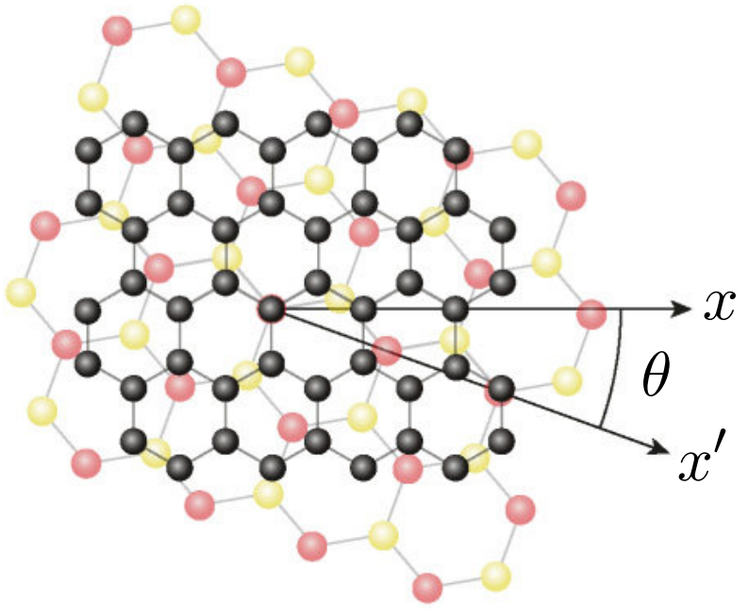
$$K^{\mathrm{sc}}_{xx}\big|_{C_3} \neq 0$$

Collinear Edelstein effect

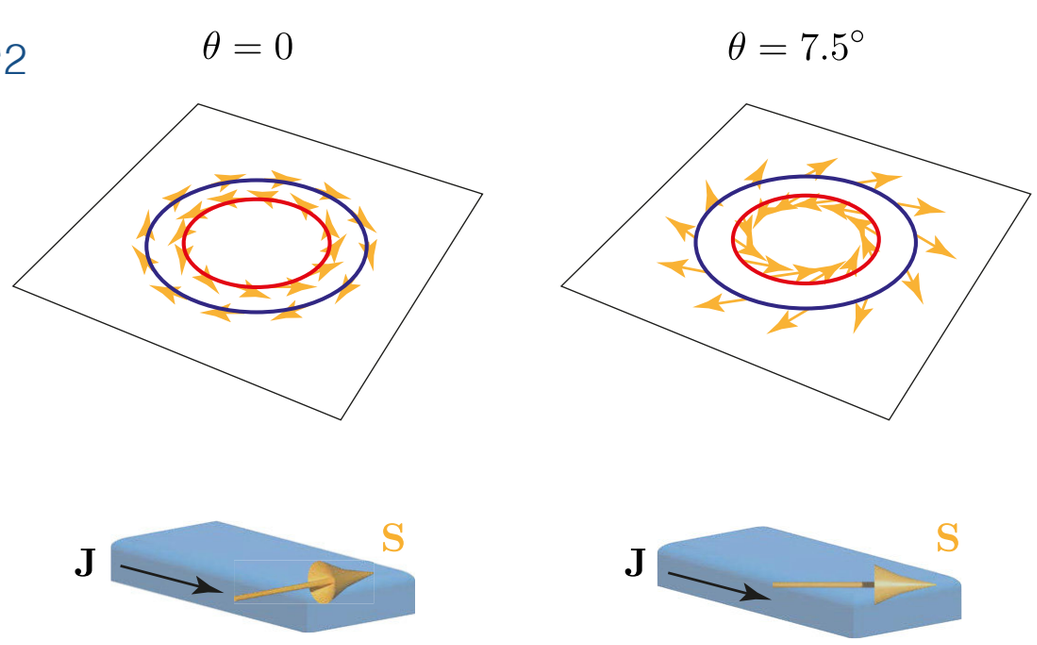
Perkins & Ferreira. Encyclopedia of CMP, 2nd Ed. (2024)

2. Spin-orbit coupling & broken symmetries

Breaking the last mirror plane: ***twisting spin textures***



G/WSe2



Standard ISGE

Li & Koshino *et al.* Phys. Rev. B 99, 075438 (2019)

A. David *et al.* Phys. Rev. B 100, 085412 (2019)

T. Namier *et al.* Phys. Rev. B 104, 195156 (2021)

Veneri *et al.* Phys. Rev. B 106, L081406 (2022)

2. Spin-orbit coupling & broken symmetries

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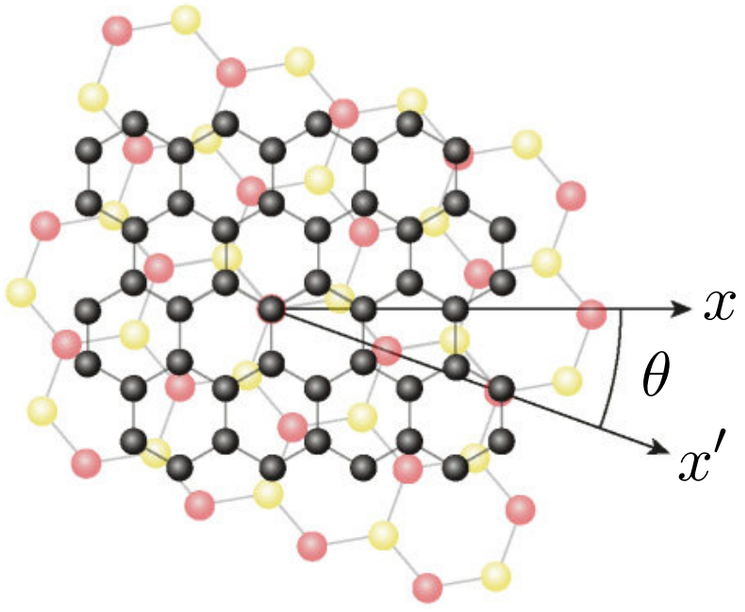
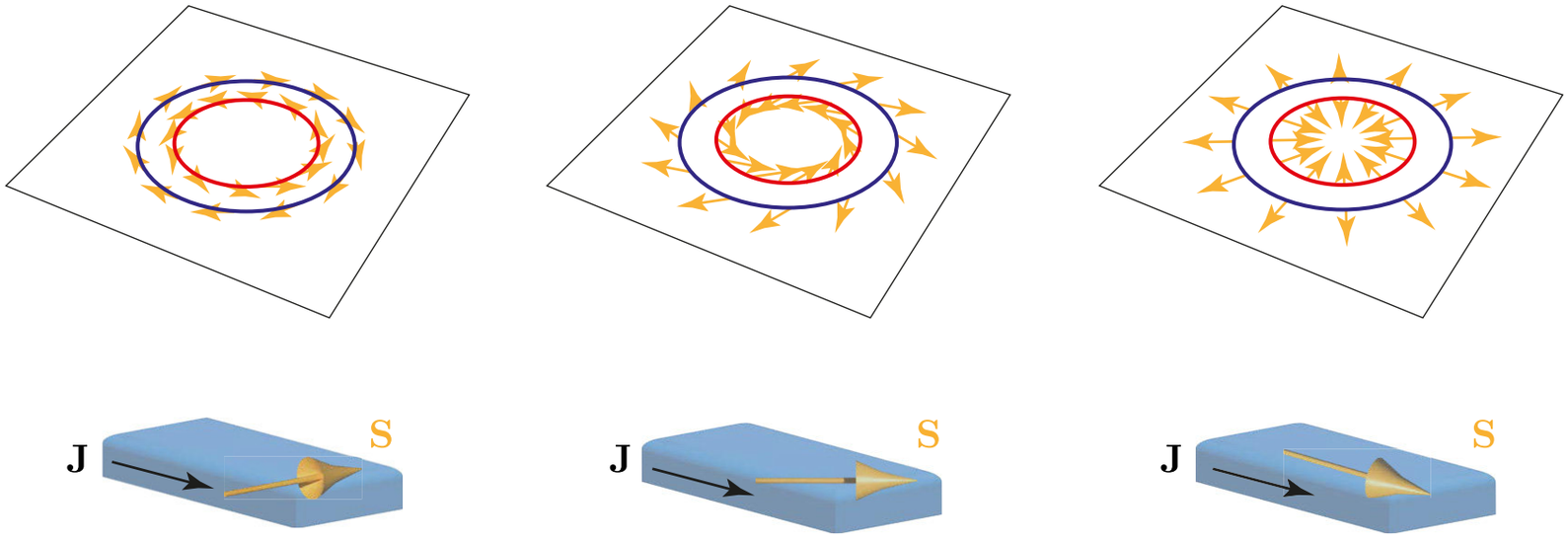


G/WSe_2

$\theta = 0$

$\theta = 7.5°$

$\theta = 13.9°$



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3a. Spin-orbit relaxation

Due to SOC and other spin-dependent effects:

$$\frac{d\hat{s}_a}{dt} = \frac{i}{\hbar}\left[\hat{s}_a, \hat{H}\right] \neq 0$$

Spin non-conservation

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Spin non-conservation

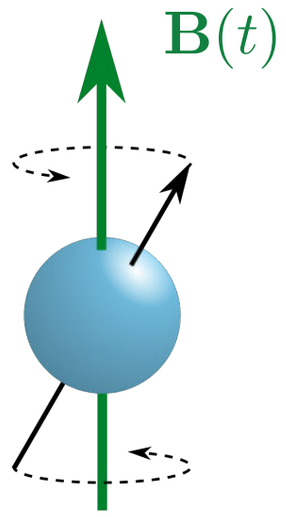
Example: Larmor precession

$$\hat{H}(t) = \mu_B \, \mathbf{B}(t) \cdot \hat{\mathbf{s}}$$

Heisenberg picture:

$$\frac{d\hat{\mathbf{s}}}{dt} = \mu_B \, \mathbf{B}(t) \times \hat{\mathbf{s}}(t)$$

field-like torque



$$\omega \propto |\mathbf{B}|$$

3a. Spin-orbit relaxation

Spin relaxation: irreversible process which erases the phase coherence among spins

*It could arise due to stochastic changes in the Larmor precession axis i.e. a random **B** field (*)*

(*) Fluctuating fields are ubiquitous in solid and can be produced via the **randomisation of momentum-space spin-orbit fields** upon multiple scattering events. Other examples include the **Overhauser field** produced by bath of nuclear spins on the electron spin and fields generated by **random magnetic impurities**.

3a. Spin-orbit relaxation

Spin relaxation: irreversible process which erases the phase coherence among spins

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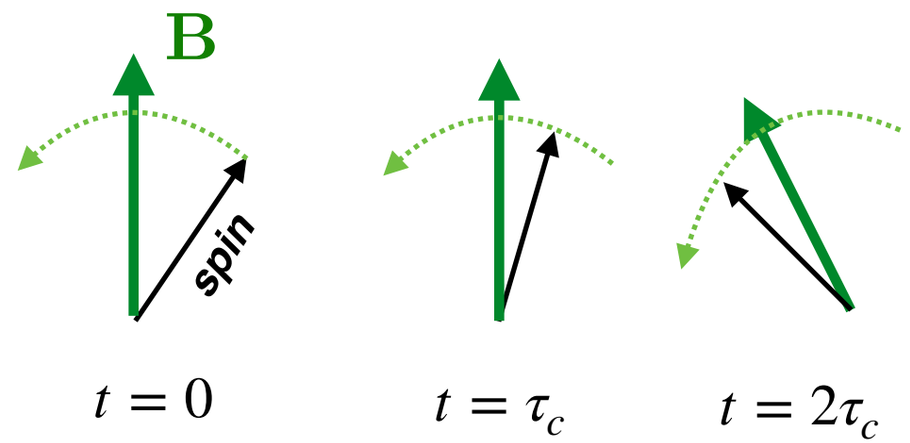
$$\Delta\phi = \omega\tau_c$$ ***precession angle***

$$\omega = \omega(B(t))$$

τ_c = *correlation/scattering time*



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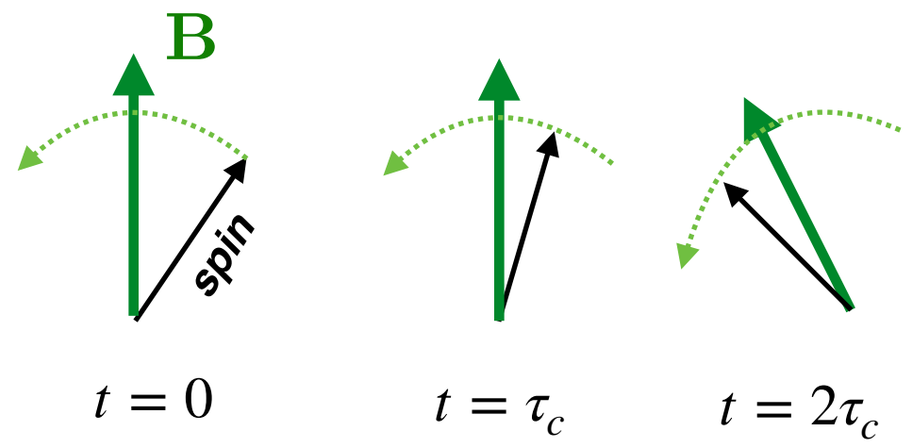


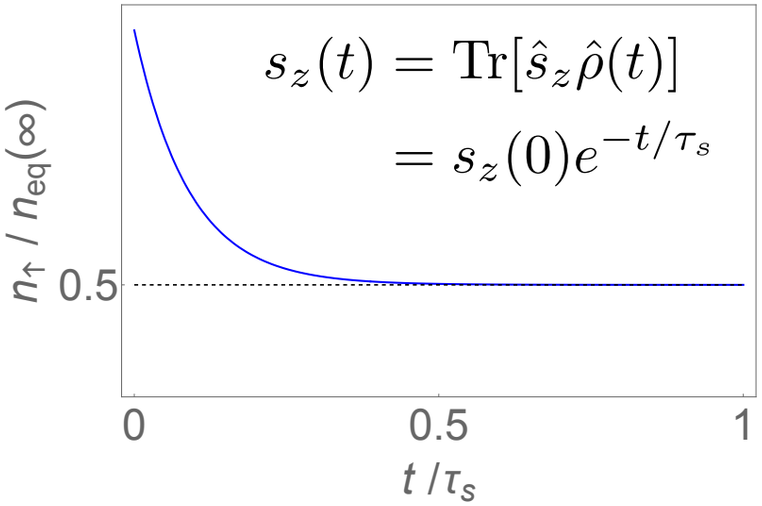
$\Delta\phi$ *undergoes a random walk*

Memory of initial state is lost at time after N *steps, when the variance equals one, i.e.* $\sigma^2 = N\Delta\phi^2 = 1$

$$\tau_s = N\tau_c \quad \rightarrow \quad 1/\tau_s = \omega^2\tau_c$$

3a. Spin-orbit relaxation

Spin relaxation: irreversible process which erases the phase coherence among spins



Prominent sources of spin relaxation include:

- **Elastic scattering** from non-magnetic impurities
- **Inelastic scattering** e.g., spin-lattice relaxation

Both mechanisms are assisted by SOC!

3a. Spin-orbit relaxation

Application: Dyakonov-Perel spin relaxation in a 2DEG with Rashba SOC

$$1/\tau_s = \omega^2 \tau_c$$

It arises due to random changes in the Rashba precession axis caused by ***impurity scattering events***

$$\Omega_{\mathrm{BR}}(\mathbf{k}) = v_{\mathrm{SO}}\,(-k_y, k_x, 0)^T$$ ⟵ *Spin precession axis is sensitive to* $\mathbf{k}$

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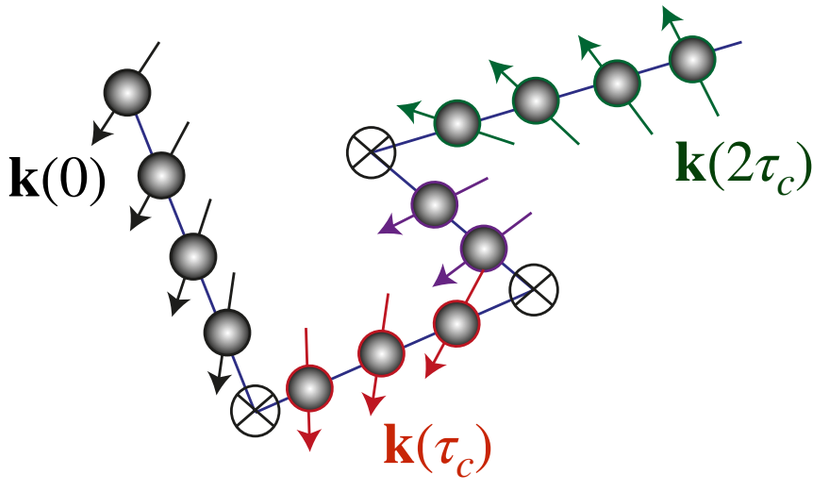
$$\left.\begin{array}{l} \omega^2 = \langle |\Omega_{\mathrm{BR}}(\mathbf{k})|^2 \rangle_{\mathrm{FS}} = v_{\mathrm{SO}}^2\, k_F^2 \\ \\ \tau_c = \tau_p \end{array}\right\} \Rightarrow \frac{1}{\tau_s} \propto \tau_p$$



3a. Spin-orbit relaxation

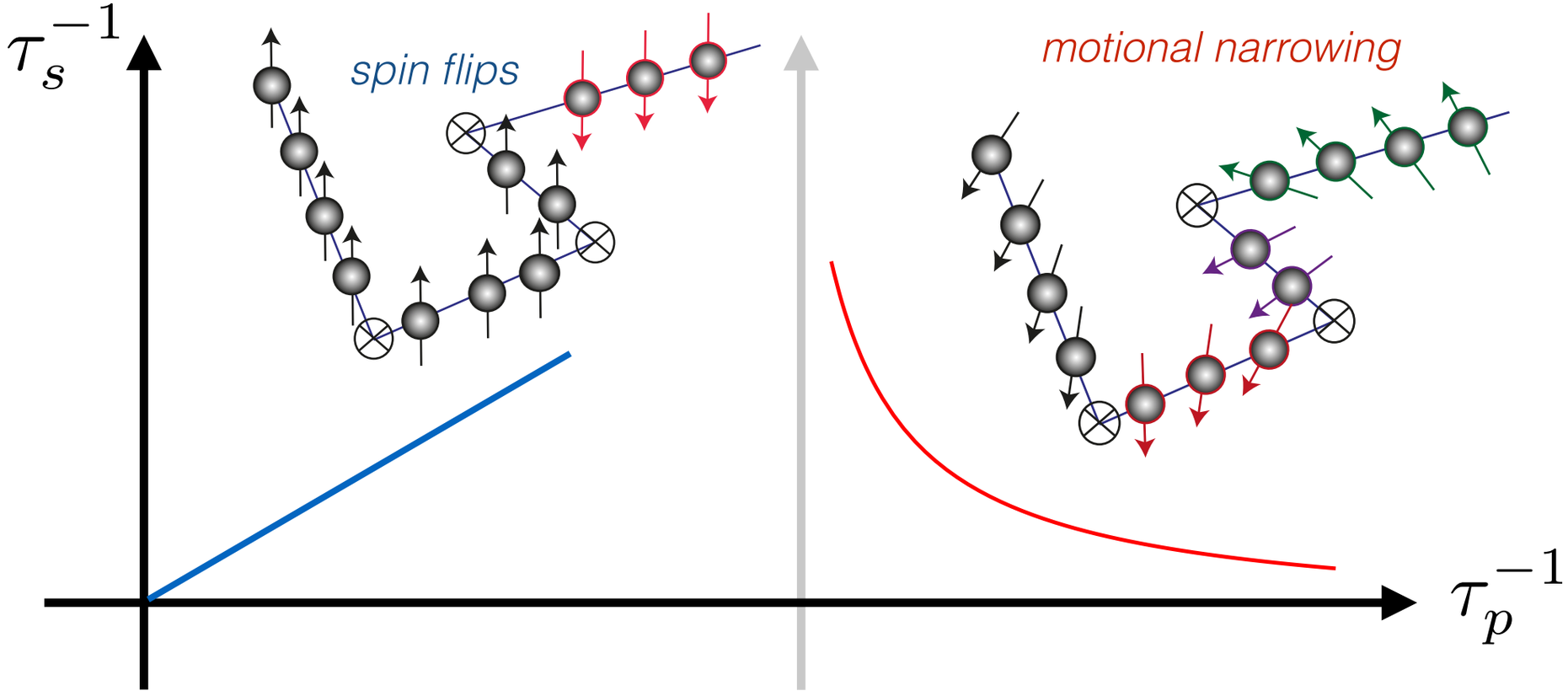
Spin-relaxation mechanisms from non-magnetic impurities:

Elliott-Yafet (centrosymmetric systems)

SO interaction leads to (usually small) spin mixing in eigenstates leading to $\tau_s \approx \left(\frac{\Delta E}{\lambda_{\mathrm{SO}}}\right)^2 \tau_p$

Dyakonov-Perel (non-centrosymmetric systems)

Electron's spin precesses in the ***k***-dependent low-symmetry SO field $\tau_s \approx \frac{1}{\tau_p} \frac{1}{\langle\,|\,\Omega_{\mathrm{SO}}(\mathbf{k})\,|\,\rangle^2}$



Elliott, PR 96, 266 (1954) [Sec. VII] | Žutic, RMP 76, 323 (2004) | Sohn, PRL 132, 246301 (2024)

3a. Spin-orbit relaxation

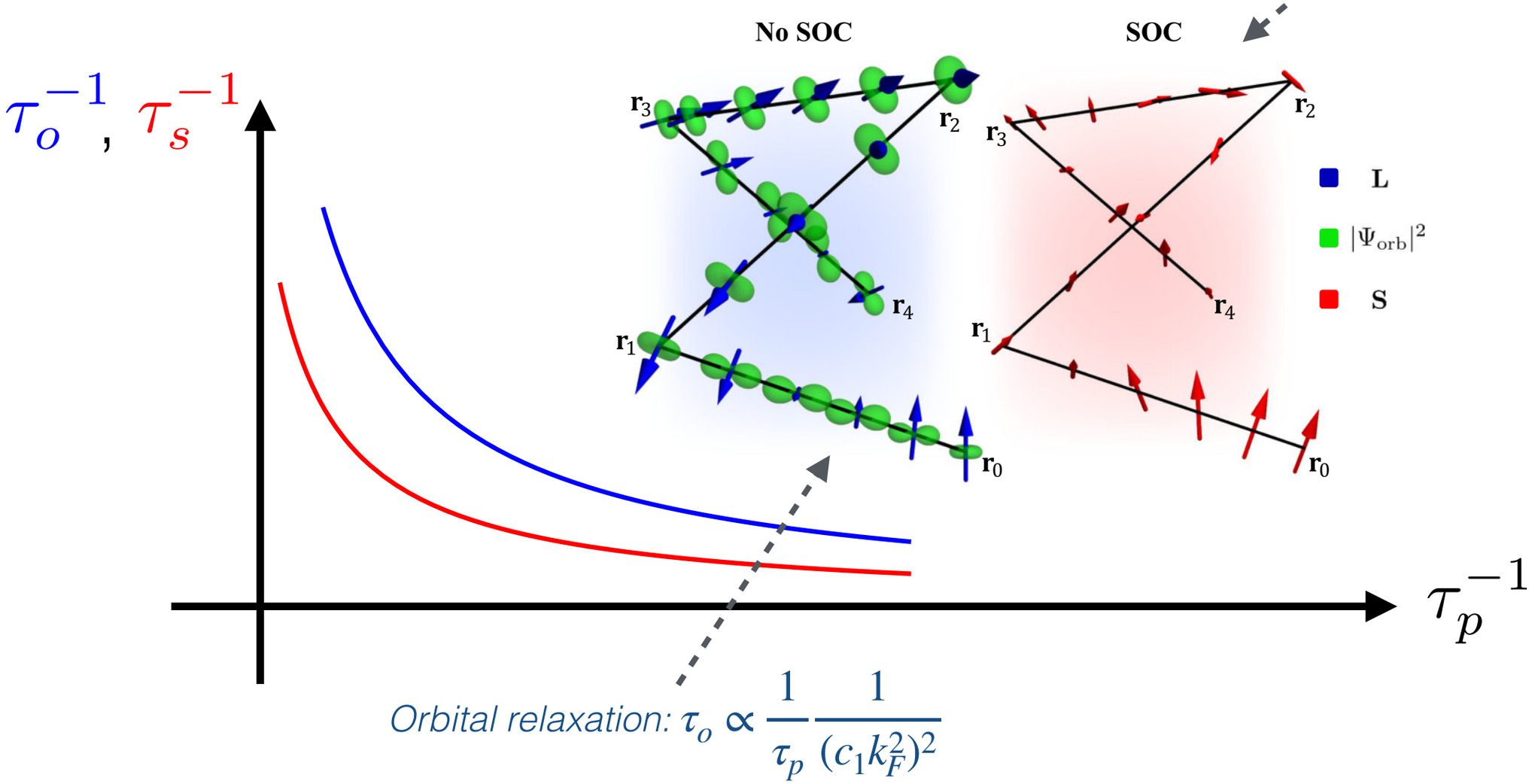
Dyakonov-Perel-like relaxation in centrosymmetric systems

Sohn, PRL 132, 246301 (2024)

$$H_{\mathbf{k}} = c_0 \mathbf{k}^2 + c_1 \left(\mathbf{k} \cdot \mathbf{L}\right)^2 + \lambda_{\mathrm{so}} \mathbf{L} \cdot \mathbf{s}$$

Luttinger p-orbital model

Spin relaxation: $\tau_s \propto \dfrac{1}{\tau_p} \dfrac{1}{\lambda_{so}^2}$



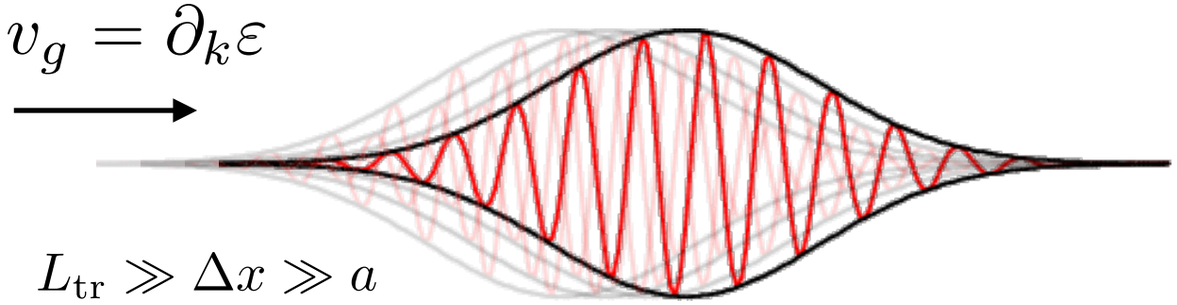
Orbital relaxation: $\tau_o \propto \dfrac{1}{\tau_p} \dfrac{1}{(c_1 k_F^2)^2}$

3b. Spin transport in metals

Semi-classical transport (Boltzmann's theory): *particle-wave duality revisited*

Wavepackets (WPs) with well defined $\mathbf{k} = \mathbf{k_c}$ (i.e., with an uncertainty much smaller than BZ size)

$$\Delta k \ll G_1 \propto a^{-1}$$



Solutions of $\hat{H}_{\mathbf{k}} |\phi_{\mathbf{k}}\rangle = \varepsilon_{\mathbf{k}} |\phi_{\mathbf{k}}\rangle$ are Bloch electronic states (waves). However, in transport problems, it is more useful to think in terms of localised wavepackets (particles).

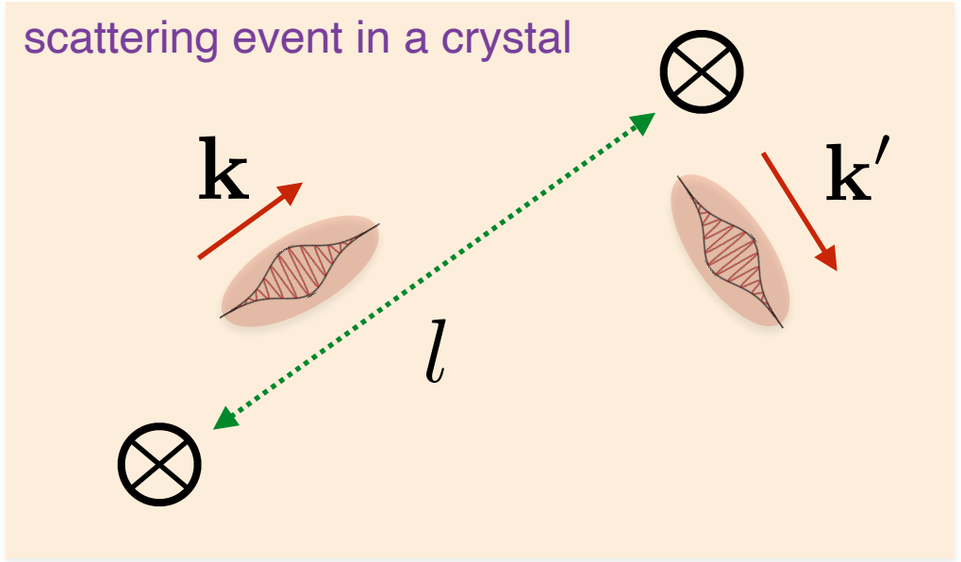
See Solid State Physics, Ashcroft and Mermin (1976)

3b. Spin transport in metals

Semi-classical transport (Boltzmann's theory): *particle-wave duality revisited*

$$\lambda_F \ll l \Leftrightarrow k_F l \gg 1$$

semiclassical condition



l = *mean free path*

- Coherent multi-impurity scattering events contribute weakly as WP only sees one impurity on average
- 6-dimensional phase space $\{\mathbf{r}, \mathbf{k}\}$ can be defined in the usual statistical sense

3b. Spin transport in metals

Semi-classical transport (Boltzmann's theory): *particle-wave duality revisited*

1. To each point $\{\mathbf{r}, \mathbf{k}\}$ assign a distribution function: $f(\mathbf{r}, \mathbf{k}, t)$

2. Next, consider its total rate of change:

$$\frac{\partial f}{\partial t} + \dot{\mathbf{r}} \cdot \nabla_{\mathbf{r}} f + \frac{d\mathbf{k}}{dt} \cdot \nabla_{\mathbf{k}} f = \left.\frac{\partial f}{\partial t}\right|_{\text{coll}}$$

$\dot{\mathbf{r}} \to \mathbf{v}_{\mathbf{k}}$ *diffusion* *external forces* $d_t\mathbf{k} \to \mathbf{F}$

L. E. Boltzmann (1918-1994)

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$\dot{\mathbf{r}} \to \mathbf{v}_{\mathbf{k}}$ *diffusion* *external forces* $d_t\mathbf{k} \to \mathbf{F}$

L. E. Boltzmann (1918-1994)

Typical case: DC electric field $\mathbf{F} = -e\mathbf{E}$

Write: $f = f_0 + \delta f$ (f_0 is the equilibrium, Fermi-Dirac function)

$$-e\mathbf{E} \cdot \mathbf{v}_{\mathbf{k}} \frac{\partial f_0(\mathbf{k})}{\partial \varepsilon} = \left.\frac{\partial f(\mathbf{k})}{\partial t}\right|_{\text{coll}}$$

acceleration term *scattering term*

Steady state & homogenous system:

$$\partial_t f, \nabla_{\mathbf{r}} f = 0$$

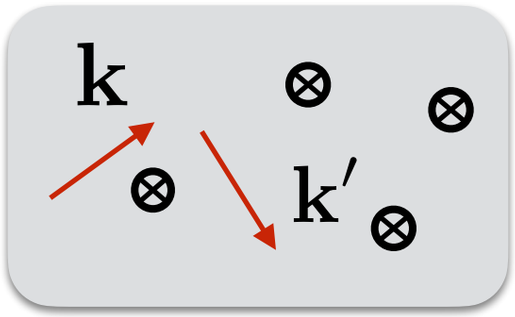
Also, to linear order in the external field:

$$\nabla_{\mathbf{k}} f = \frac{\partial f}{\partial \varepsilon_{\mathbf{k}}} \frac{\partial \varepsilon_{\mathbf{k}}}{\partial \mathbf{k}} \approx \frac{\partial f_0}{\partial \varepsilon_{\mathbf{k}}} \mathbf{v}_{\mathbf{k}}$$

3b. Spin transport in metals

Semi-classical transport (Boltzmann's theory): *particle-wave duality revisited*

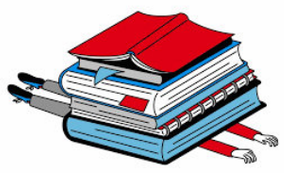
$$-e\mathbf{E}\cdot\mathbf{v}_{\mathbf{k}}\frac{\partial f_0(\mathbf{k})}{\partial\varepsilon} = \left.\frac{\partial f(\mathbf{k})}{\partial t}\right|_{\text{coll}}$$



$$= -\sum_{\mathbf{k}'}\left[\delta f(\mathbf{k}) - \delta f(\mathbf{k}')\right] W_{\mathbf{k}\to\mathbf{k}'}$$

transition rate

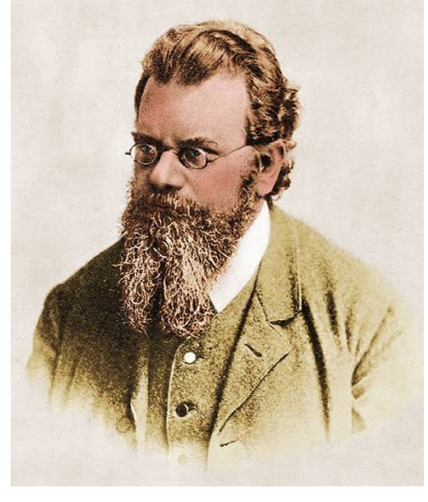
L. E. Boltzmann (1918-1994)



We must have $\sum_{\mathbf{k}}\left.\frac{\partial f(\mathbf{k})}{\partial t}\right|_{\text{coll}} = -\sum_{\mathbf{k}}\sum_{\mathbf{k}'}\left[\delta f(\mathbf{k}) - \delta f(\mathbf{k}')\right] W_{\mathbf{k}\to\mathbf{k}'} = 0$. Interpret this result.

3b. Spin transport in metals

Semi-classical transport (Boltzmann's theory): *particle-wave duality revisited*



L. E. Boltzmann (1918-1994)

$W_{\mathbf{k}\to\mathbf{k}'}$ can be computed quantum mechanically, but a microscopic model is required. Consider a disorder landscape of random, short-ranged impurities:

$$V_{\mathrm{imp}}(\mathbf{r}) = \sum_{\{\mathbf{r}_i\}} u_0\, \delta(\mathbf{r} - \mathbf{r}_i)$$

scattering potential strength

δ-function is often justified due to screening

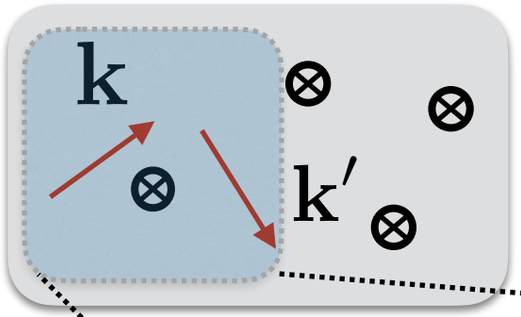
set of impurity positions

3b. Spin transport in metals

Semi-classical transport (Boltzmann's theory): *particle-wave duality revisited*

n_{imp} = impurity concentration

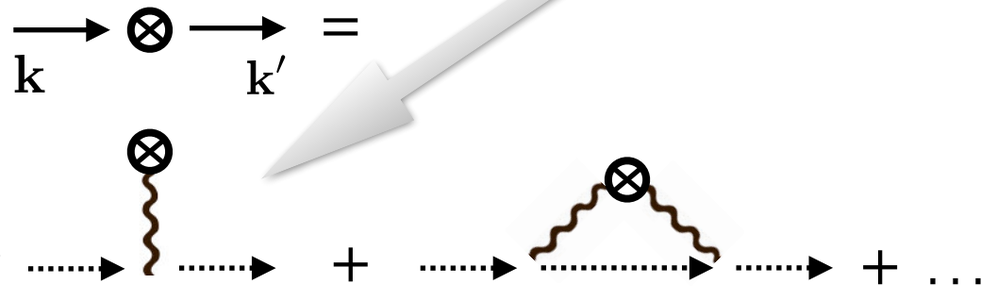
$\varrho(\varepsilon_F)$ = DoS at Fermi level



Total scattering rate is:

$$\hat{T} \approx u_0$$

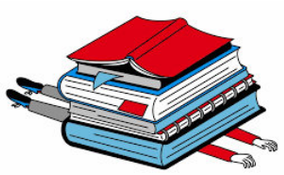
1st Born diagram



Generalised Golden rule

$$W_{\mathbf{k}\to\mathbf{k}'} = 2\pi\, n_{\mathrm{imp}} \left|\langle \mathbf{k}| \hat{T} |\mathbf{k}'\rangle\right|^2 \delta(\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}'})$$

T-matrix



Derive the result above for the *T*-matrix of parabolic-band electrons. Do you expect any significant differences between the **2D** and **3D** cases? What about systems of *massless* fermions?

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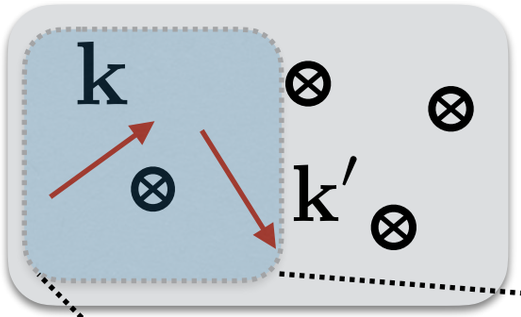

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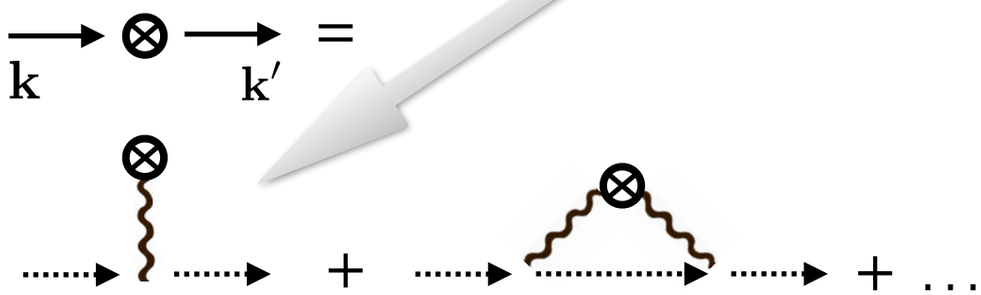

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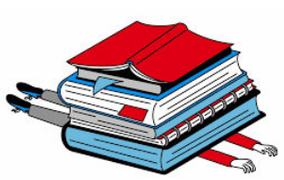
T-matrix

Total scattering rate is: $\Gamma_{\mathbf{k}} = \sum_{\mathbf{k}'} W_{\mathbf{k}\to\mathbf{k}'}$. For a parabolic band, one has:

$$\Gamma_{k_F} \propto n_{\mathrm{imp}}\, \varrho(\varepsilon_F)\, |T(\varepsilon_F)|^2 \propto \begin{cases} n_{\mathrm{imp}}\, \varrho(\varepsilon_F)\, u_0^2, & u_0\, \varrho(\varepsilon_F) \ll 1 \quad \text{(weak scattering regime)} \\ n_{\mathrm{imp}} [\varrho(\varepsilon_F)]^{-1}, & u_0\, \varrho(\varepsilon_F) \gg 1 \quad \text{(strong scattering regime)} \end{cases}$$



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3b. Spin transport in metals

Semi-classical transport (Boltzmann's theory): *particle-wave duality revisited*

The transport equation can be solved exactly in many cases of interest,
but an often employed approximation is

$$-e\mathbf{E}\cdot\mathbf{v}_{\mathbf{k}}\frac{\partial f_0(\mathbf{k})}{\partial\varepsilon} = -\sum_{\mathbf{k}}\sum_{\mathbf{k}'}\left[\delta f(\mathbf{k}) - \delta f(\mathbf{k}')\right] W_{\mathbf{k}\to\mathbf{k}'} \approx -\frac{\delta f}{\tau_{\mathbf{k}}}$$

relaxation time approximation (**RTA**)

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dominated by Fermi surface!

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$$\delta f(\mathbf{k}) = e\,\tau_{\mathbf{k}}\,\mathbf{E}\cdot\mathbf{v}_{\mathbf{k}}\frac{\partial f_0(\mathbf{k})}{\partial\varepsilon} \underset{\boldsymbol{T=0}}{=} -e\,\tau_{\mathbf{k}}\,\mathbf{E}\cdot\mathbf{v}_{\mathbf{k}}\,\delta(\varepsilon_{\mathbf{k}}-\varepsilon_F)$$

Non-equilibrium quantities can now be easily computed :

Charge carrier density: $$\mathbf{j}_c = \frac{g_s}{V}\sum_{\mathbf{k}}(-e\mathbf{v}_{\mathbf{k}})f(\mathbf{k})$$

- $g_s = 2$ is a spin degeneracy factor
- V is the volume
- $v_{\mathbf{k}} = v_k\,\mathbf{e}_{\mathbf{k}}$ (rotational symmetry)
- ϱ = DoS with spin included

3b. Spin transport in metals

Semi-classical transport (Boltzmann's theory): *particle-wave duality revisited*

The transport equation can be solved exactly in many cases of interest,
but an often employed approximation is

$$-e\mathbf{E}\cdot\mathbf{v}_{\mathbf{k}}\frac{\partial f_0(\mathbf{k})}{\partial\varepsilon} = -\sum_{\mathbf{k}}\sum_{\mathbf{k}'}\left[\delta f(\mathbf{k}) - \delta f(\mathbf{k}')\right] W_{\mathbf{k}\to\mathbf{k}'} \approx -\frac{\delta f}{\tau_{\mathbf{k}}}$$

relaxation time approximation (**RTA**)

$$\delta f(\mathbf{k}) = e\,\tau_{\mathbf{k}}\,\mathbf{E}\cdot\mathbf{v}_{\mathbf{k}}\frac{\partial f_0(\mathbf{k})}{\partial\varepsilon} \underset{T=0}{=} -e\,\tau_{\mathbf{k}}\,\mathbf{E}\cdot\mathbf{v}_{\mathbf{k}}\,\delta(\varepsilon_{\mathbf{k}}-\varepsilon_F)$$

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- $v_{\mathbf{k}} = v_k\,\mathbf{e}_{\mathbf{k}}$ (rotational symmetry)
- ϱ = DoS with spin included

$$\mathbf{j}_c = g_s\int\frac{d^3\mathbf{k}}{(2\pi)^3}\,(-e\,\mathbf{v}_{\mathbf{k}})\,\delta f(\mathbf{k}) = \hat{\sigma}\cdot\mathbf{E}$$

where

$$\sigma_{ij} = \frac{1}{3}\,e\,\varrho(\varepsilon_F)\,v_F^2\tau_F\,\delta_{ij} \qquad (i,j=x,y,z)$$

electric conductivity tensor

3b. Spin transport in metals

Semi-classical transport (Boltzmann's theory): *particle-wave duality revisited*

Continuity equation & constitutive relations

First, introduce charge density: $n(\mathbf{r}) = \frac{g_s}{V} \sum_{\mathbf{k}} (-e) f(\mathbf{r}, \mathbf{k})$

3b. Spin transport in metals

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Next, integrate 2 sides of Boltzmann equation over momentum space:

$$-e \frac{g_s}{V} \sum_{\mathbf{k}} \boxed{\frac{\partial f}{\partial t} + \mathbf{v_k} \cdot \nabla_{\mathbf{r}} f - e\mathbf{E} \cdot \mathbf{v_k} \frac{\partial f_0}{\partial \varepsilon} = \left. \frac{\partial f}{\partial t} \right|_{\text{coll}}} \longrightarrow \sum_{\mathbf{k}} \left. \frac{\partial f(\mathbf{r}, \mathbf{k})}{\partial t} \right|_{\text{coll}} = 0$$

Detailed balance condition:

3b. Spin transport in metals

Semi-classical transport (Boltzmann's theory): *particle-wave duality revisited*

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Detailed balance condition:

$$\frac{\partial n}{\partial t} + \nabla_{\mathbf{r}} \left[\frac{g_s}{V} \sum_{\mathbf{k}} (-e\mathbf{v_k}) f(\mathbf{r}, \mathbf{k}) \right] = 0 \quad \Rightarrow \quad \boxed{\frac{\partial n}{\partial t} + \nabla \cdot \mathbf{j}_c = 0}$$

Number conservation of electrons

3b. Spin transport in metals

Semi-classical transport (Boltzmann's theory): *particle-wave duality revisited*

Continuity equation & constitutive relations

An important **constitutive relation** can also be derived:

$$\mathbf{j}_c(\mathbf{r}) = \sigma_c \mathbf{E} + D\boldsymbol{\nabla} n$$

Drift ***Diffusion***

Making use of the Einstein relation $\sigma_c = e^2 \varrho D$, one may cast the constitutive equation as $\mathbf{j}_c = \sigma_c \left(\mathbf{E} + \frac{1}{e} \nabla \mu \right) \equiv \sigma_c \boldsymbol{\mathscr{E}}$.

3b. Spin transport in metals

Two-channel Mott model (Valet and Fert, 1993)

T. Valet

A. Fert

$$\frac{\partial f_\sigma}{\partial t} + \mathbf{v}_{\sigma\mathbf{k}} \cdot \nabla_{\mathbf{r}} f_\sigma - e\mathbf{E} \cdot \mathbf{v}_{\sigma\mathbf{k}} \frac{\partial f_{0\sigma}}{\partial \varepsilon} = \left. \frac{\partial f_\sigma}{\partial t} \right|_{\text{coll}}$$

$$\sigma = \uparrow, \downarrow$$

3b. Spin transport in metals

Two-channel Mott model (Valet and Fert, 1993)

T. Valet

A. Fert

$$\left.\frac{\partial f_\sigma}{\partial t}\right|_{\text{coll}} = \left.\frac{\partial f}{\partial t}\right|_{\text{coll}}^{\sigma\to\sigma} + \left.\frac{\partial f}{\partial t}\right|_{\text{coll}}^{\sigma\to\sigma'}$$

spin-conserving + ***spin-flip processes***

3b. Spin transport in metals

Two-channel Mott model (Valet and Fert, 1993)

T. Valet

A. Fert

Spin-flip terms:

$$\sum_{\mathbf{k}'} [W_{\bar{\sigma}\mathbf{k}'\to\sigma\mathbf{k}}\delta f_{\bar{\sigma}}(\mathbf{k}') - W_{\sigma\mathbf{k}\to\bar{\sigma}\mathbf{k}'}\delta f_{\sigma}(\mathbf{k})]$$

$\bar{\sigma} = -\sigma$

Total scattering rates:

$$\frac{1}{\tau_\uparrow} = \frac{1}{\tau_{\uparrow\uparrow}} + \frac{1}{\tau_{\uparrow\downarrow}}$$

$$\frac{1}{\tau_\downarrow} = \frac{1}{\tau_{\uparrow\uparrow}} + \frac{1}{\tau_{\downarrow\uparrow}}$$

$\tau_{\uparrow\downarrow}, \tau_{\downarrow\uparrow} \equiv \tau_{\mathrm{sf}}$ ***"spin flip time"***

3b. Spin transport in metals

Two-channel Mott model (Valet and Fert, 1993)

$$\mathbf{j}_\sigma(\mathbf{r}) = \frac{1}{V}\sum_{\mathbf{k}}(-ev_{\mathbf{k}})f_\sigma(\mathbf{r},\mathbf{k})$$

$$j_s(\mathbf{r}) = j_\uparrow(\mathbf{r}) - j_\downarrow(\mathbf{r})$$

spin current density

$$n_\sigma(\mathbf{r}) = \frac{1}{V}\sum_{\mathbf{k}}(-e)f_\sigma(\mathbf{r},\mathbf{k})$$

$$s(\mathbf{r}) = n_\uparrow(\mathbf{r}) - n_\downarrow(\mathbf{r})$$

spin accumulation density

T. Valet

A. Fert

3b. Spin transport in metals

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$$s(\mathbf{r}) = n_\uparrow(\mathbf{r}) - n_\downarrow(\mathbf{r})$$

spin accumulation density

T. Valet

A. Fert

Steady-state continuity equations:

Charge current

$$\nabla\cdot(\mathbf{j}_\uparrow + \mathbf{j}_\downarrow) = 0$$

Spin current

$$\nabla\cdot(\mathbf{j}_\uparrow - \mathbf{j}_\downarrow) = -\frac{\delta n_\uparrow(\mathbf{r}) - \delta n_\downarrow(\mathbf{r})}{\tau_{\mathrm{sf}}}$$

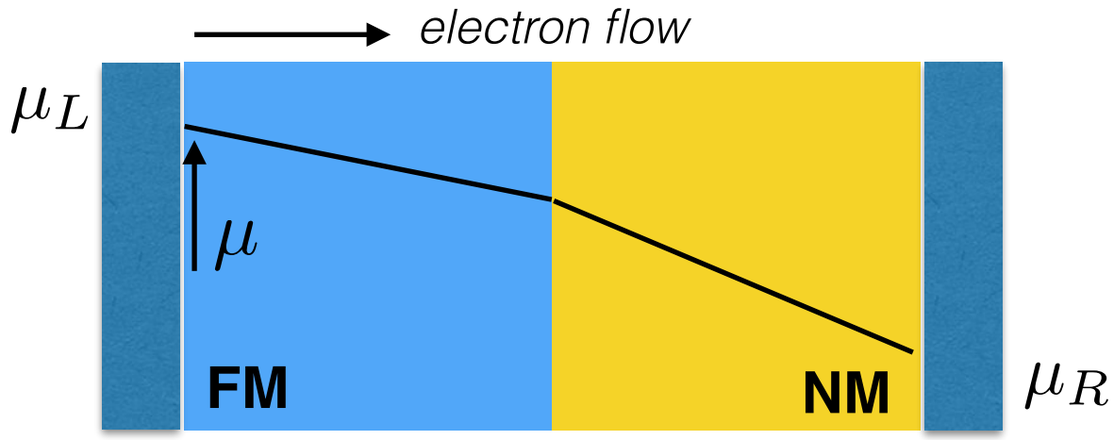
spin flip time

In normal metals,
$\tau_{sf} \gg \tau_{\uparrow\uparrow}$ leading to $l_s \gg l$

Moreover, in ferromagnetic metals the bands are exchange-split, and thus $\tau_\uparrow \neq \tau_\downarrow$

3b. Spin transport in metals

Spin interface resistance & the GMR effect



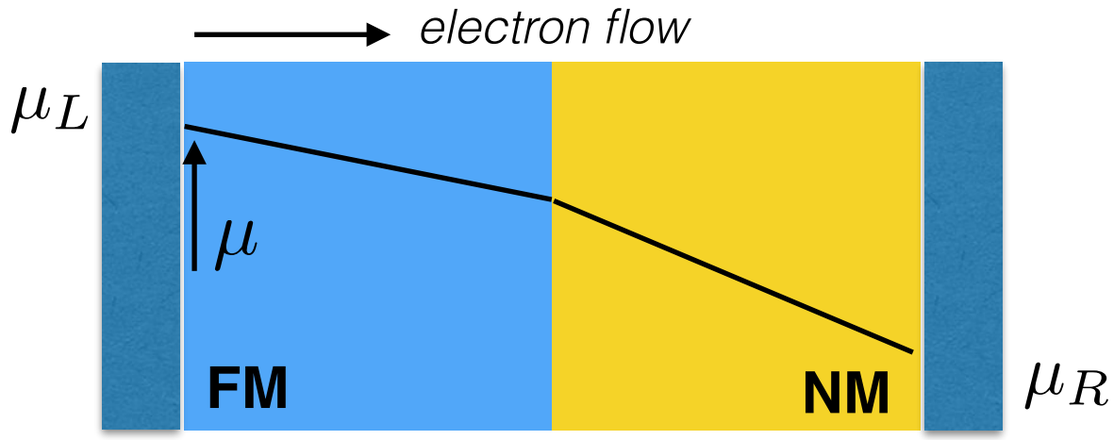
- Fully polarised spin current is injected at LHS
- Spin current is vanishing small at the other end, due to spin relaxation in the NM

Diffusive regime: lateral dimensions $\gg l, l_s$

Son, PRL 52, 2271 (1987) | Valet and Fert, PRB 48, 7102 (1993) | Yu and Flatte, PRB 66, 201202(R) (2002)

3b. Spin transport in metals

Spin interface resistance & the GMR effect



Constitutive relation + spin continuity equation:

(1) $$\mathbf{j}_{\uparrow,\downarrow} = (\sigma_{\uparrow,\downarrow}/e)\,\boldsymbol{\nabla}\mu_{\uparrow,\downarrow}$$

(2) $$\nabla \cdot (\mathbf{j}_{\uparrow} - \mathbf{j}_{\downarrow}) = -\frac{\delta n_{\uparrow}(\mathbf{r}) - \delta n_{\downarrow}(\mathbf{r})}{\tau_{\mathrm{sf}}}$$

Son, PRL 52, 2271 (1987) | Valet and Fert, PRB 48, 7102 (1993) | Yu and Flatte, PRB 66, 201202(R) (2002)

3b. Spin transport in metals

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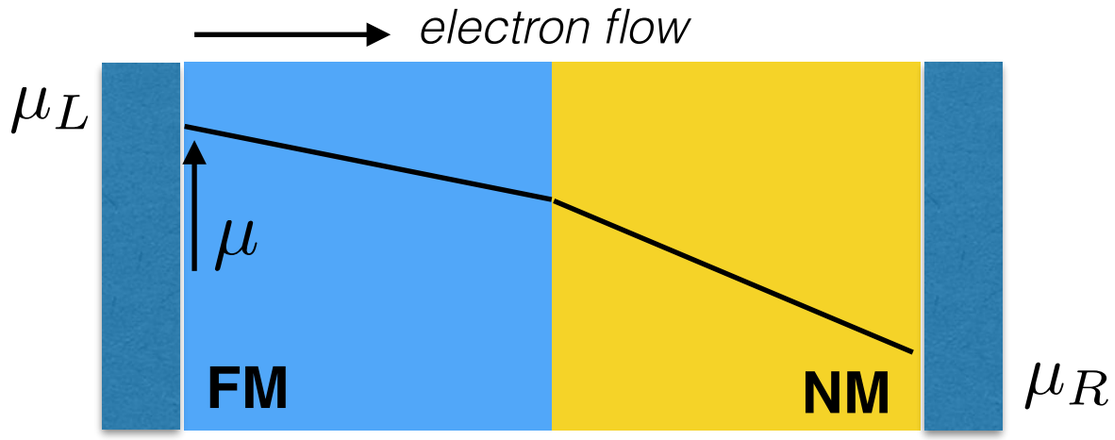


Constitutive relation + spin continuity equation:

(1) $\mathbf{j}_{\uparrow,\downarrow} = (\sigma_{\uparrow,\downarrow}/e)\,\boldsymbol{\nabla}\mu_{\uparrow,\downarrow}$

(2) $\nabla \cdot (\mathbf{j}_{\uparrow} - \mathbf{j}_{\downarrow}) = -\dfrac{\delta n_{\uparrow}(\mathbf{r}) - \delta n_{\downarrow}(\mathbf{r})}{\tau_{\mathrm{sf}}}$

spin diffusion equation

$$\nabla^2(\mu_{\uparrow} - \mu_{\downarrow}) = -\frac{\mu_{\uparrow} - \mu_{\downarrow}}{l_s^2}$$

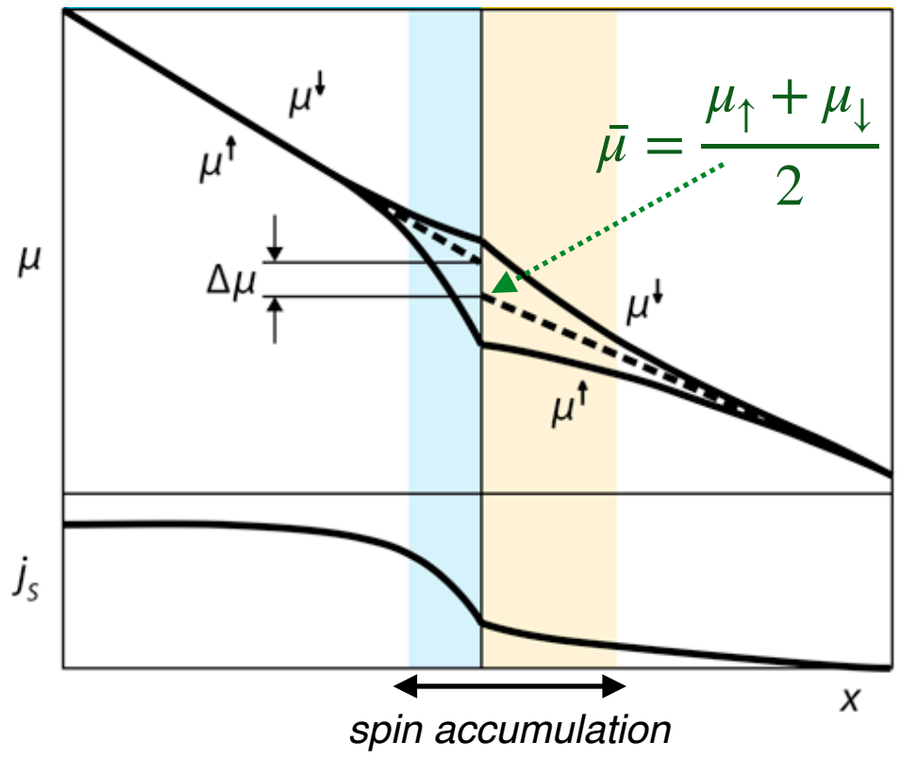
$l_{s,m} = \sqrt{D_m \tau_{\mathrm{sf},m}}$ (m = NM, FM)

Son, PRL 52, 2271 (1987) | Valet and Fert, PRB 48, 7102 (1993) | Yu and Flatte, PRB 66, 201202(R) (2002)

3b. Spin transport in metals

Spin interface resistance & the GMR effect

- Majority spins ($\downarrow$) are preferably transmitted
- Size of spin accumulation region is governed by $l_{s,\mathrm{NM}}$, $l_{s,\mathrm{FM}}$



Physics Viewpoint: https://physics.aps.org/articles/v8/83

Son, PRL 52, 2271 (1987) | Valet and Fert, PRB 48, 7102 (1993) | Yu and Flatte, PRB 66, 201202(R) (2002)

3b. Spin transport in metals

Spin interface resistance & the GMR effect

- Majority spins ($\downarrow$) are preferably transmitted
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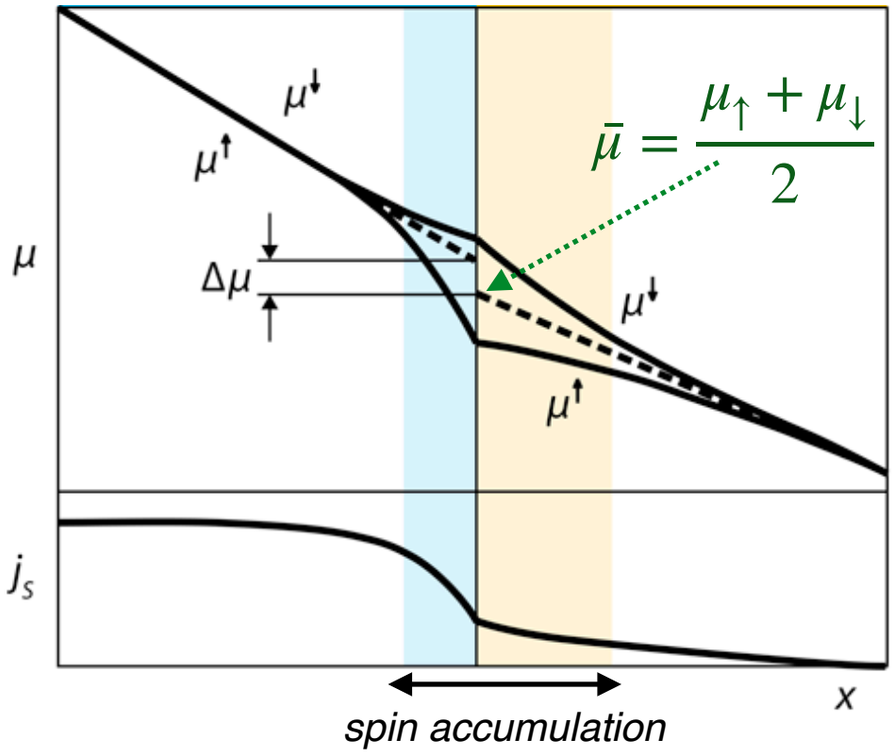
The spin-average chemical potential is discontinuous at $x = 0$, thus creating a voltage difference

$$R = \frac{\bar{\mu}_{\mathrm{FM}}(0) - \bar{\mu}_{\mathrm{NM}}(0)}{eI}$$

"Spin-coupled interface resistance"
is a key concept GMR physics!



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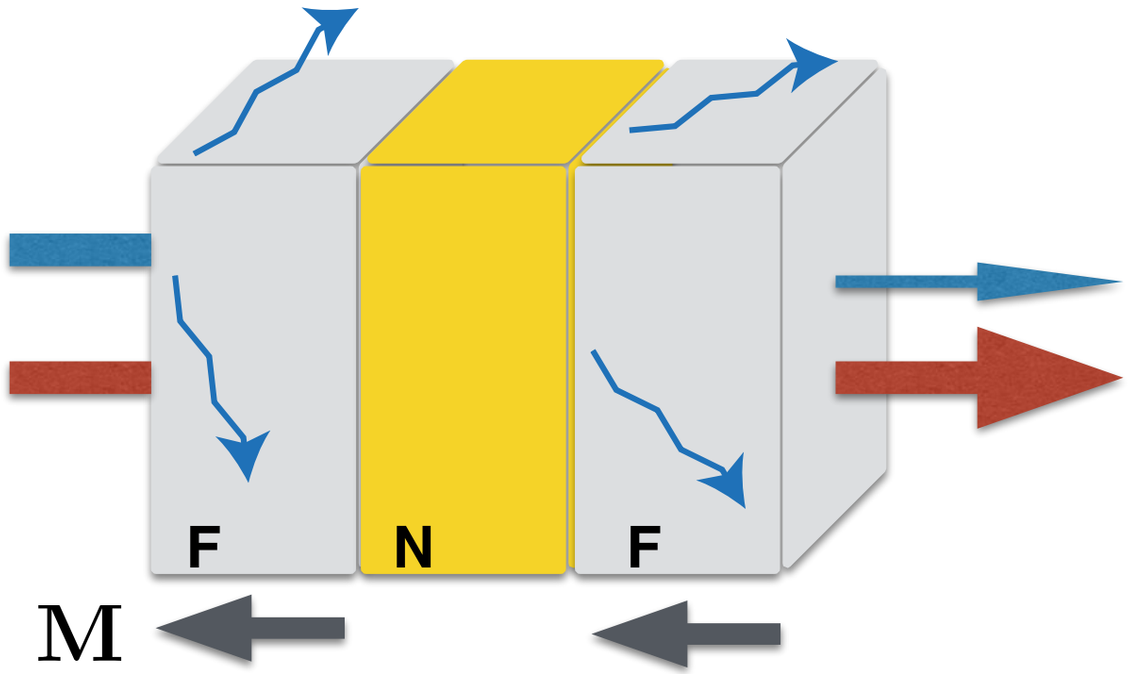
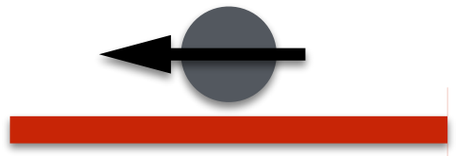
Son, PRL 52, 2271 (1987) | Valet and Fert, PRB 48, 7102 (1993) | Yu and Flatte, PRB 66, 201202(R) (2002)

3c. Spin transport in metals

Spin interface resistance & the GMR effect



majority spins
[“down”]



minority spins
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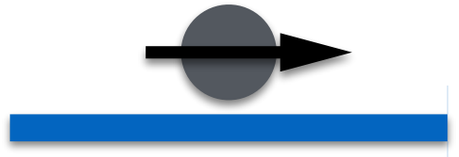

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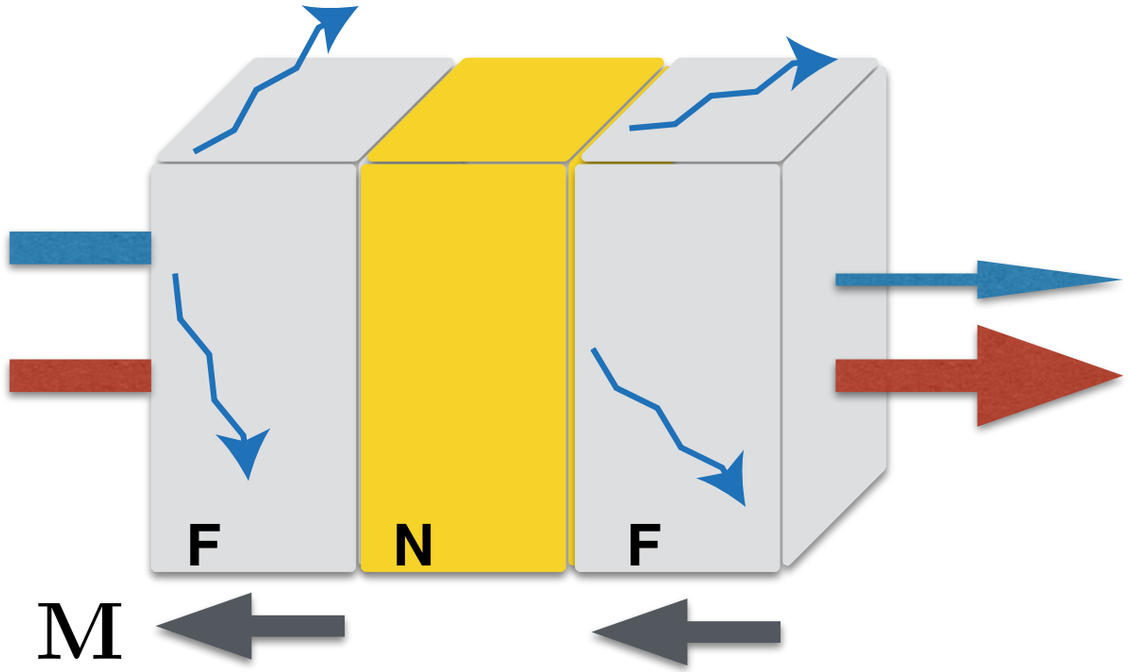
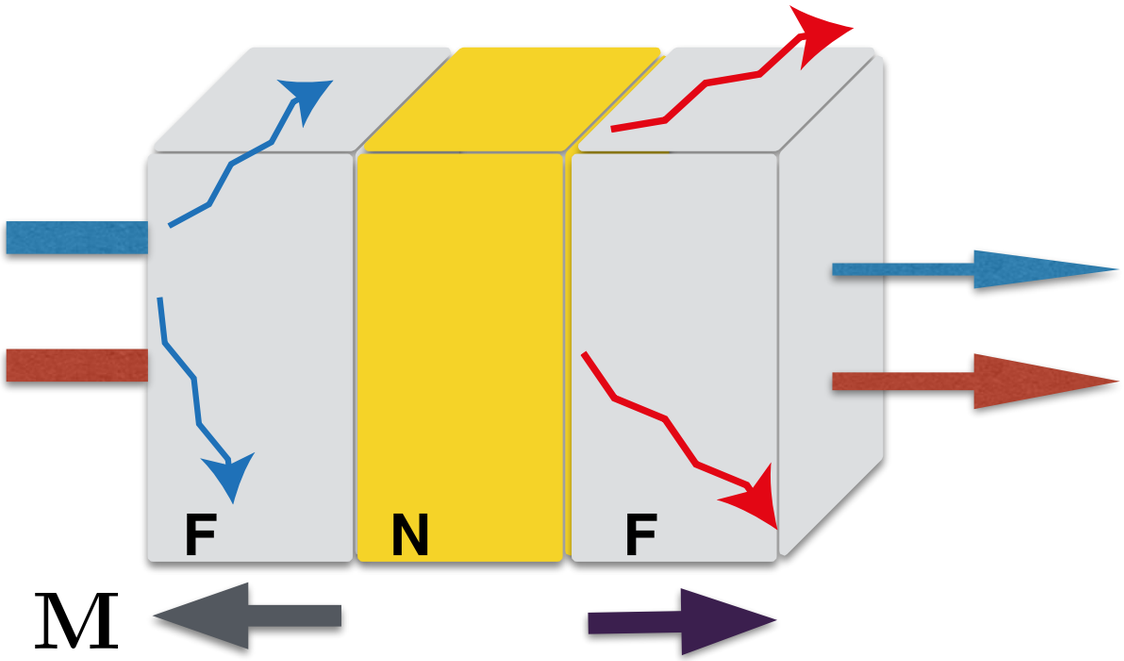
3c. Spin transport in metals

Spin interface resistance & the GMR effect

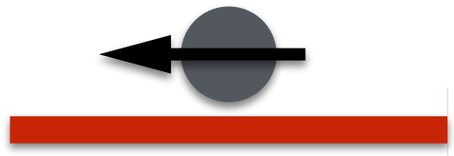
Parallel config.



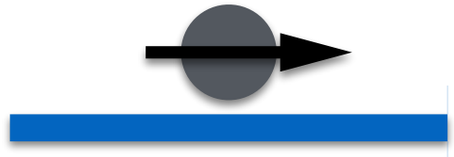
Antiparallel config.



majority spins ["down"]



minority spins ["up"]



$$R_{\uparrow\downarrow} > R_{\text{parallel}}$$

- Interfacial spin accumulation picture offers a compelling explanation
- Spin-dependent scattering within the FM layers (not discussed here) is also important

Son, PRL 52, 2271 (1987) | Valet and Fert, PRB 48, 7102 (1993) | Yu and Flatte, PRB 66, 201202(R) (2002)

3c. Coupled charge-spin transport effects enabled by SOC

In Secs. 3a-b, **SOC** was a source of **spin and orbit relaxation**, but how does it modify the electrodynamic responses of solids?

- Part of the answer was given earlier in Sec. 1b: **SHE and ISGE**, but there is more!

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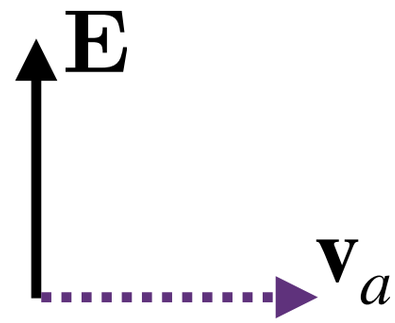
- SOC can endow energy bands with a spin Berry curvature [even in high-symmetry crystals], which modifies the *semiclassical equations of motion*:

$$\frac{d\langle \mathbf{r} \rangle}{dt} = \frac{1}{\hbar}\nabla_{\mathbf{k}}\varepsilon_{n\sigma} - \frac{d\langle \mathbf{k} \rangle}{dt} \times \Omega_{n\sigma}(\mathbf{k})$$

$$\frac{d\langle \mathbf{k} \rangle}{dt} = -\frac{e}{\hbar}\left[\mathbf{E} + \frac{d\langle \mathbf{r} \rangle}{dt} \times \mathbf{B}\right]$$

→ *anomalous velocity*

(intrinsic SHE)



Xiao *et al.* RMP 82, 1959 (2010)

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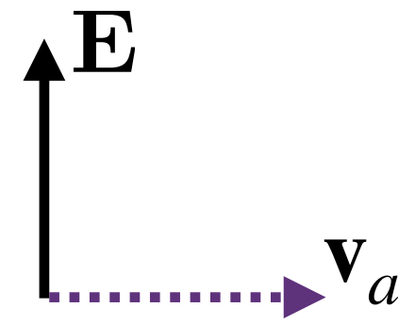


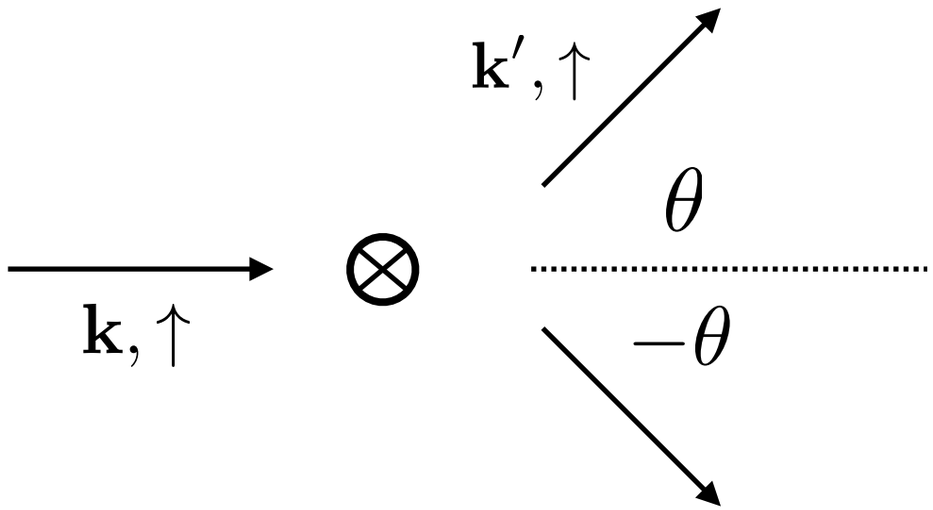
Xiao *et al.* RMP 82, 1959 (2010)

- Through disorder, SOC gives rise to *extrinsic electrodynamic responses*

Sinova et al. RMP 87, 1213 (2015)

3c. Coupled charge-spin transport effects enabled by SOC

Example: extrinsic spin Hall effect



left-right asymmetry

$$\sigma(\theta) \propto \left|\langle \mathbf{k}|\hat{T}|\mathbf{k}'\rangle\right|^2 \neq \sigma(-\theta)$$

[breaks micro-reversibility, $W_{\mathbf{k}\to\mathbf{k}'} \neq W_{\mathbf{k}'\to\mathbf{k}}$]

Gradhand *et al.*, PRL 104, 186403 (2010) | Fert & Levy, PRL 106, 157209 (2011) | Ferreira *et al.*, PRL 112, 066601 (2014)

3c. Coupled charge-spin transport effects enabled by SOC

Example: extrinsic spin Hall effect

Intuition in 2D: $\hat{H}_{so} = \lambda_{so} \hat{L}_z \hat{s}_z$ ➡ *SOC experienced near impurity*

[neglect spin flips]

Consider a WP experiencing SOC for a time δt: $|\psi_{\mathbf{k}}(t)\rangle = e^{-i\hat{H}_{\mathrm{so}}t} |\mathbf{k}, \uparrow\rangle$

Gradhand *et al.*, PRL 104, 186403 (2010) | Fert & Levy, PRL 106, 157209 (2011) | Ferreira *et al.*, PRL 112, 066601 (2014)

3c. Coupled charge-spin transport effects enabled by SOC

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Recall that $\hat{L}_z$ is the generator of rotations in coordinate space!

$$e^{-i\lambda_{\mathrm{so}}\delta t\,\hat{L}_z\hat{s}_z}\,|\mathbf{k},\uparrow\rangle = \hat{R}_z(\lambda_{\mathrm{so}}\delta t)\,|\mathbf{k},\uparrow\rangle = |\mathbf{k}_{\delta\theta},\uparrow\rangle$$

$$\delta\theta = \lambda_{\mathrm{so}}\delta t$$

Gradhand *et al.*, PRL 104, 186403 (2010) | Fert & Levy, PRL 106, 157209 (2011) | Ferreira *et al.*, PRL 112, 066601 (2014)

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$$\delta\theta = \lambda_{\mathrm{so}}\delta t$$

$$e^{-i\lambda_{\mathrm{so}}\delta t\,\hat{L}_z\hat{s}_z}\,|\mathbf{k},\downarrow\rangle = \hat{R}_z(-\lambda_{\mathrm{so}}\delta t)\,|\mathbf{k},\downarrow\rangle = |\mathbf{k}_{-\delta\theta},\downarrow\rangle$$

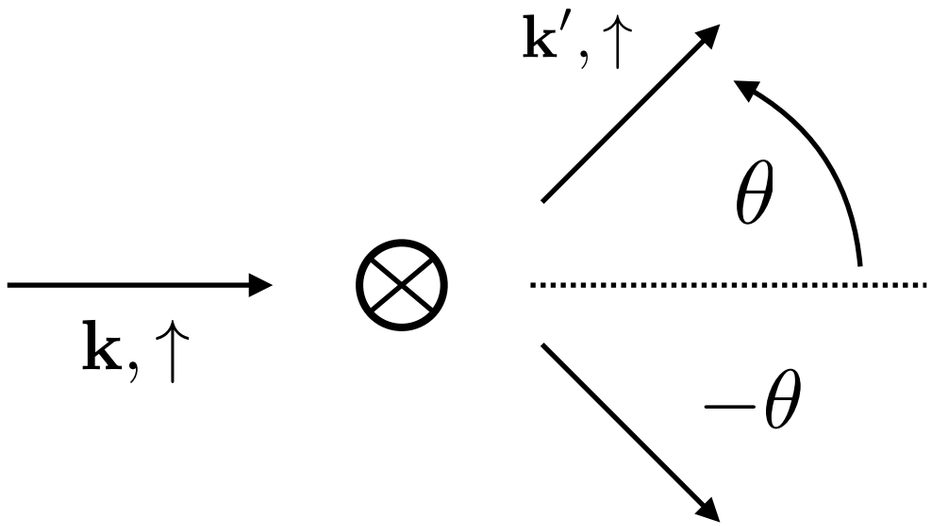
Time reversal symmetry

$$\sigma_{\uparrow}(\theta) = \sigma_{\downarrow}(-\theta)$$

Gradhand *et al.*, PRL 104, 186403 (2010) | Fert & Levy, PRL 106, 157209 (2011) | Ferreira *et al.*, PRL 112, 066601 (2014)

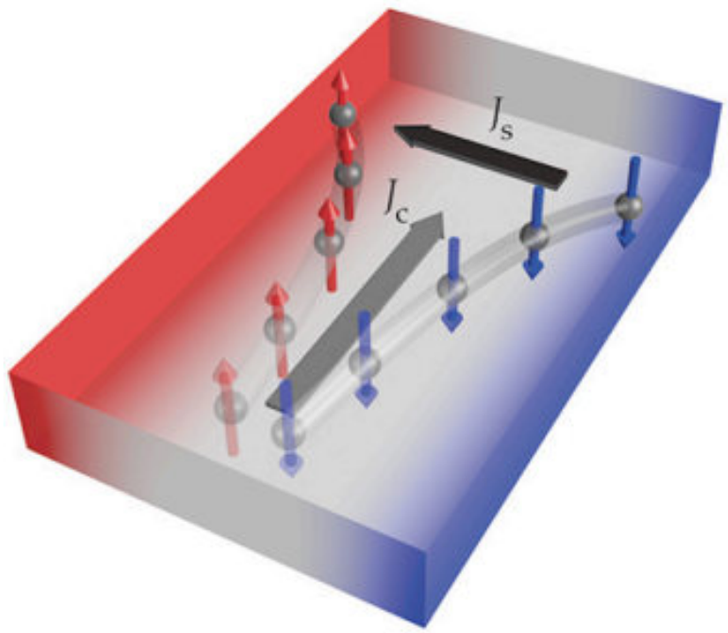
3c. Coupled charge-spin transport effects enabled by SOC

Example: Extrinsic Spin Hall effect



$$\sigma(\theta) \propto |\langle \mathbf{k}|\hat{T}|\mathbf{k}'\rangle|^2 \neq \sigma(-\theta)$$

Solution of Boltzmann equation now ***has new relaxation times***: $\tau_{\uparrow}^{\perp}$ and $\tau_{\downarrow}^{\perp}$



This mechanism is called **skew scattering** and dominates the SHE in samples with high electronic mobility

$$\sigma_{\mathrm{sH}}^{\mathrm{s.k.}} \propto \sigma_{xx}$$

Gradhand *et al.*, PRL 104, 186403 (2010) | Fert & Levy, PRL 106, 157209 (2011) | Ferreira *et al.*, PRL 112, 066601 (2014)

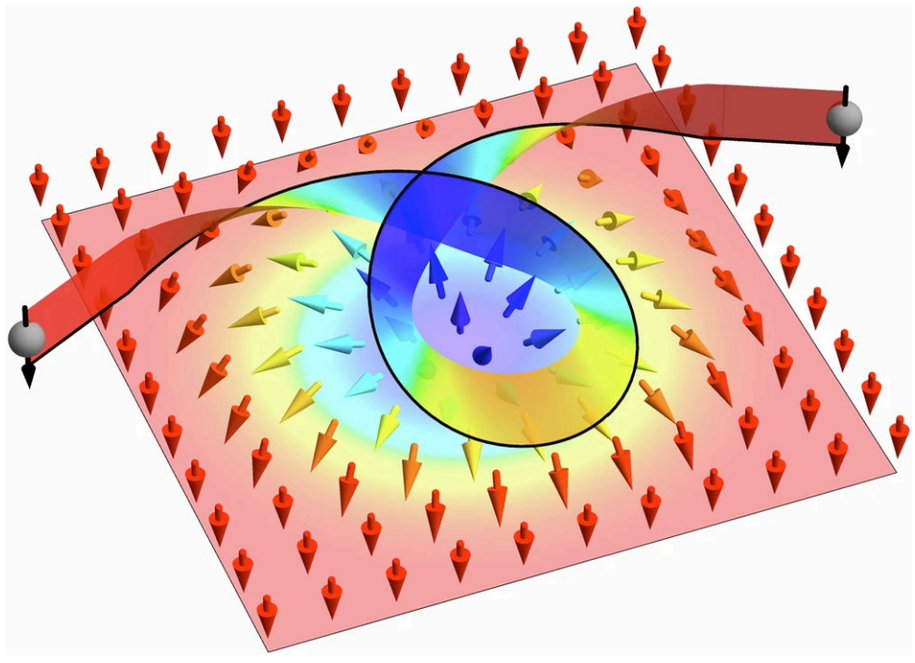
3d. Orbital Hall effect in low-SOC metals

Orbital Hall effect

Predicted in 2005, the OHE has been detected in 2023 a series of experiments with light metals:

Bernevig, PRL 95, 066601 (2005) I Choi, Nature 619, 52 (2023) I Lyalin, PRL 131, 156702 (2023) I Sala PRL 131, 156703 (2023)

Orbital Hall currents are believed to be ubiquitous given that SOC is not essential!



Topological OHE

B. Göbel, L. Schimpf & I. Mertig,
Comm. Phys. 8, 17 (2025)

3d. Orbital Hall effect in low-SOC metals

Orbital Hall effect

Physical origin of OAM?

For a pure Bloch state, the (intra-atomic) OAM is absent: $\langle \psi_{n\mathbf{k}} | \hat{L}_z | \psi_{n\mathbf{k}} \rangle = 0$

Usually a linear combination of cubic harmonics (s, p_x, p_y, p_z, *etc.)*

However, flow of OAM can be in principle generated provided orbitals hybridise

Hybridisation occurs due to interband transitions induced by ***E*** fields

Go, PRL 121, 086602 (2018)

3d. Orbital Hall effect in low-SOC metals

Orbital Hall effect

Modern theory of orbital magnetisation: Intra and inter-atomic OAM: $\hat{\mathbf{L}} = \frac{m_e}{2}\left(\hat{\mathbf{r}} \times \hat{\mathbf{v}} - \hat{\mathbf{v}} \times \hat{\mathbf{r}}\right)$

Computed from $\{\varepsilon_n(\mathbf{k}); |n(\mathbf{k})\rangle\} \longmapsto \langle n\mathbf{k}|\hat{\mathbf{L}}|n'\mathbf{k}'\rangle$

Thonhauser PRL 95, 137205 (2005) | Bhowal, PRB 103, 195309 (2021) | Pezo PRB 106, 104414 (2022) | Bush, PRR 5, 043052 (2023)

Definition is **intuitive**, but $\hat{r}$ operator is problematic for systems with periodic boundary conditions.

Correct evaluation of non-equilibrium orbital currents is currently subject of debate.

This issue has been overcome in the context of equilibrium OAM (magnetisation) in systems with broken $\mathscr{T}$ symmetry

$$\mathbf{m}_{\mathrm{orb}}(\mu, T) = -\frac{e}{2}\sum_n f_n(\mu, T)\,\langle n|\,\mathbf{r} \times \mathbf{v}|n\rangle$$

(Xiao, Shi, Niu, 2005, T. Thonhauser, Vanderbilt, and Resta, 2005, …)

3d. Orbital Hall effect in low-SOC metals

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Similar to the SHE, it is believed that two major mechanisms contribute to the OHE:

intrinsic and extrinsic

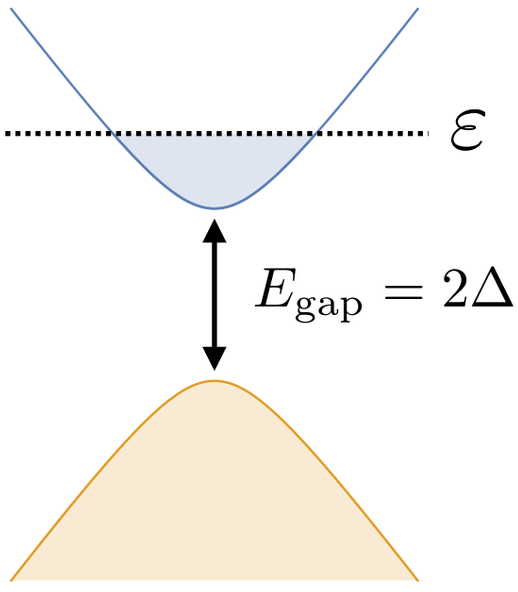
orbital texture of eigenstates (orbital Berry curvature)

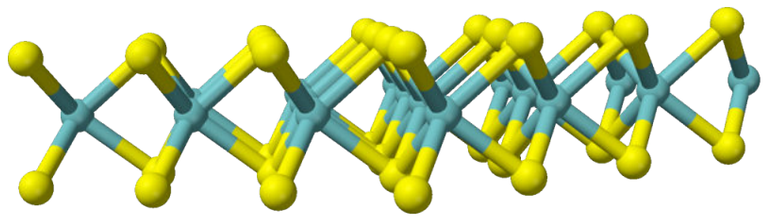
OAM-dependent scattering

3d. Orbital Hall effect in low-SOC metals

Orbital Hall effect

Minimal OHE model: massive 2D Dirac bands (+ random impurities), no SOC!



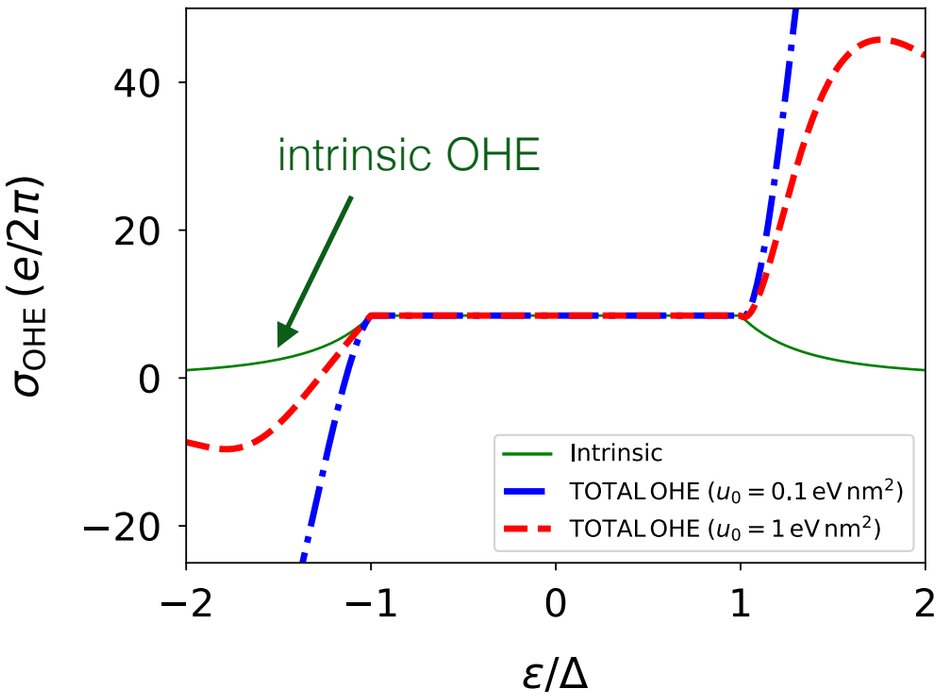


$$\hat{V}_{\rm dis}(\mathbf{x}) = \sum_i u_0\, \delta(\mathbf{x} - \mathbf{x}_i)$$

Veneri, Rappoport & Ferreira. Phys. Rev. Lett. 134, 136201 (2025)

3d. Orbital Hall effect in low-SOC metals

Orbital Hall effect



$$n = 10^{13}\,\mathrm{cm}^{-2} \qquad E_{\mathrm{gap}} = 1.0\,\mathrm{eV}$$

- Strong dependence of σ_{OHE} with scattering potential
- Extrinsic & intrinsic responses have opposite parities

Veneri, Rappoport & Ferreira. Phys. Rev. Lett. 134, 136201 (2025)

3d. Orbital Hall effect in low-SOC metals

Orbital Hall effect

What is causing the strong extrinsic response?

$$L_z(\mathbf{k}) = \mp\hbar \frac{m_e v^2 \Delta}{E_{\mathbf{k}}^2}$$

Wavepackets have opposite OAM at *K* / *K*’ points

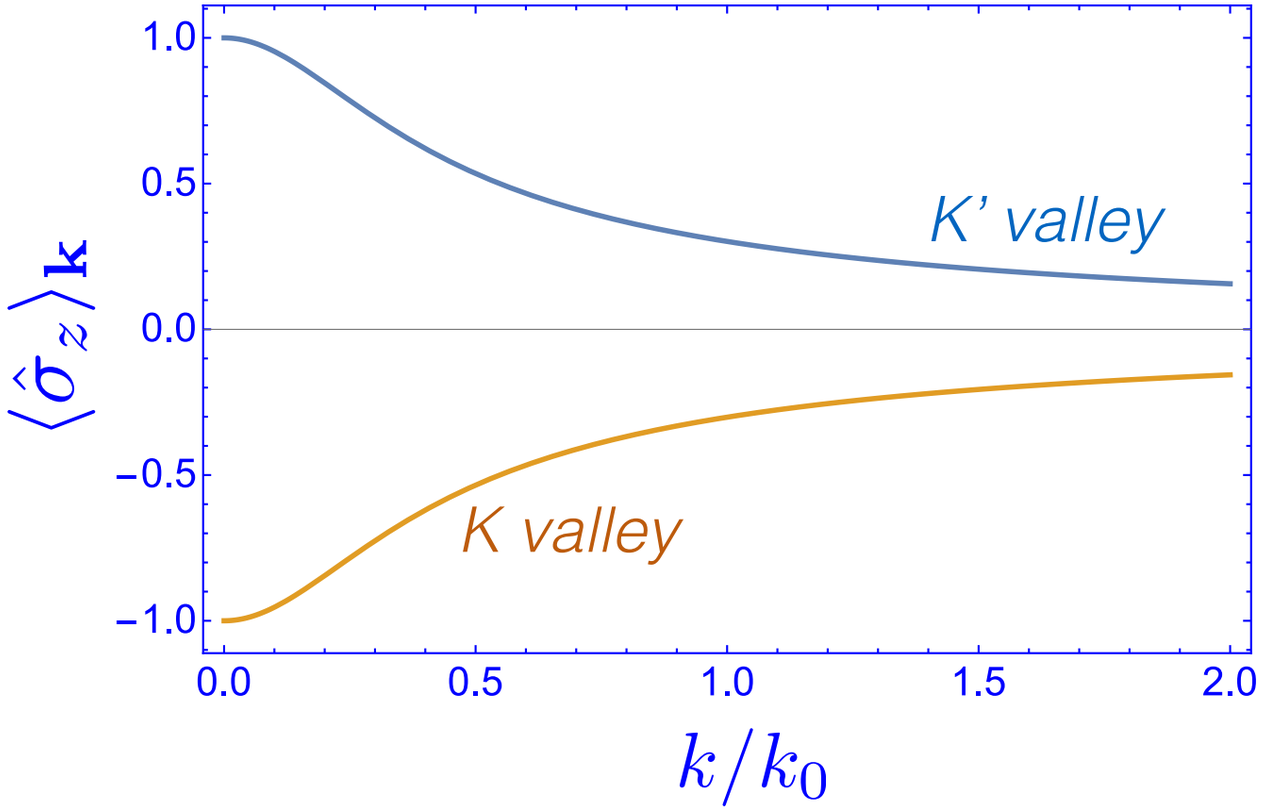
Veneri, Rappoport & Ferreira. Phys. Rev. Lett. 134, 136201 (2025)

3d. Orbital Hall effect in low-SOC metals

Orbital Hall effect

What is causing the strong extrinsic response?

Pseudo-spin texture of conduction electrons

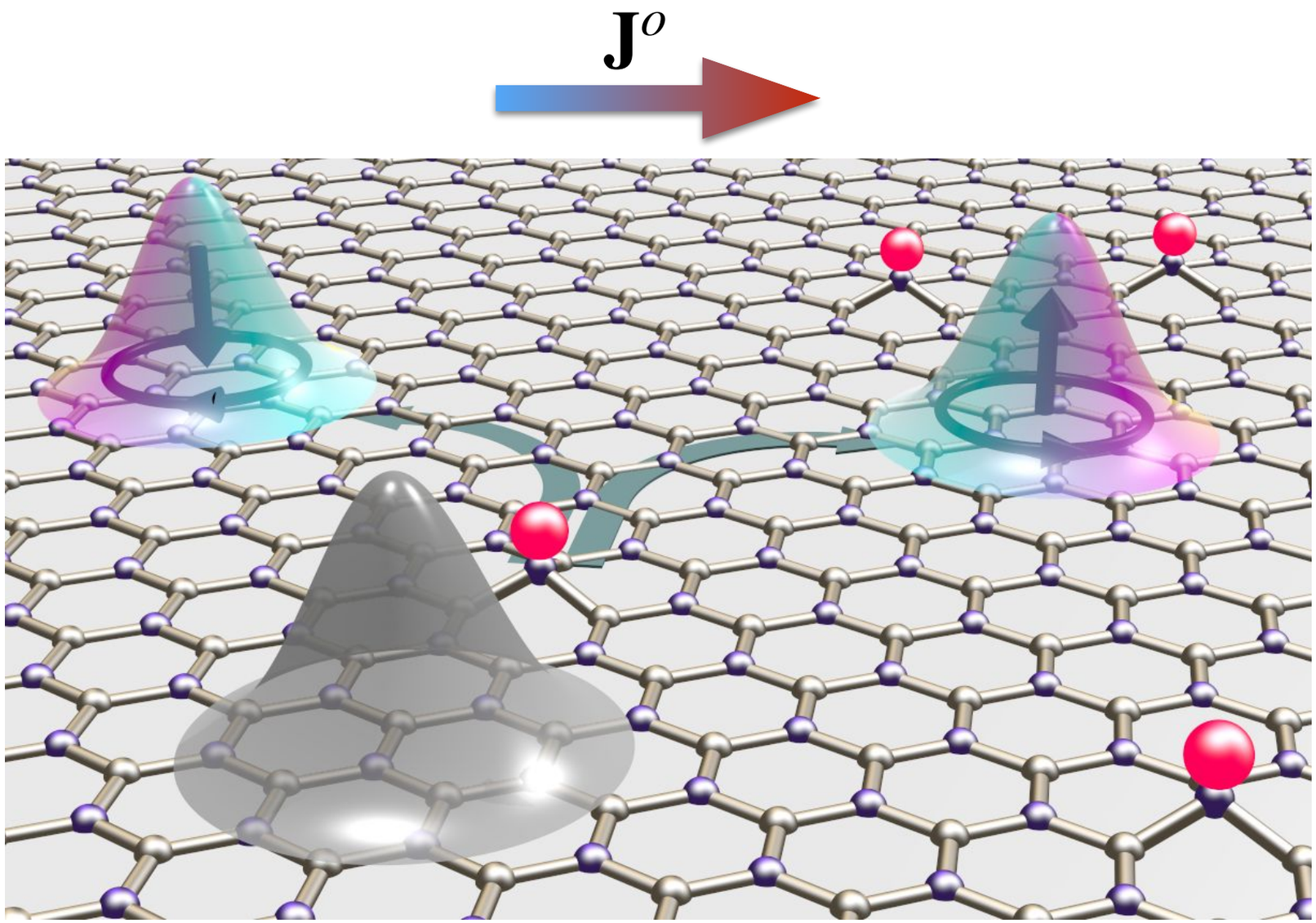


This defines a quantisation axis $\| \hat{z}$ *for orbital skew scattering!*

Veneri, Rappoport & Ferreira. Phys. Rev. Lett. 134, 136201 (2025)

3d. Orbital Hall effect in low-SOC metals

Orbital Hall effect



Orbital skew scattering *[without SOC]*

Veneri, Rappoport & Ferreira. **Phys. Rev. Lett. 134, 136201 (2025)**

End

Thank you for your attention!

Contact: aires.ferreira at york.ac.uk