A Short Journey Through Spin-Orbitronics

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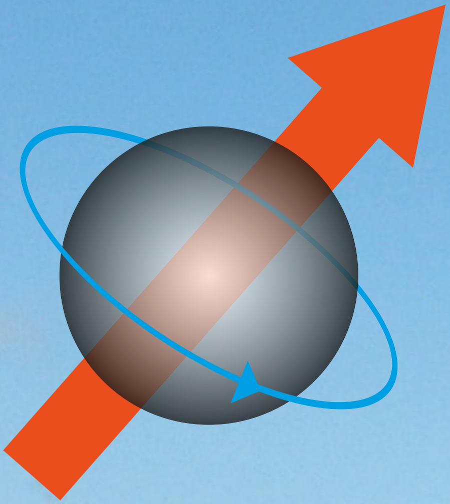


2024 European School on Magnetism

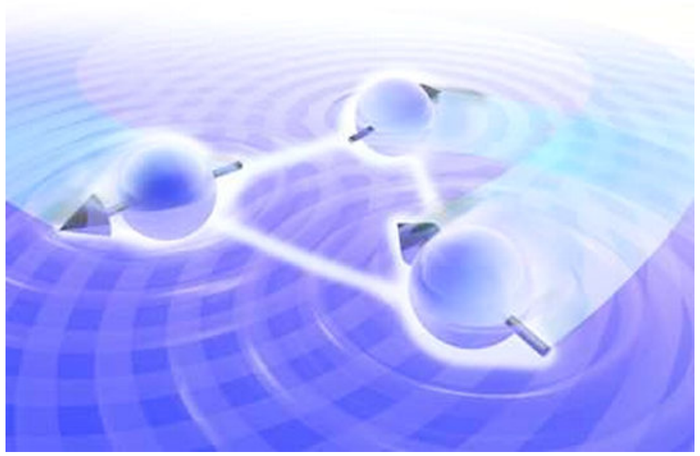
Spintronics

"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



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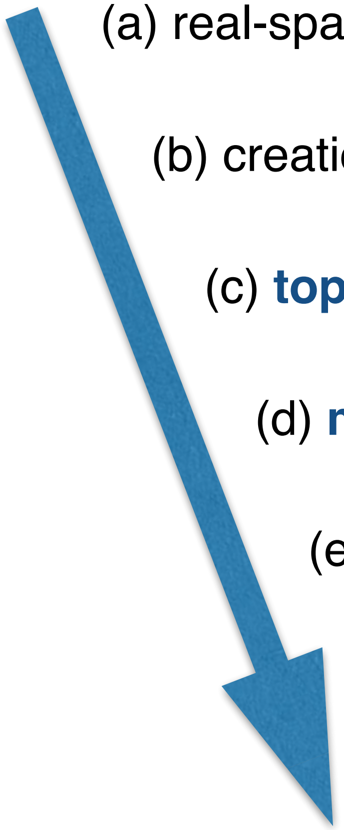


(a) real-space **spin textures** in magnetic systems

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

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

(d) **magnetisation dynamics**

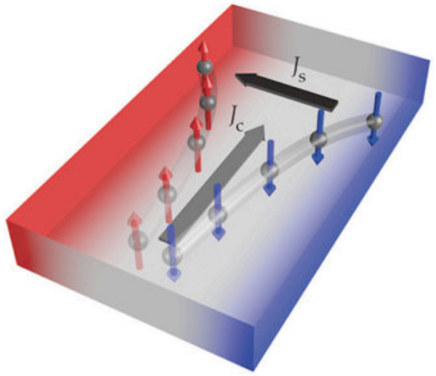
(e) spin and orbital moment **relaxation**

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

…

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) …

Timeline



Spin Hall effect (Prediction)

70s

Spin current

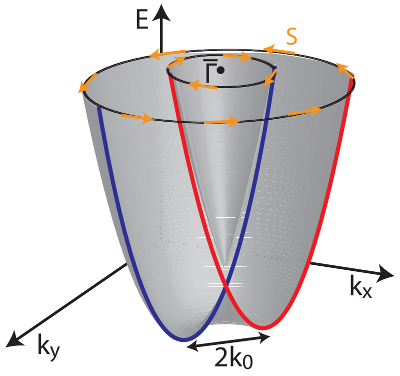
Spin-polarised currents (FM/SC junctions)

Spin-valve effect (SV) [giant magneto-resistance (GMR)]

80s

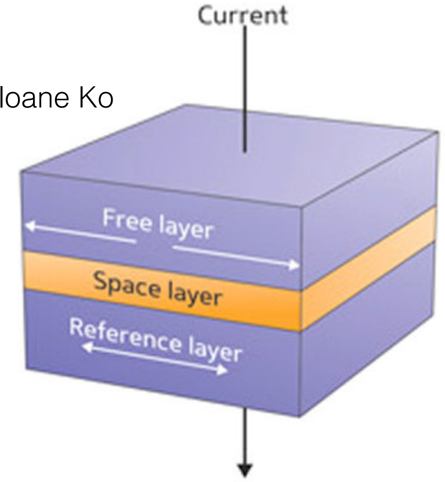
GMR

Broken symmetry & spin galvanic effects (SGEs)



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

© 2010 Viloane Ko



Bulk SV effects & Perpendicular GMR

90s

CPP-GMR

Optical spin injection & detection in Semiconductors (SCs)

All-metal room-T LSVs

2D spintronics

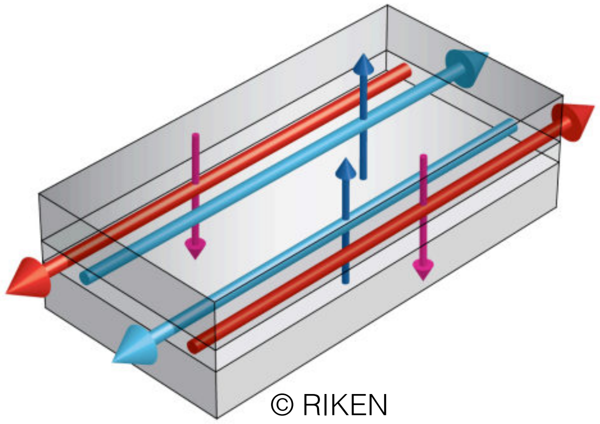
magnonics

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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STT-MRAM

10s

SOT, AFs

Antiferromagnetic (AF) metal spintronics

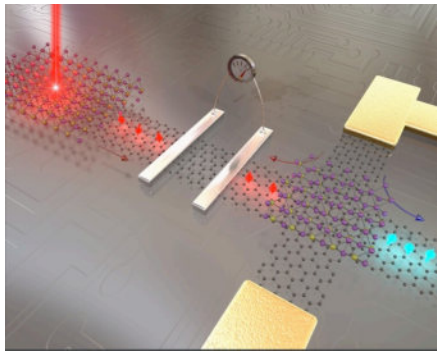
Spin-orbit torque (SOT)

20s

On-going

Orbitronics

Altermagnets



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Outline

Today's focus: Some fundamentals of spintronics and orbitronics

1. Spin currents & orbital currents in solids
2. Spin-orbit coupling in **k**-space & broken symmetries
3. Spin relaxation & out-of-equilibrium (transport) processes

Next Week [Felix Casanova]:

➡ Discovery of spin Hall effect (SHE)

➡ Spin-momentum locking in topological insulators

➡ Inverse spin galvanic effect

and more!

Notation for this lecture

- ***bold*** *symbols for vector/pseudo-vector quantities*
- *acronyms:* ***SO*** *= spin-orbit;* ***SOC*** *= spin-orbit coupling;* ***OAM*** *= orbital angular momentum*
- *Natural units with $\hbar = 1$:*

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*:*

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

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

[mixed states]

- ***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:*

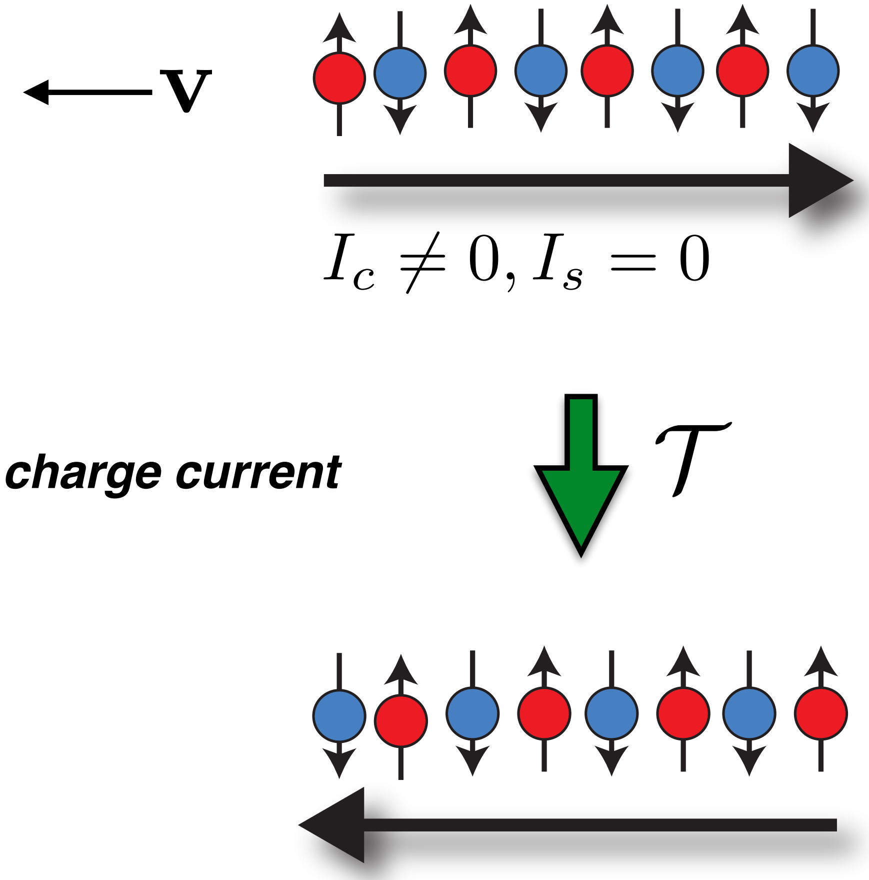
Mirror reflection about the yz-plane

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

1. Spin and orbital currents

- ***Intuitive definition***

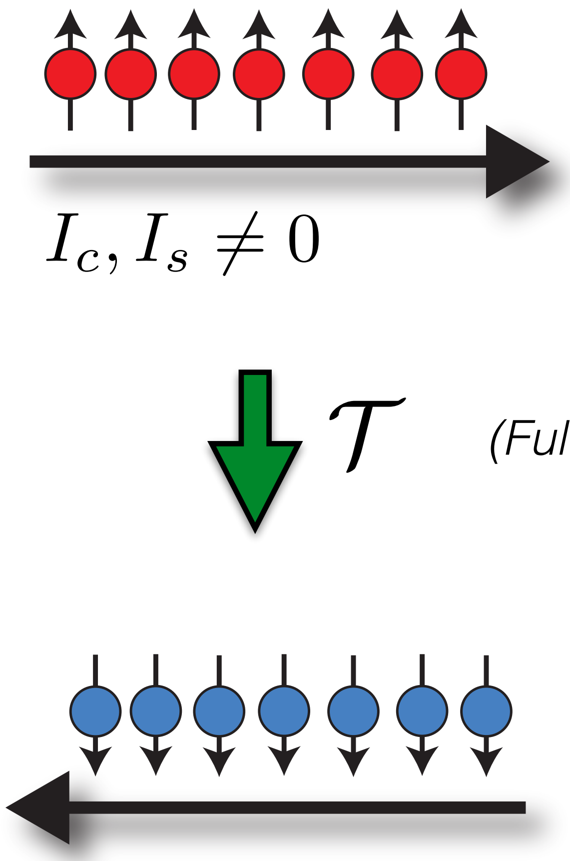
charge current $$I_c = \sum_{\sigma=\uparrow,\downarrow} I_\sigma = I_\uparrow + I_\downarrow$$ → **spin current** $$I_s = \sum_{\sigma=\uparrow,\downarrow} s_\sigma I_\sigma = I_\uparrow - I_\downarrow$$



$$I_c \neq 0, I_s = 0$$

Pure charge current $\mathcal{T}$

$$I_c \to -I_c$$



$$I_c, I_s \neq 0$$

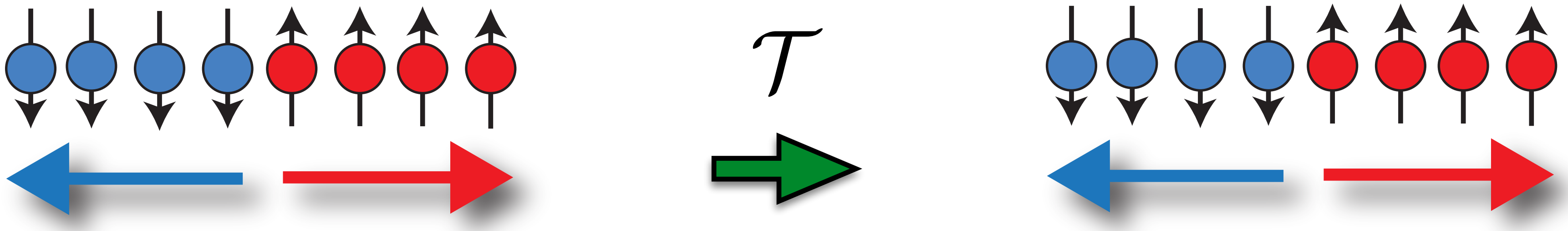
$\mathcal{T}$ *(Fully)* ***spin-polarised current***

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

1. Spin and orbital currents

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

Pure spin currents:



Invariant under $\mathscr{T}$

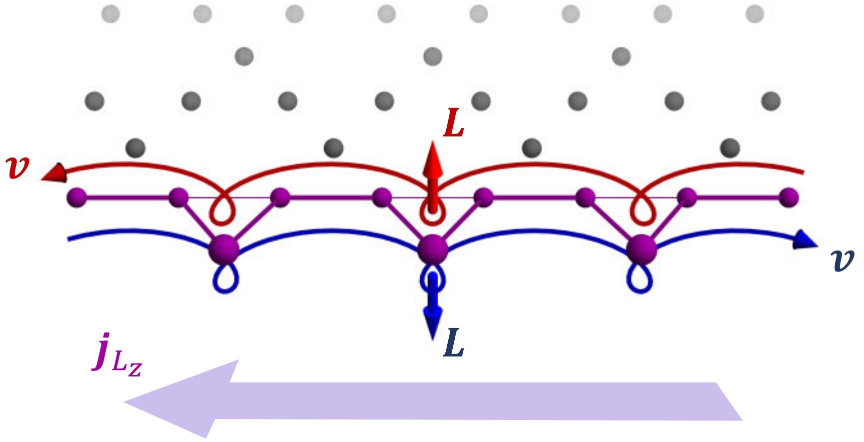
(non-dissipative)

- 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)

Pure orbital currents:

- OAM version of a spin current
- Exist irrespective of orbital composition
- Do not require SOC!



Bush, PRR 5, 043052 (2023)

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)

1. 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:

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

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: $$\hat{\mathbf{j}}_s^a = \frac{\hbar}{4}\left\{\hat{\mathbf{v}}, \hat{s}^a\right\}$$ → *anti-commutator*

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

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

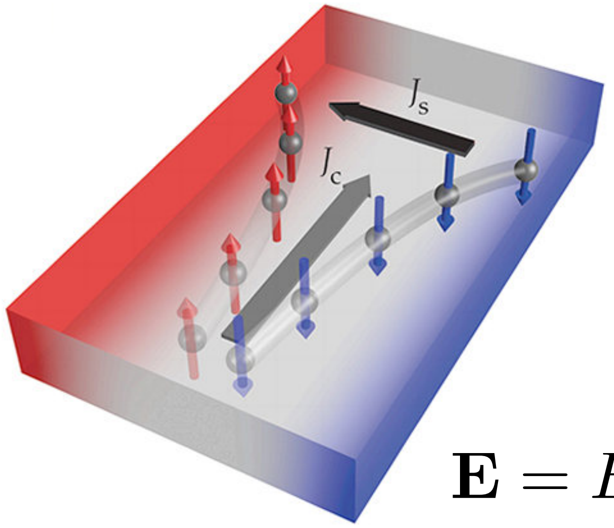
spin sink/source *term*
or 'torque density' usually due to SOC

Orbital current operator: can be defined in an analogous fashion with $\hat{s}^a \rightarrow \hat{L}^a$

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

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

Spin and orbital currents: role of symmetries



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

Which kinds of non-equilibrium effects can emerge in a given material?

Spin Hall effect (SHE): $$j^a_{s,j} = \sigma^a_{jx}\, E_x$$

Consider a crystal structure with 3 perpendicular mirror planes

Under $x \to -x$, we have $E_x \to -E_x$ but $j^z_{s,x} \to +j^z_{s,x}$. ➡ $\sigma^z_{xx} = 0$

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 ⟹	✗	✗	✗	✗	✗	✓	✗	✓	✗

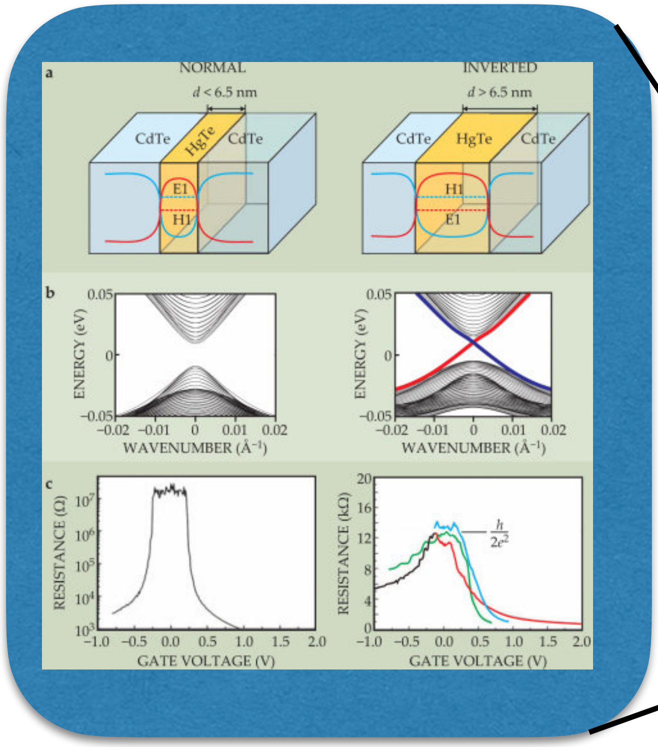
± = same (opposite) parity

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

$\hat{U}_x\, \hat{s}_z\, \hat{U}_x = -\hat{s}_z$ and $\hat{U}_x\, \hat{v}_x\, \hat{U}_x = -\hat{v}_x$ ➡ $\hat{U}_x\, \hat{j}^z_{s,x}\, \hat{U}_x = +\hat{j}^z_{s,x}$

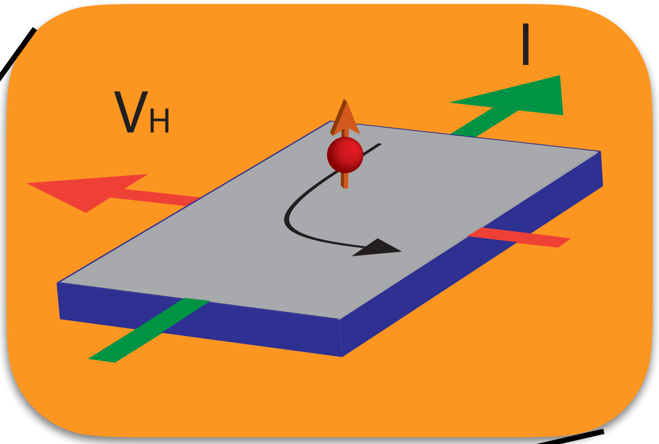
2. Spin-orbit coupling & broken symmetries

Z2 Topological Insulator



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

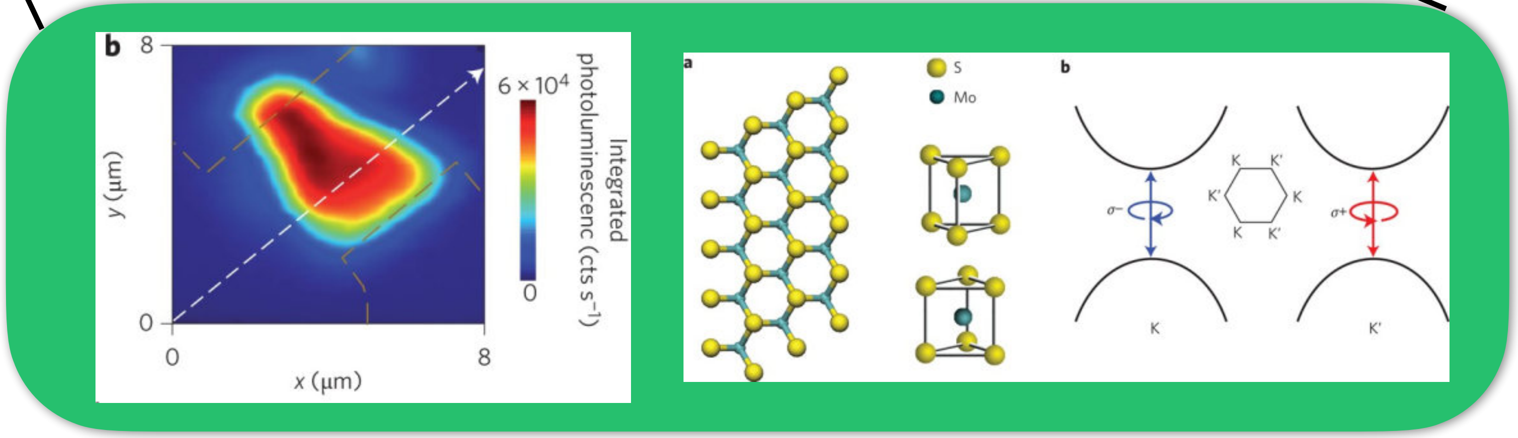
Spin/Anomalous Hall effects



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

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

Excitonic spin-valley coherence

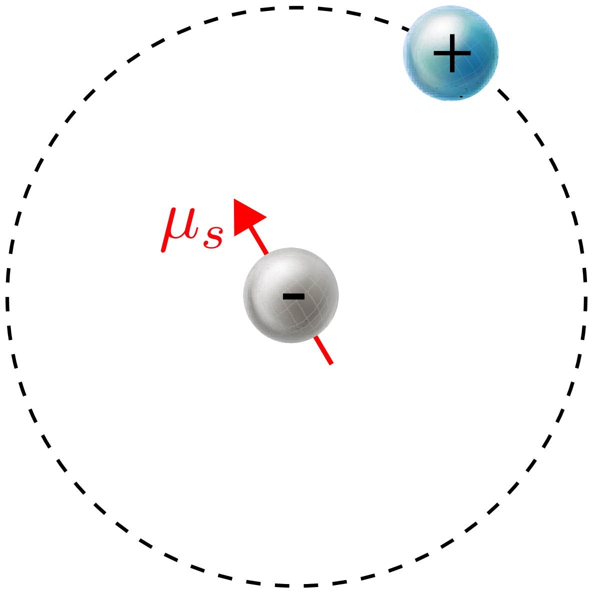


G. Wang *et al.*,
Rev. Mod. Phys. 90, 021001 (2018)

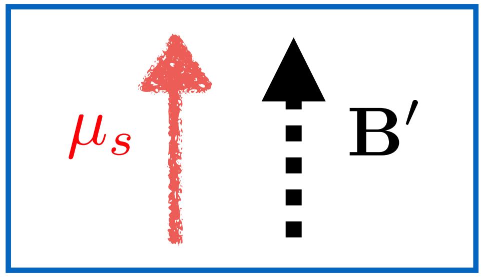
2. Spin-orbit coupling & broken symmetries

Revisiting atomic physics

➡ Electron experiences a magnetic field in its rest frame



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

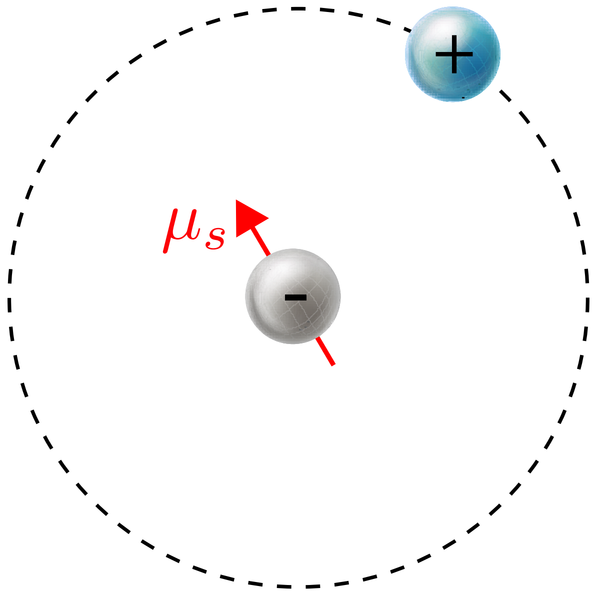


$$\mathbf{B}' \simeq -\frac{1}{c^2}\mathbf{v} \times \mathbf{E}$$

2. Spin-orbit coupling & broken symmetries

Revisiting atomic physics

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

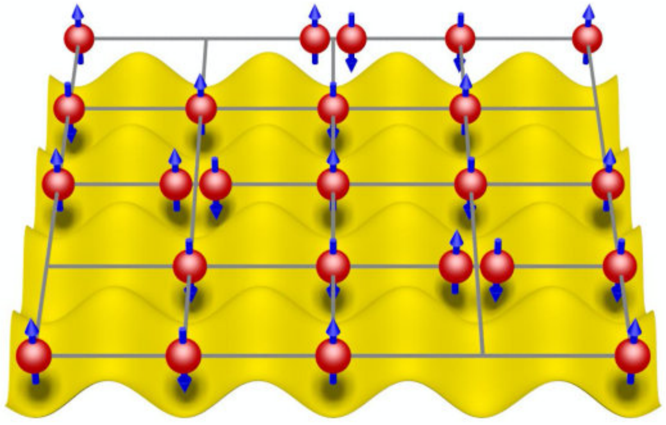


$$V_{\mathrm{SO}} = \frac{1}{2m^2c^2}(\nabla V \times \mathbf{p}) \cdot \mathbf{s}$$

- Even a H atom is affected by SOC (fine structure)
- SOC strength grows as Z^3 - Z^4

2. Spin-orbit coupling & broken symmetries

SOC in a crystal lattice



➡ **Symmetry-independent SOC**

✳ **Exists in every crystal structure**

(stems from atomic SOC)

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

✳ **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**

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

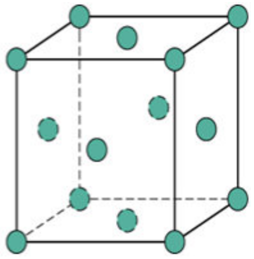
✳ **time-reversal symmetry**

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

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

Kramers degeneracy

- SOC lifts band degeneracies (orbital splitting)



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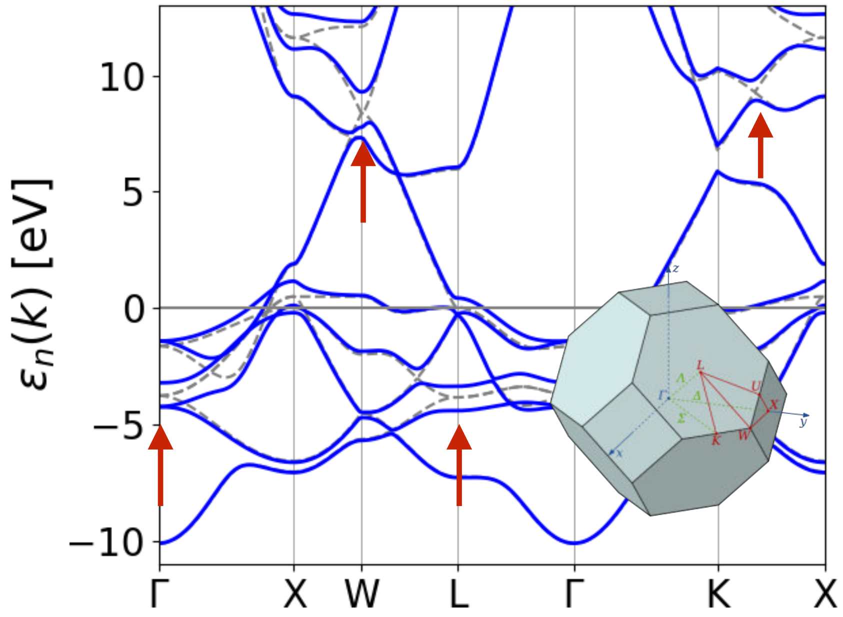


2. Spin-orbit coupling & broken symmetries

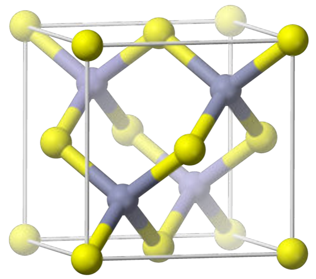
SOC in a crystal lattice

➡ **Symmetry-dependent SOC**

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

✳ Dresselhaus interaction (bulk inversion asymmetry)

G. Dresselhaus. ‘55



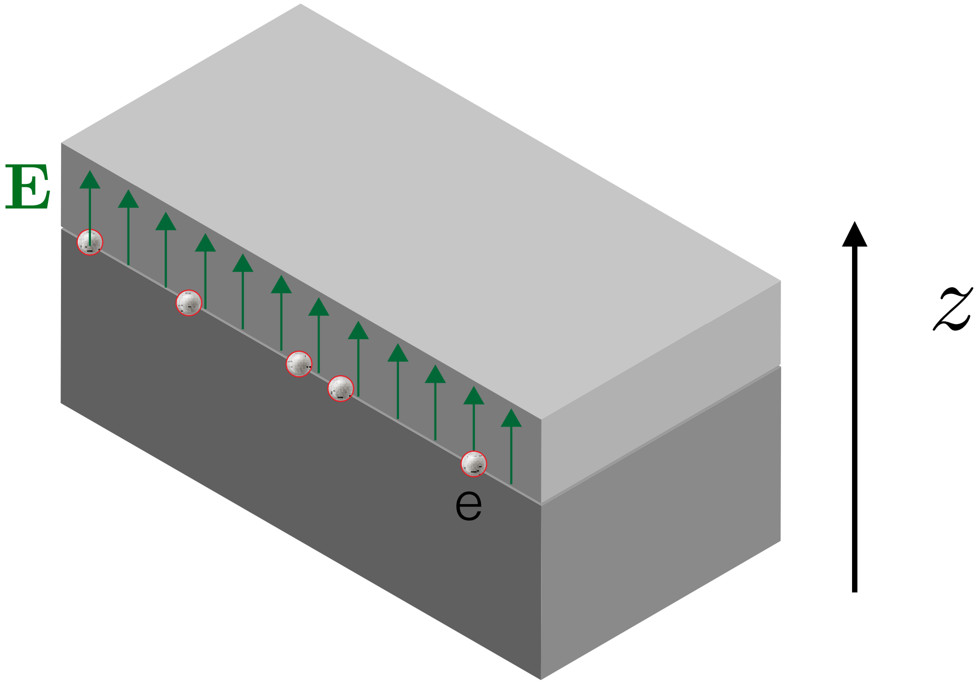
✳ Bychkov-Rashba interaction (structural inversion asymmetry @ surface/interface)

Y. A. Bychkov, E. I. Rashba, ‘84

2. Spin-orbit coupling & broken symmetries

Symmetry breaking

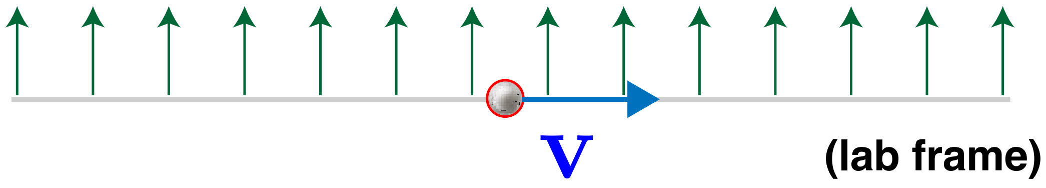
➡ **The Rashba effect**

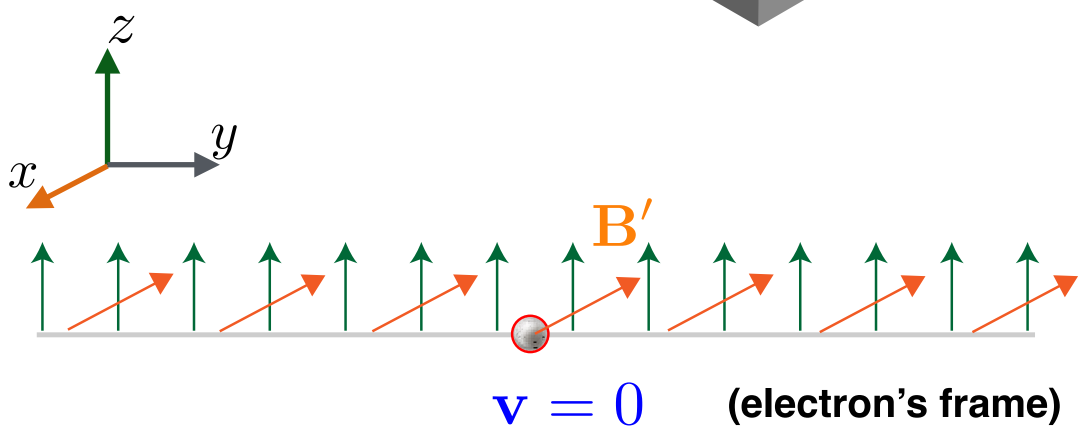


Non-relativistic band dispersion of a 2D electron gas:

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

Relativist frame change:





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

in-plane effective SO field

2. Spin-orbit coupling & broken symmetries

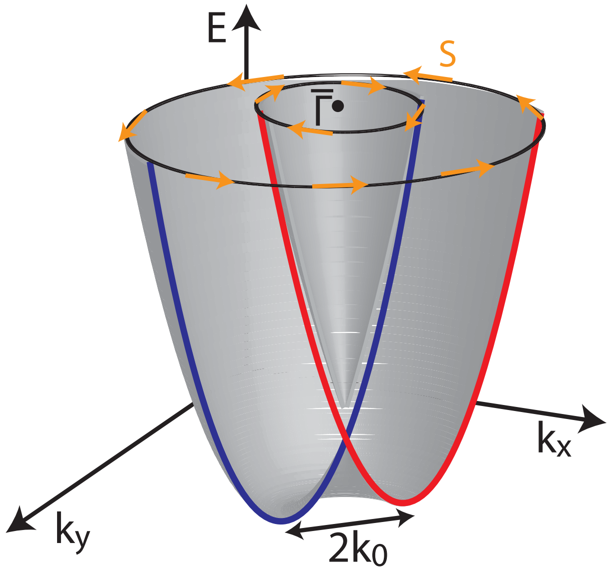
Symmetry breaking

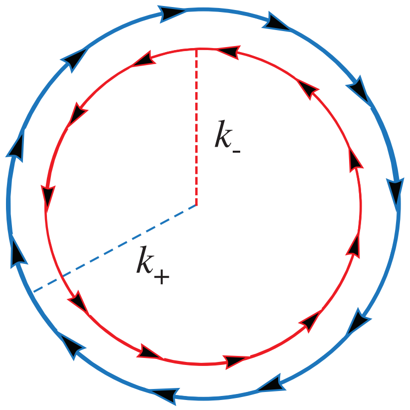
➡ **The Rashba effect**

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

✳ **BR spin-orbit field**

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





***k*-space spin texture**

$$\boxed{\mathbf{s}_n(\mathbf{k}) = \langle u_{n\mathbf{k}} | \,\hat{\mathbf{s}}\, | u_{n\mathbf{k}} \rangle}$$

spin-orbit entangled Fermi surface

2. Spin-orbit coupling & broken symmetries

Time reversal symmetry

➡ **Anti-unitary symmetries**

Fermi-Dirac distribution function

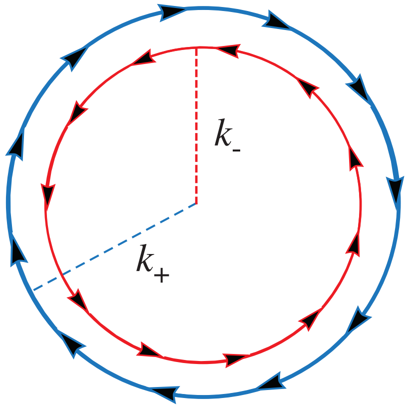
$$\mathbf{s}_{\text{eq.}} = \text{Tr}\left[\hat{\mathbf{s}}\,\hat{\rho}_{\text{eq}}\right] = \sum_{n,\mathbf{k}} f_n(\mathbf{k})\, s_n(\mathbf{k}) = 0$$

single-electron picture

This holds in general for a TR-invariant system:

$$\mathcal{T}^{-1}\hat{\mathbf{s}}\,\mathcal{T} = -\hat{\mathbf{s}} \quad ➡ \quad \mathbf{s}_{\text{eq.}} = 0$$

***k*-space Rashba spin texture**



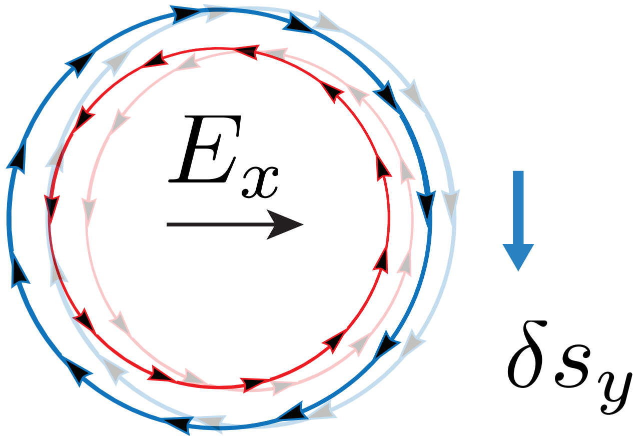
$$s_n(\mathbf{k}) = -s_n(-\mathbf{k})$$

2. Spin-orbit coupling & broken symmetries

Out-of-equilibrium physics are different!

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

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



Inverse spin-galvanic (Edelstein) effect: $\delta s_y = K_{yx}\,E_x$

Broken $z \to -z$ symmetry

Sanity check:

$x \to -x$: $\{s_y, E_x\} \to \{-s_y, -E_x\}$

$y \to -y$: $\{s_y, E_x\} \to \{s_y, E_x\}$

More about the ISGE next Week [Felix Casanova]

3a. Spin-orbit relaxation

Due to SOC and other spin-dependent effects:

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

Spin non-conservation

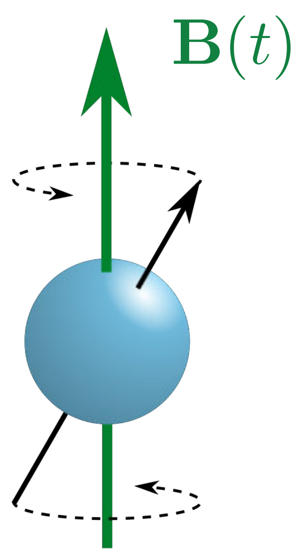
Example: **Larmor precession**

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

Heisenberg picture:

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

field-like torque



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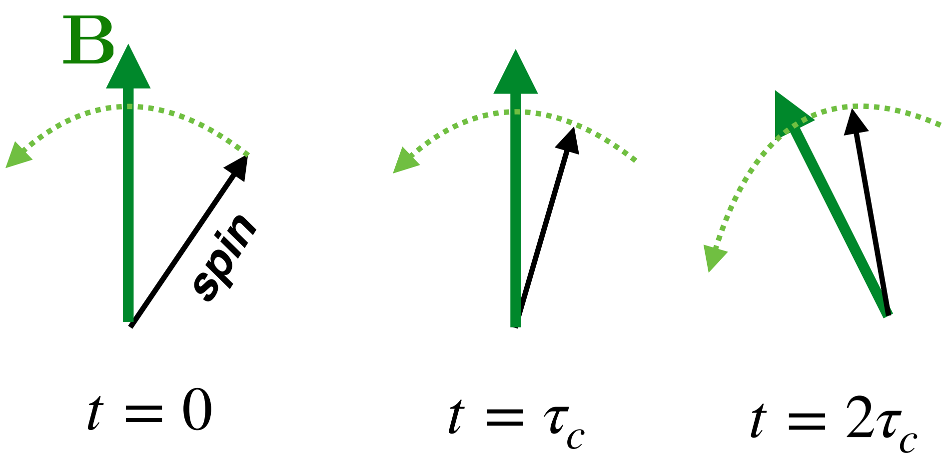
3a. Spin-orbit relaxation

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 (*)*

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



τ_c = *correlation (scattering) time*

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

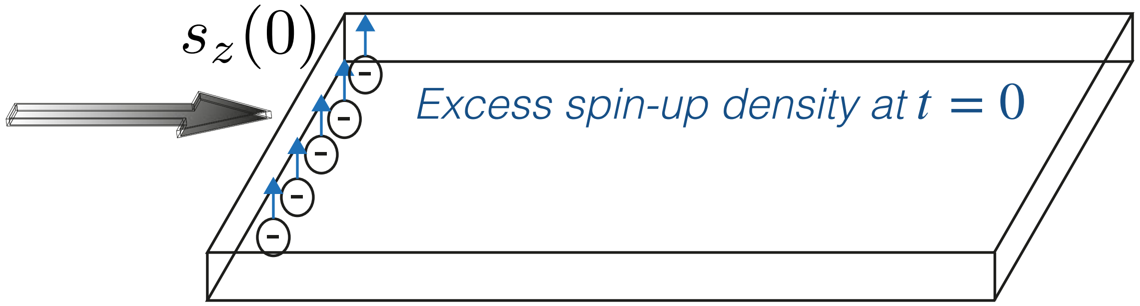
Memory of initial state is lost at time after N *steps,*
when the variance equals one, i.e. $\sigma^2 = N\Delta\phi^2 = 1$

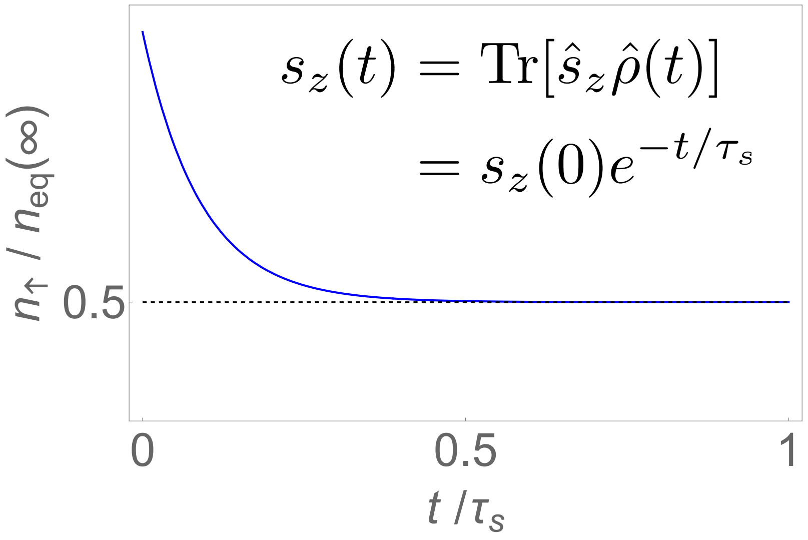
$$1/\tau_s = \omega^2\tau_c$$

(*) 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





$$s_z(t) = \mathrm{Tr}[\hat{s}_z \hat{\rho}(t)]$$
$$= s_z(0)e^{-t/\tau_s}$$

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

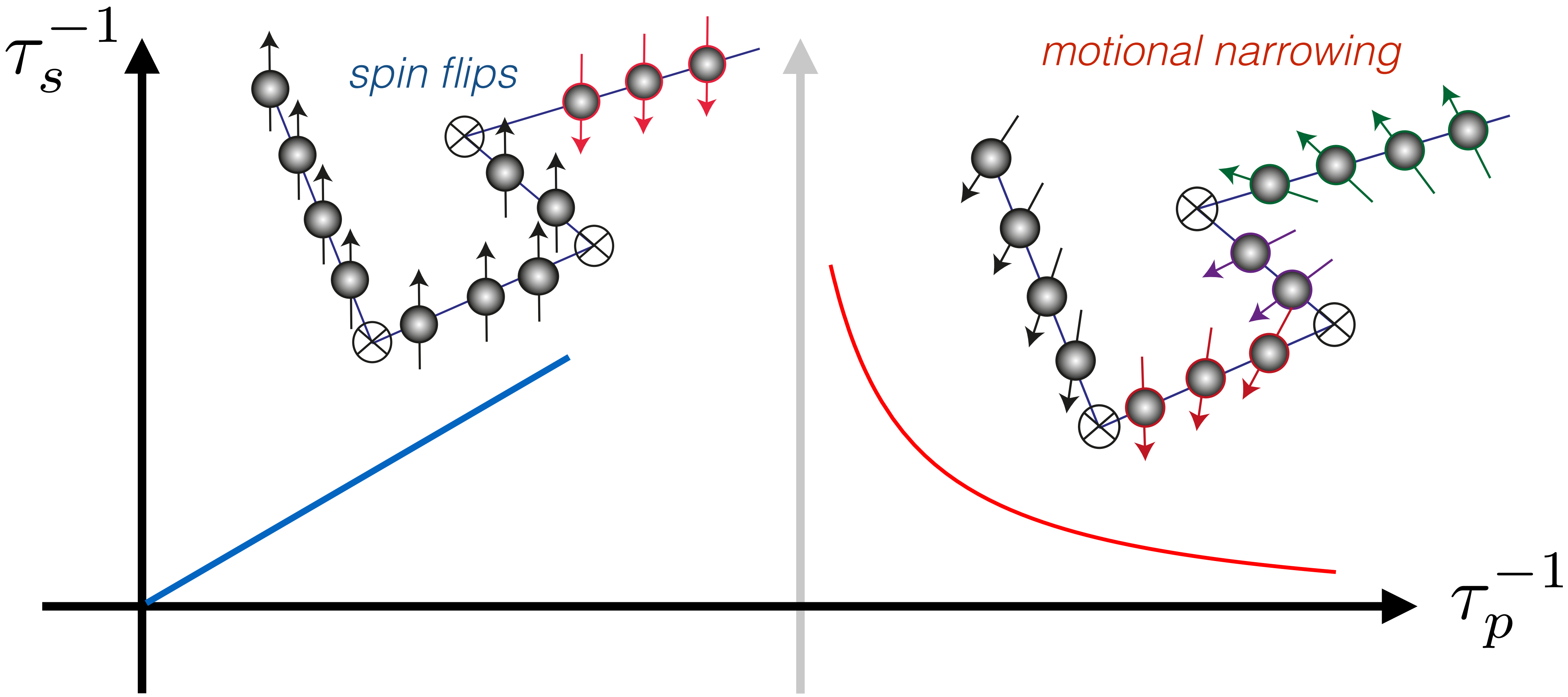
Spin-relaxation mechanisms from non-magnetic impurities:

Elliott-Yafet (centrosymmetric systems)

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

Dyakonov-Perel (non-centrosymmetric systems)

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



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

3a. Spin-orbit relaxation

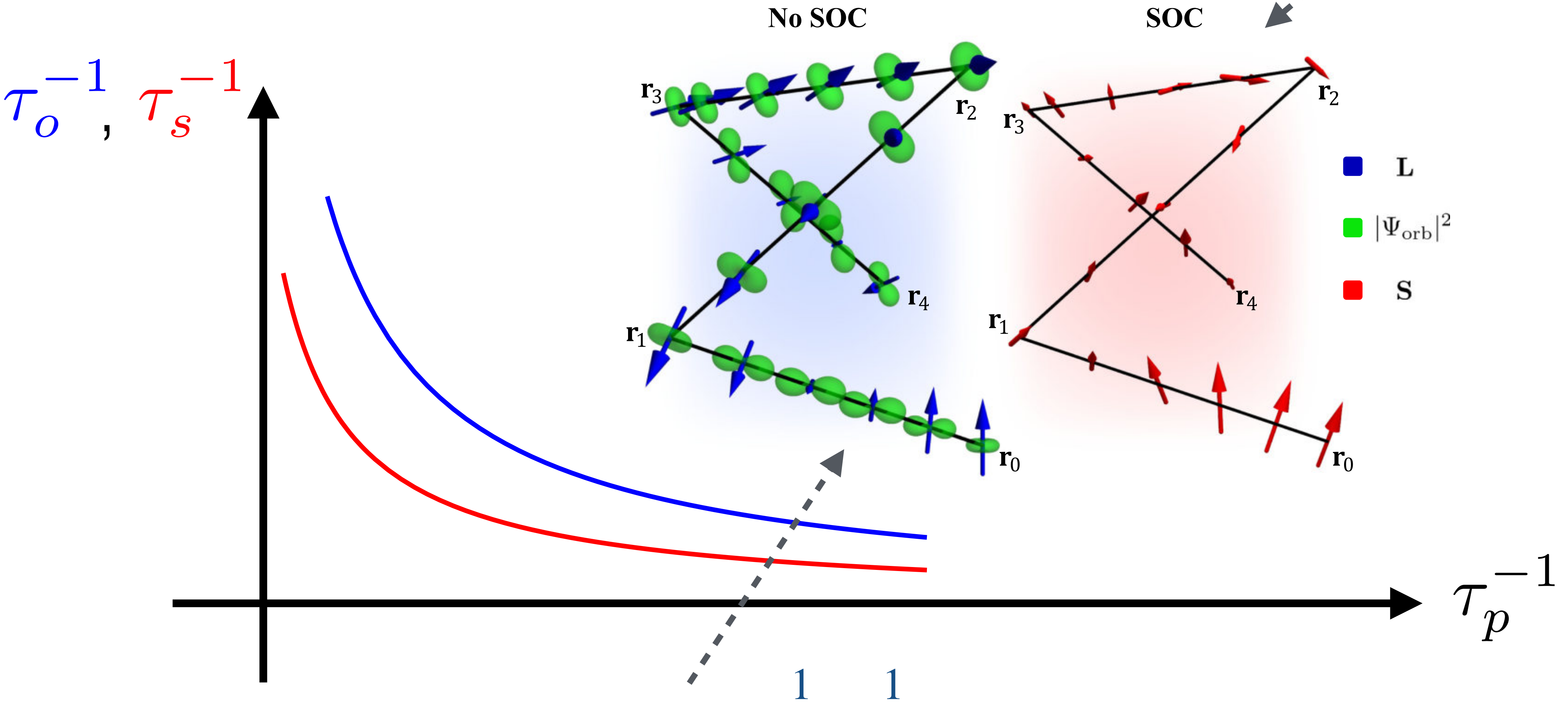
Dyakonov-Perel-like relaxation in centrosymmetric systems

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: $\tau_s \propto \frac{1}{\tau_p}\frac{1}{\lambda_{SO}^2}$

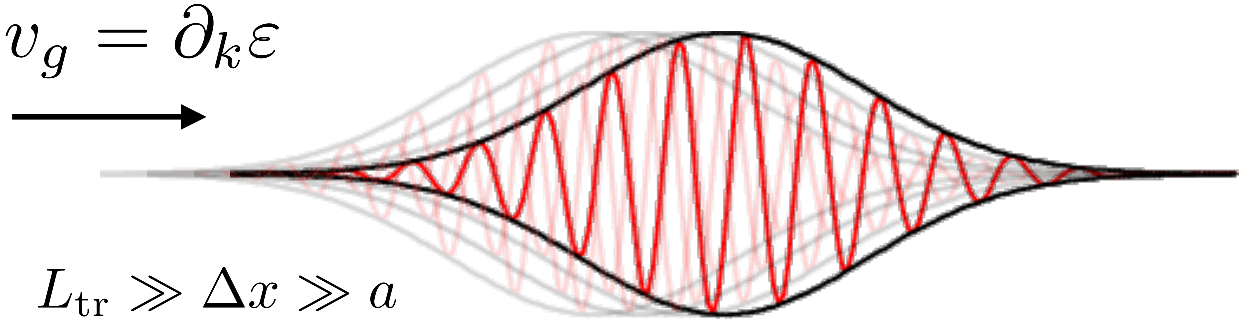


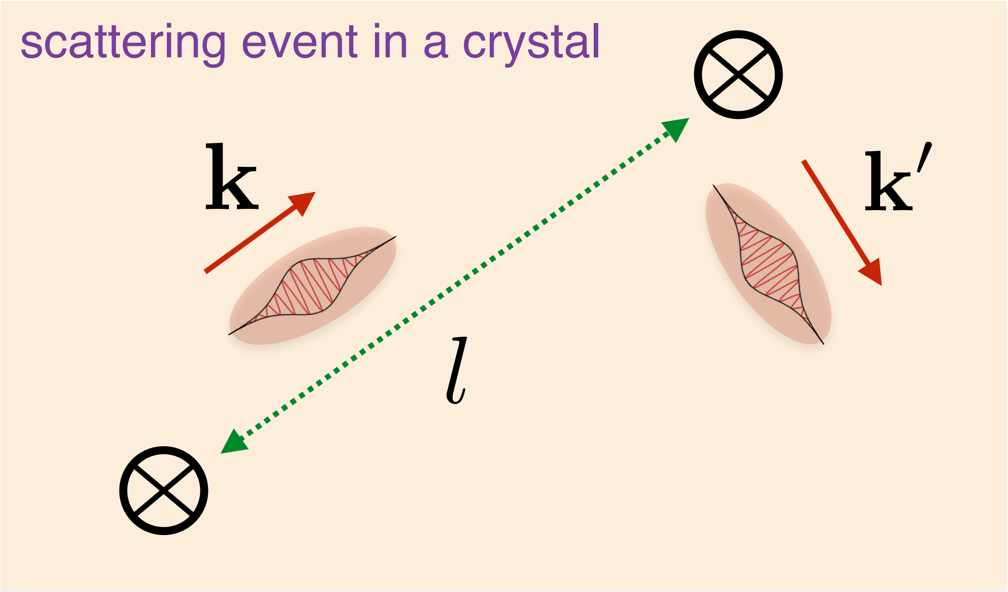
Orbital relaxation: $\tau_o \propto \frac{1}{\tau_p}\frac{1}{(c_1 k_F^2)^2}$

3b. Spin transport in metals

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

Wavepackets (WPs) with well defined $\mathbf{k} = \mathbf{k}_\mathbf{c}$ (i.e., with an uncertainty much smaller than BZ size) $\Delta k \ll G_1 \propto a^{-1}$





semiclassical condition

$$\boxed{\lambda_F \ll l \Leftrightarrow k_F l \gg 1}$$

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

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).

Solid State Physics,
Ashcroft and Mermin (1976)

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:

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

$\dot{\mathbf{r}} \to \mathbf{v}_{\mathbf{k}}$ *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)

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

acceleration term *scattering term*

Steady state &
homogenous system:

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

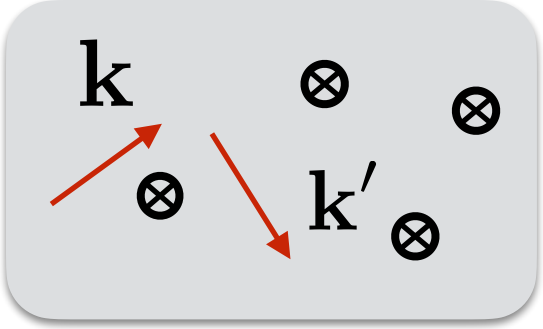
Also, to linear order in
the external field:

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

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)

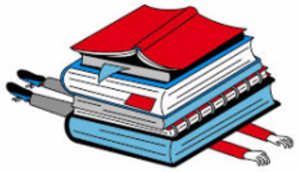
$W_{\mathbf{k}\to\mathbf{k}'}$ can be computed quantum mechanically, but a microscopic model is required.
Consider a disorder landscape of random, short-ranged impurities:

scattering potential strength

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

δ-function is justified due to screening

set of impurity positions



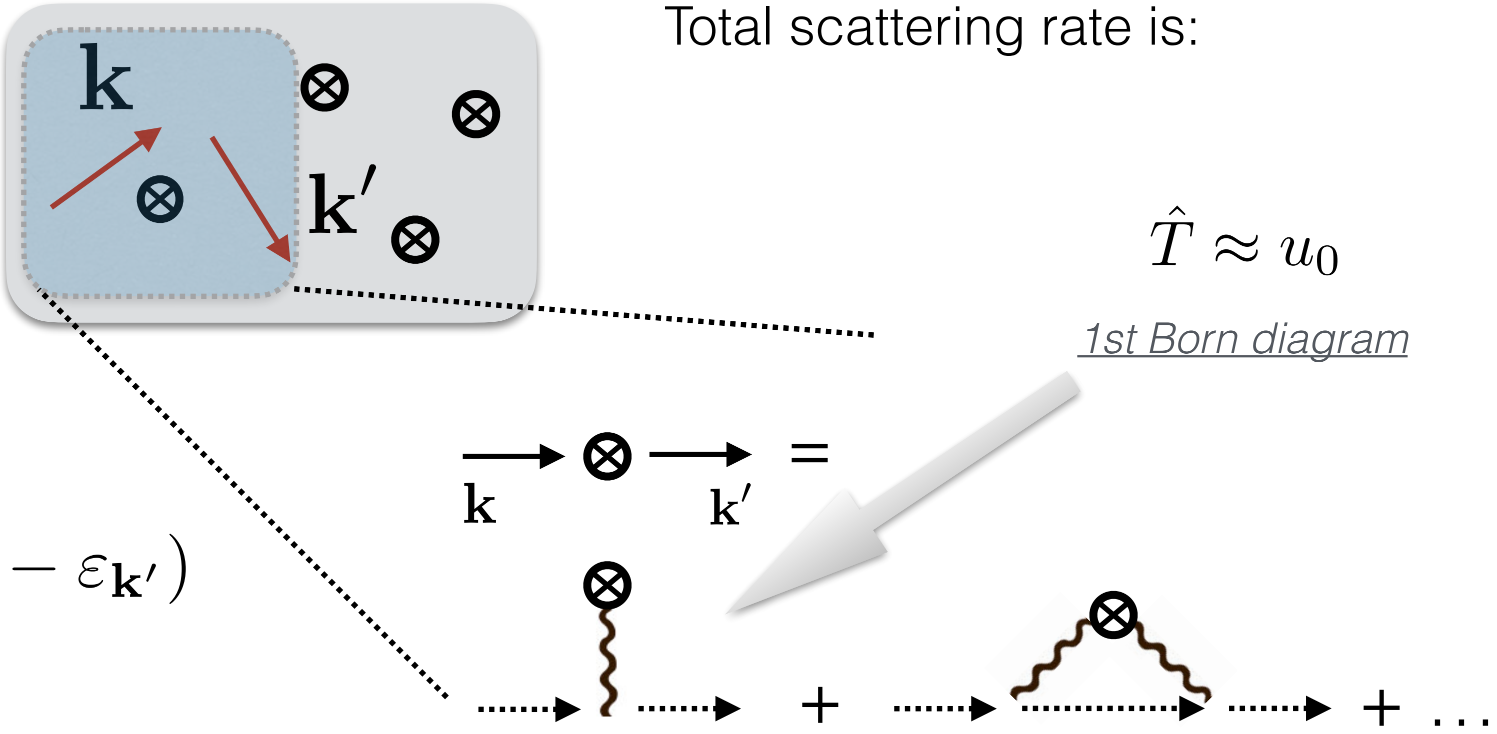
Show that $\sum_{\mathbf{k}}\left.\frac{\partial f(\mathbf{k})}{\partial t}\right|_{\text{coll}}=-\sum_{\mathbf{k}}\sum_{\mathbf{k}'}\left[\delta f(\mathbf{k})-\delta f(\mathbf{k}')\right]W_{\mathbf{k}\to\mathbf{k}'}=0$ and interpret this result.

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

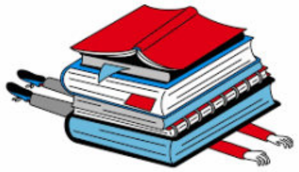
Generalised Golden rule

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

T-matrix

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

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



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?

3b. Spin transport in metals

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

The transport equation can be solved exactly 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**)

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

Non-equilibrium quantities can now be easily computed :

- $g_s = 2$ 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

Charge carrier density:

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

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

where

$$\boxed{\sigma_{ij} = \frac{1}{3}\,e\,\varrho(\varepsilon_F)\,v_F^2\tau_F\,\delta_{ij}}$$

$(i, j = x, y, z)$

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

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

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

Detailed balance condition:

$$\sum_{\mathbf{k}}\left.\frac{\partial f(\mathbf{r},\mathbf{k})}{\partial t}\right|_{\text{coll}} = 0$$

$$\frac{\partial n}{\partial t} + \nabla_{\mathbf{r}}\left[\frac{g_s}{V}\sum_{\mathbf{k}}(-e\mathbf{v}_{\mathbf{k}})f(\mathbf{r},\mathbf{k})\right] = 0$$

$$\boxed{\frac{\partial n}{\partial t} + \nabla\cdot\mathbf{j}_c = 0}$$

Number conservation of electrons

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

$$\mathbf{j}_c(\mathbf{r}) = \underbrace{\sigma_c\,\mathbf{E}}_{\textit{Drift}} + \underbrace{D\boldsymbol{\nabla}n}_{\textit{Diffusion}}$$

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

3b. Spin transport in metals

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

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

T. Valet

A. Fert

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

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

Spin-flip terms:

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

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

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)


T. Valet


A. Fert

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

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

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

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

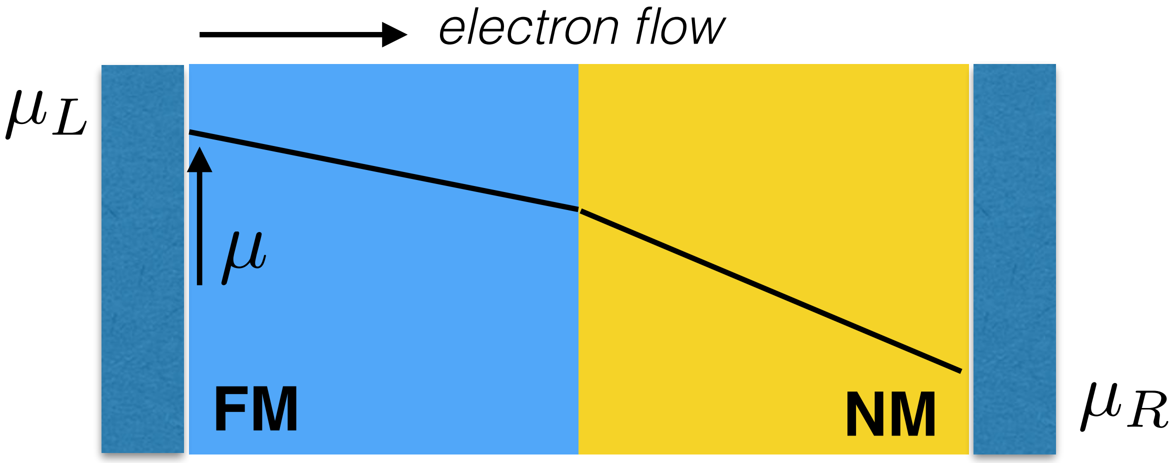
In normal metals,
$\tau_{sf} \gg \tau_{\uparrow\uparrow}$ leading to $l_s \gg l$

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



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

Constitutive relation + spin continuity equation:

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

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

spin diffusion equation

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

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

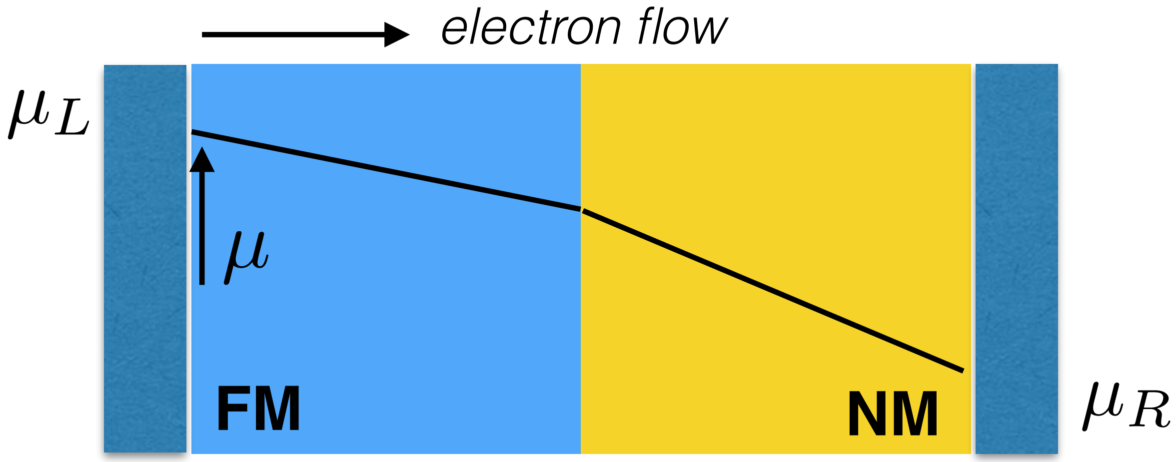
Son, PRL 52, 2271 (1987) I Valet and Fert, PRB 48, 7102 (1993) I Yu and Flatte, PRB 66, 201202(R) (2002)

3b. Spin transport in metals

Spin interface resistance & the GMR effect

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

spin diffusion equation

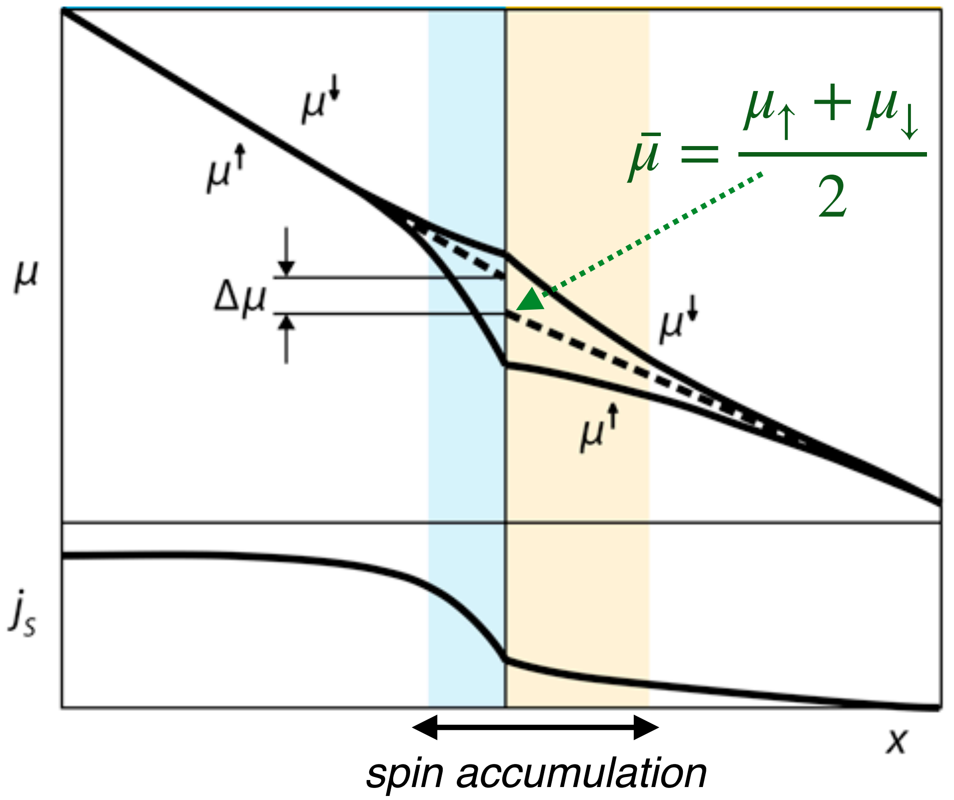


Diffusive regime: lateral dimensions $\gg l, l_s$

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



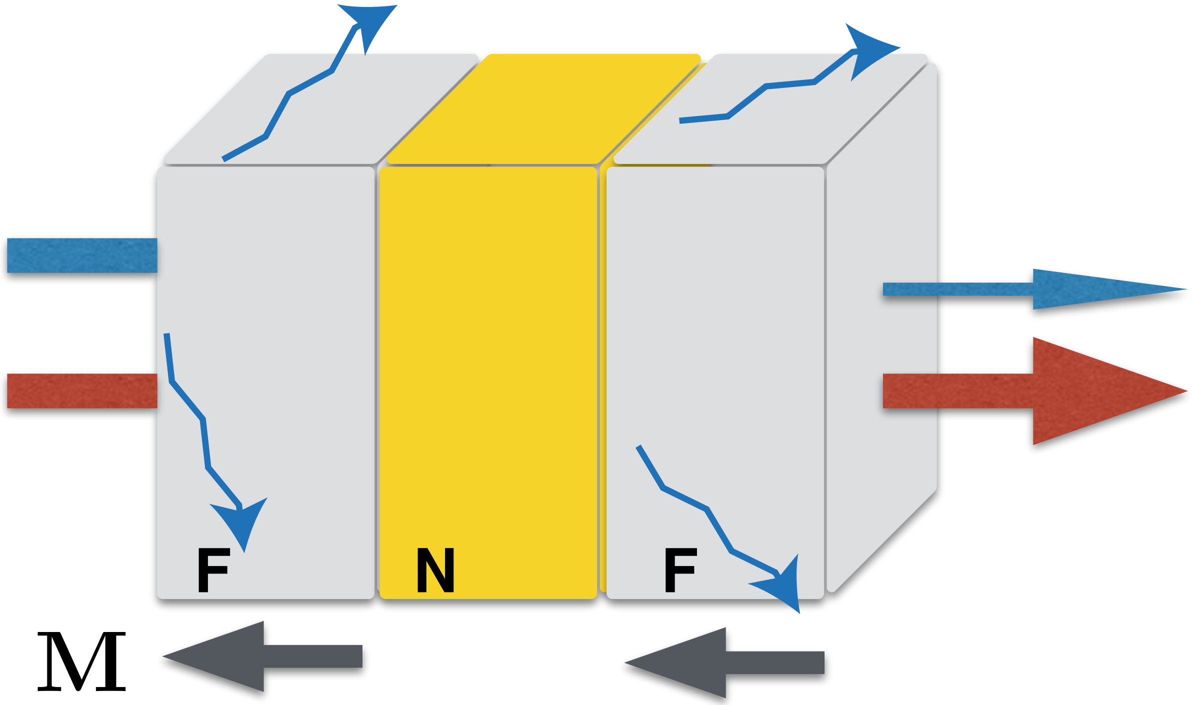
Physics Viewpoint: https://physics.aps.org/articles/v8/83

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

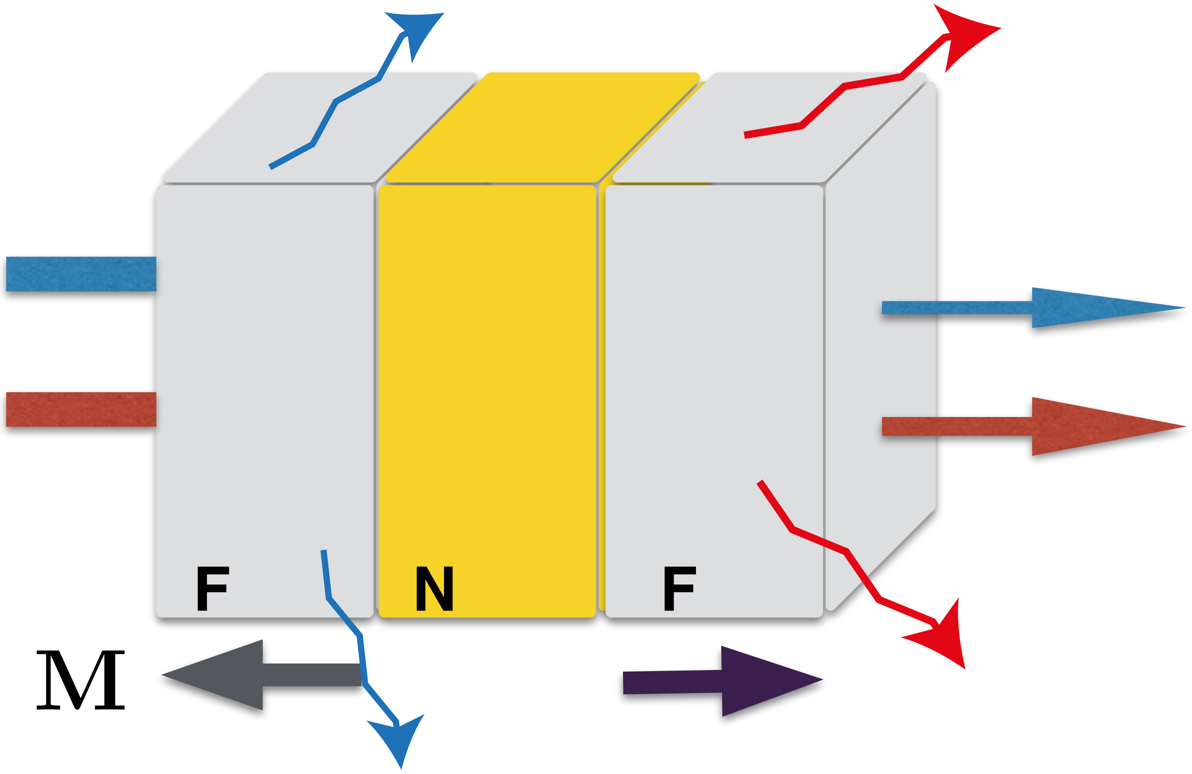
3c. Spin transport in metals

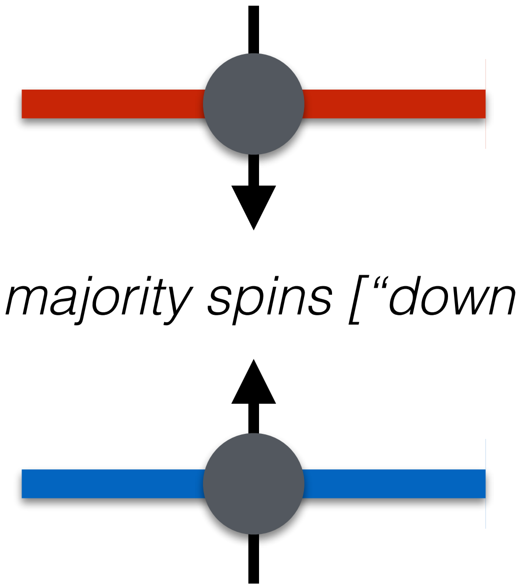
Spin interface resistance & the GMR effect

Parallel config.



Antiparallel config.





majority spins [“down”]

minority spins [“up”]

Conduction occurs in parallel, and thus:

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

- ➡ Interfacial spin accumulation picture offers a compelling explanation
- ➡ Spin-dependent scattering within the FM layers 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?

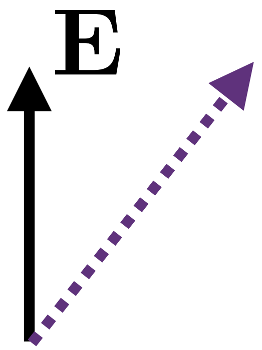
- SOC can endow energy bands with a Berry curvature [even in high-symmetry systems], which modifies the *semiclassical equations of motion*: Xiao RMP 82, 1959 (2010)

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

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

→ *anomalous velocity*

(intrinsic SHE)



- Low-symmetry SOC allows for direct/inverse *spin galvanic effects*

  [next week @ ESM]

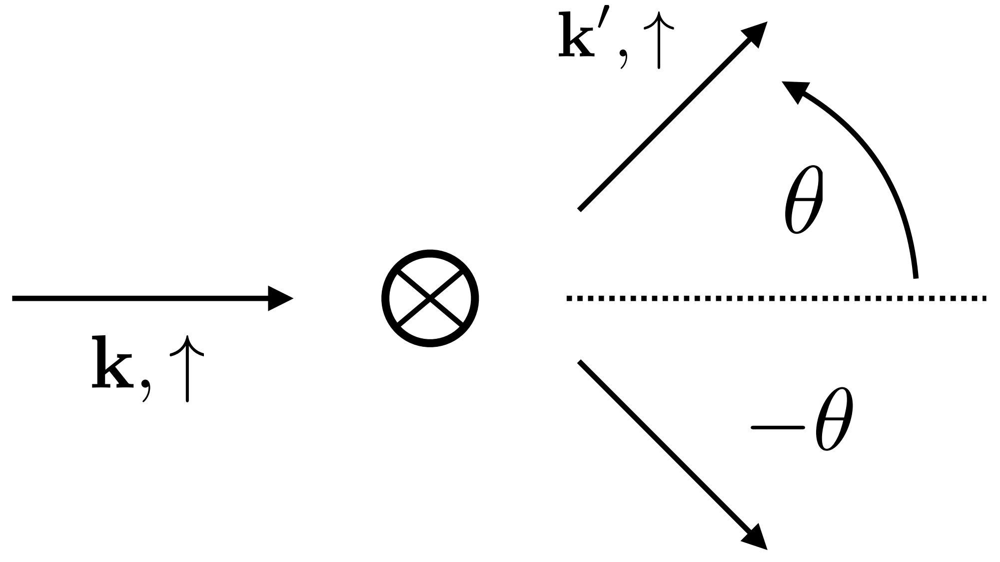
- Through disorder, SOC gives rise to *extrinsic electrodynamic responses* (e.g. extrinsic SHE) even if intrinsic mechanisms are weak or absent

  [next week @ ESM]

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

Example: Extrinsic Spin Hall effect

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



Intuition in 2D: Consider a WP experiencing SOC for a time δt

$$\boxed{\delta\theta = \lambda_{\rm so}\delta t}$$

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

(recall that $\hat{L}_z$ is the generator of rotations in coordinate space)

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

Time reversal symmetry

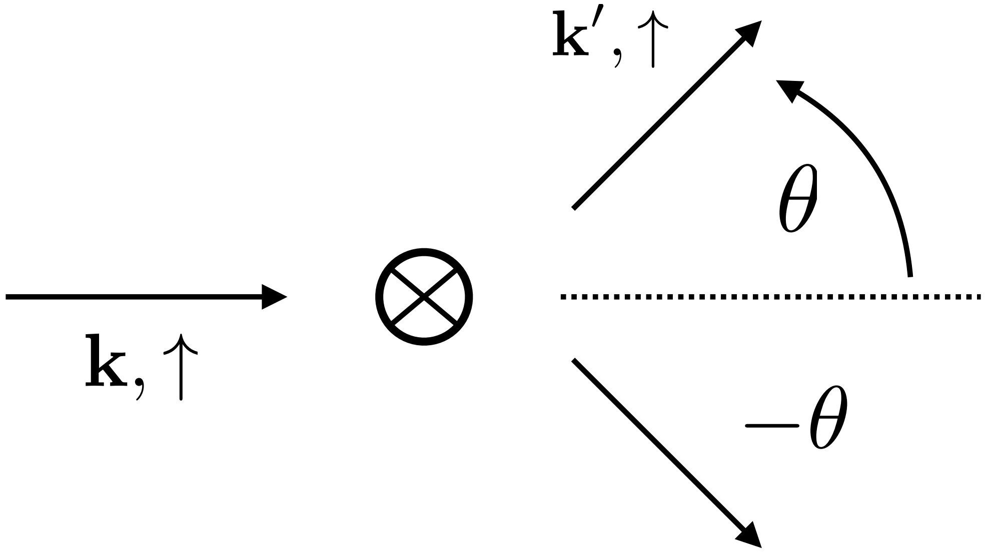
$$\sigma_\uparrow(\theta) = \sigma_\downarrow(-\theta)$$

Gradhand, PRL 104, 186403 (2010) I Fert & Levy, PRL 106, 157209 (2011) I Ferreira, PRL 112, 066601 (2014)

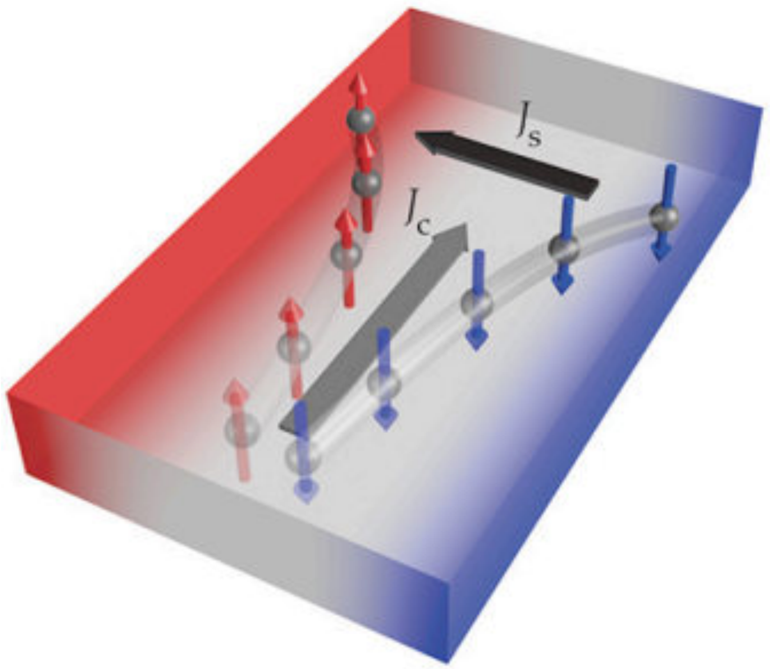
3c. Coupled charge-spin transport effects enabled by SOC

Example: Extrinsic Spin Hall effect

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



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

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

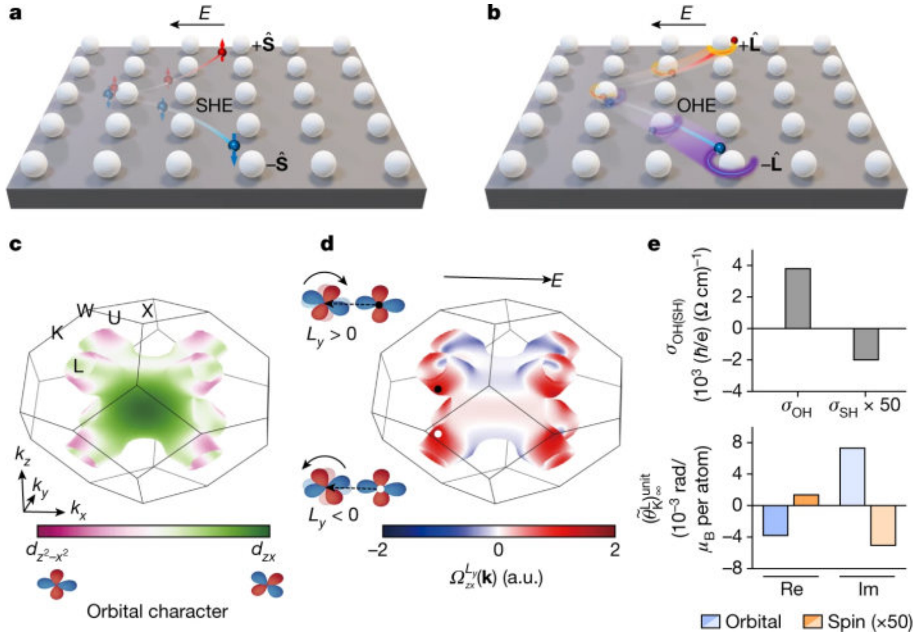
Gradhand, PRL 104, 186403 (2010) I Fert & Levy, PRL 106, 157209 (2011) I Ferreira, PRL 112, 066601 (2014)

3d. Orbital Hall effect in low-SOC metals

Orbital Hall effect

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

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



OAM can be generated locally provided orbitals <u>hybridise</u>

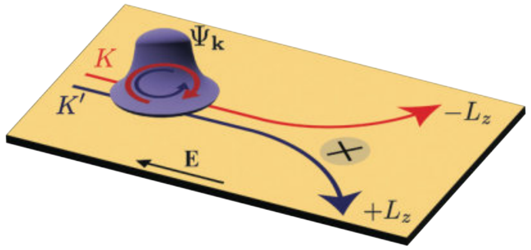
Hybridisation occurs due to interband transitions induced by ***E*** fields

Go, PRL 121, 086602 (2018)

The role of **extrinsic contributions** is now under scrutiny by the community

Orbital skew scattering

Veneri, arXiv:2408.04492 (2024)



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

(*) 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** and physically sound, but $\hat{r}$ operator is not well defined for systems with periodic boundary conditions.

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

End

Thank you for your attention!

Contact: aires.ferreira at york.ac.uk