Quantum spin transport

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Outline

- Introduction to quantum transport
- Spin-dependent magnitudes
- Case studies:

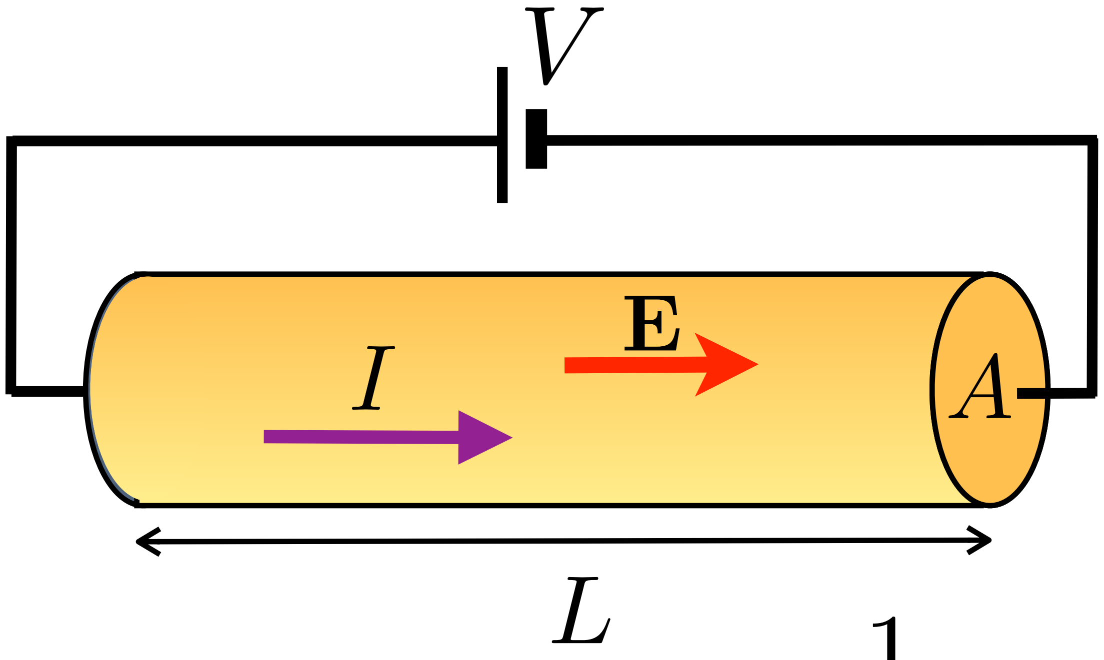
  1. The Datta-Das transistor
  2. Spin-polarized currents without B fields (with TRS)
  3. Two-current model for FM electrodes: spin thermoelectrics

Electric current

Classical description
Non equilibrium
Ohm's law

Georg Simon Ohm
(1789-1854)

$$V = RI$$



$$I = GV$$

$$G = \frac{1}{R}$$ conductance

$$\sigma = \frac{1}{\rho}$$ conductivity

Local expression: The application of an electric field generates a current density

$$\mathbf{j} = \sigma \mathbf{E}$$

Electronic transport regimes

Relevant longitudes

- L Size of the system in the direction of the current
- λ_F Fermi wavelength
- L_e Elastic mean free path

The carrier loses momentum information (direction) - collisions with static defects

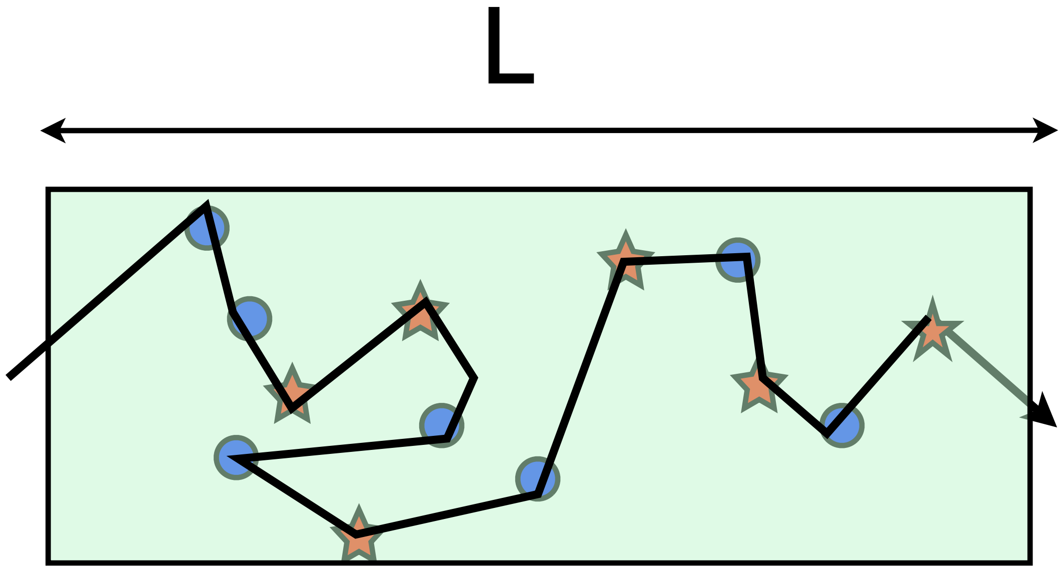
- L_ϕ Phase relaxation length

The wavefunction loses phase coherence - vibrations, electron-electron interaction, internal degrees of freedom of the impurities (spin)

Electronic transport regimes

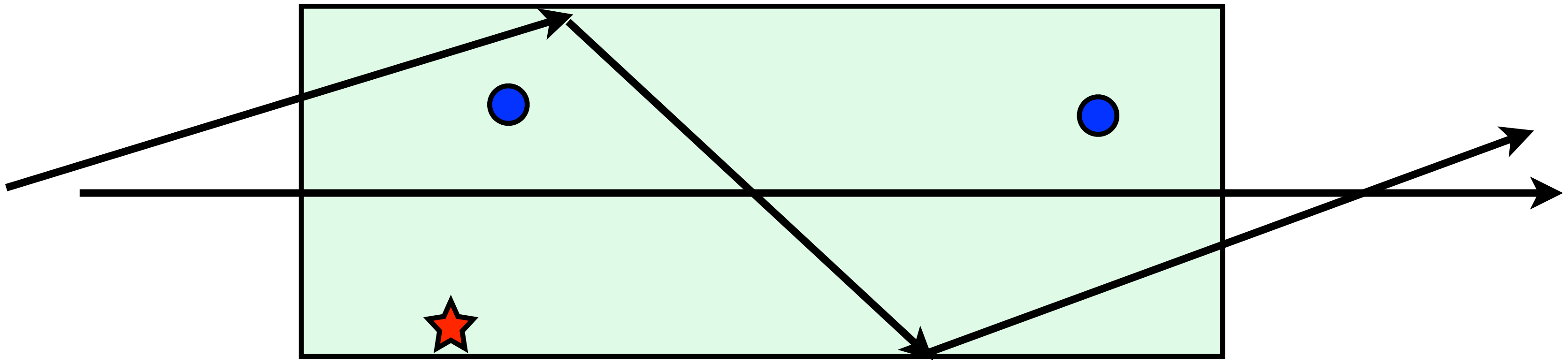
- Classical transport (incoherent, diffusive)

$$L \gg L_e, L_\phi$$



- Ballistic quantum transport (coherent)

$$L \ll L_e, L_\phi$$



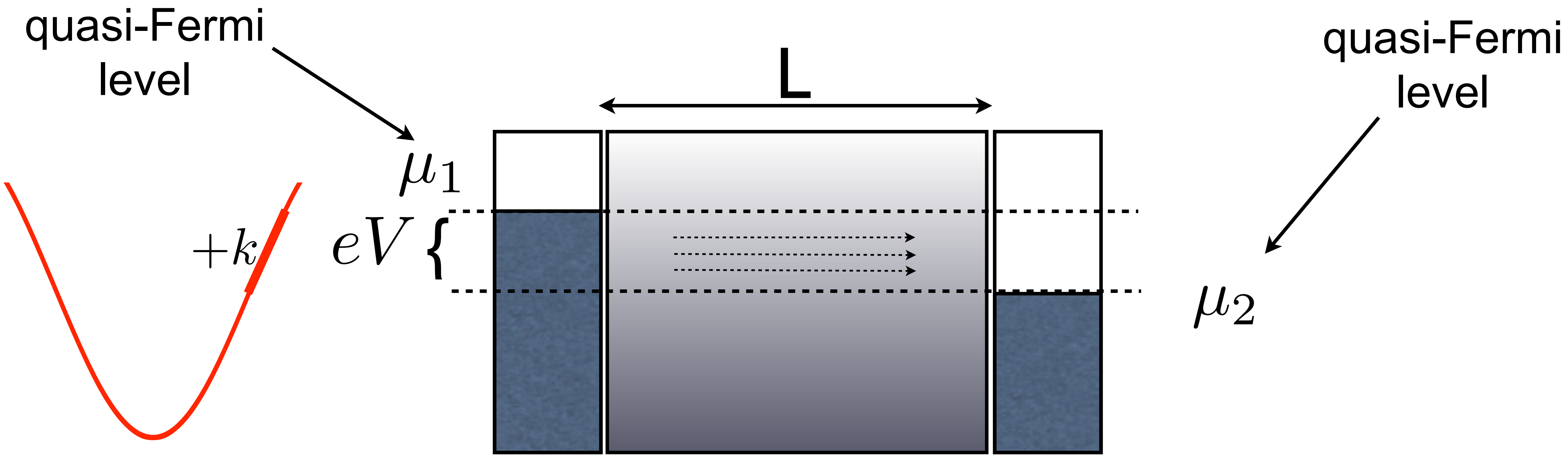
Some characteristic magnitudes (at 4 K)

	2DEG GaAs	Metals	Graphene	SWNT
n	4×10^{11} cm^{-2}	$10^{21} - 10^{23}$ cm^{-3}	$10^{11} - 10^{12}$ cm^{-2}	10^{11} cm^{-2}
L_e	$100 - 10^4$ nm	$1 - 10$ nm	50 nm to 3 μm	1 μm
λ_F	40 nm	0.5 nm	$2\sqrt{\pi/n}$	0.74 nm
L_ϕ	100 nm	0.5 μm	0.5 μm	3 μm

n: carrier density

Ballistic transport in one dimension (1D)

Reflectionless contacts, T=0 K, one mode



$$I = \Delta n\, e\, v$$

Δn : carrier density contributing to the currrent (with positive velocity)

$$\Delta n = D_{1D}^{e^+}(E)\,\Delta E$$

$$D_{1D}^{e^+}(E) = \frac{1}{\pi\hbar v}$$

$$\Delta E = eV$$

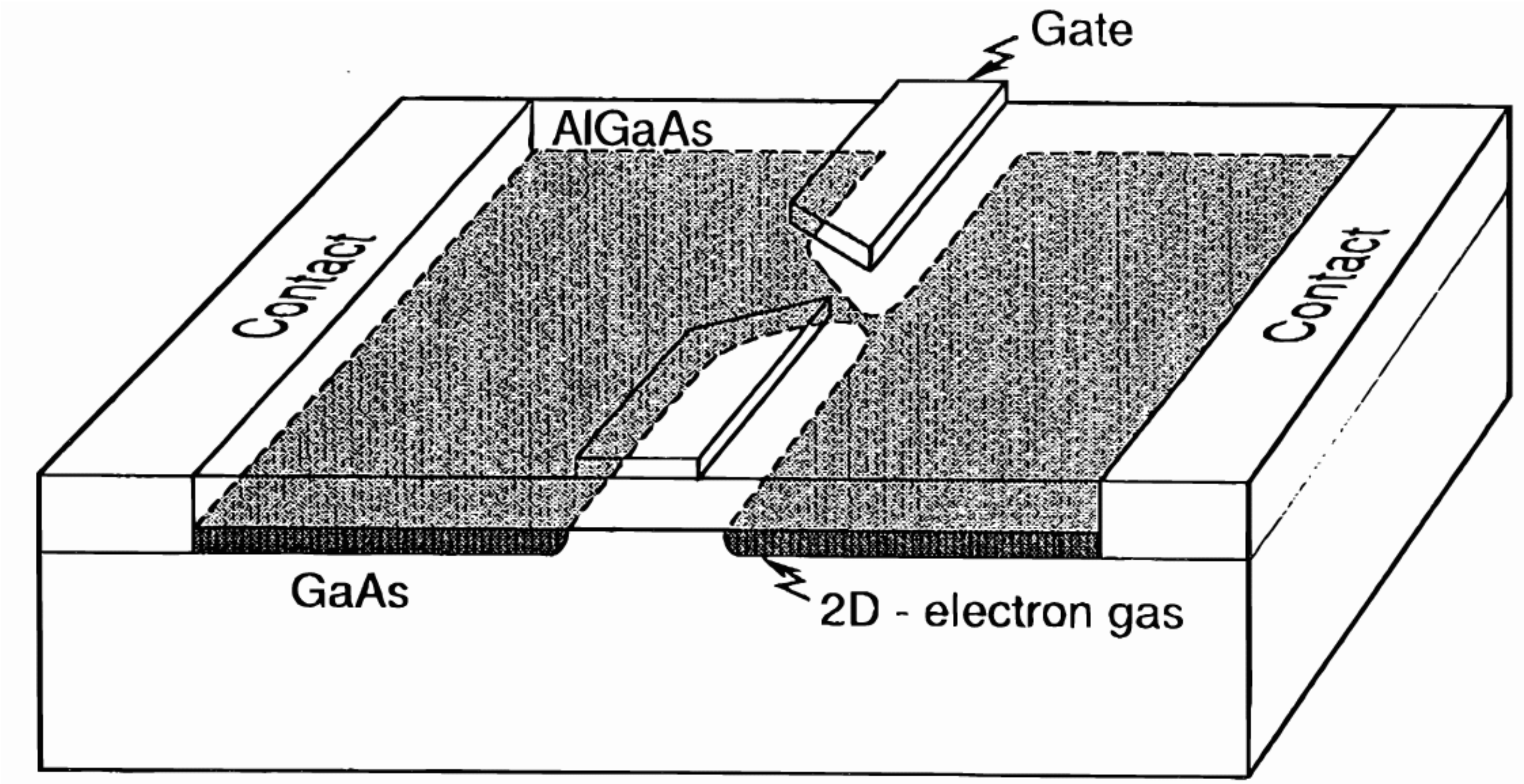
$$I = \frac{2e^2}{h}V$$

$$\boxed{G = \frac{2e^2}{h}}$$

G independent of L

conductance quantization

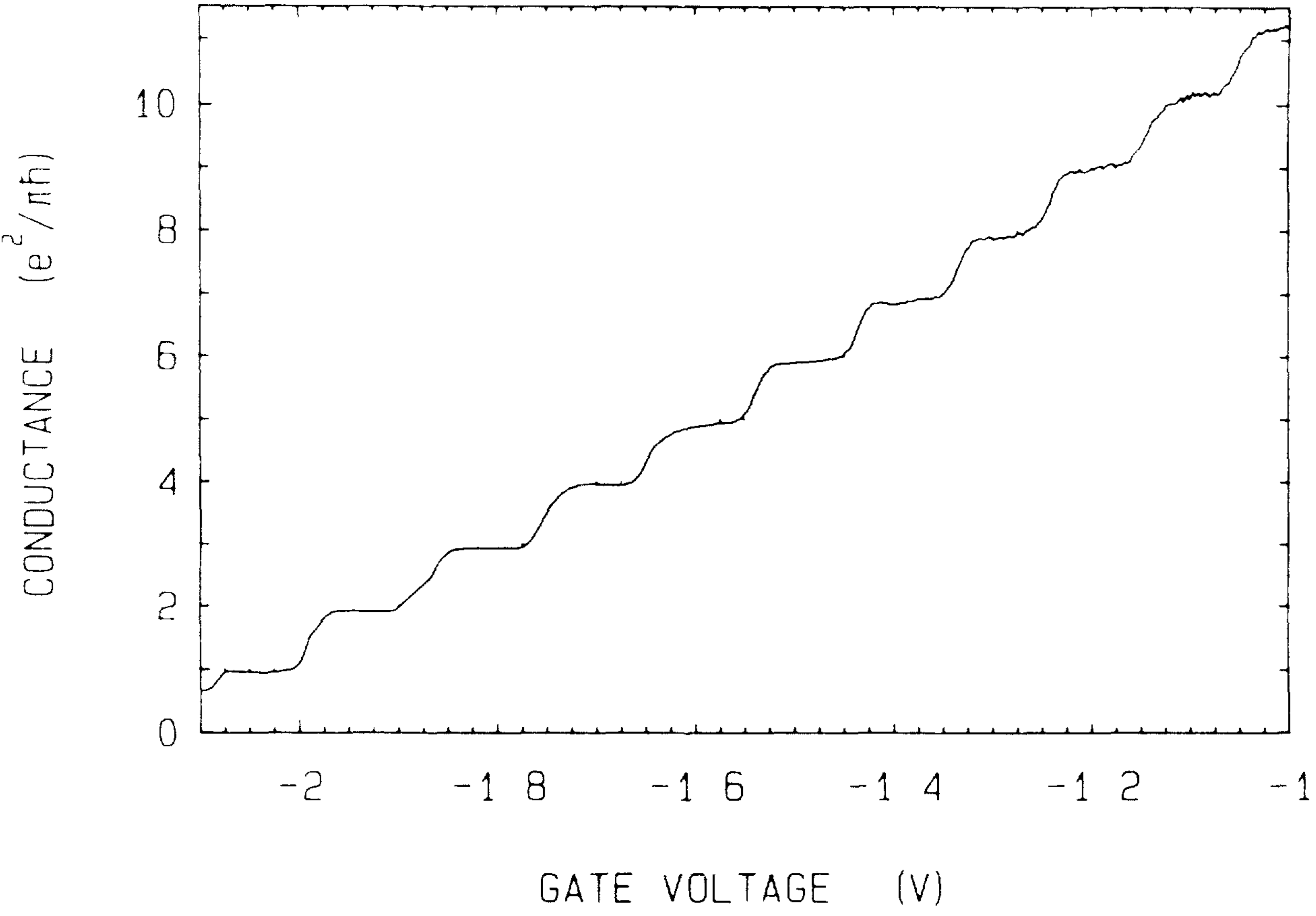
Quantum point contact (QPC) in a bidimensional electron gas (2DEG)

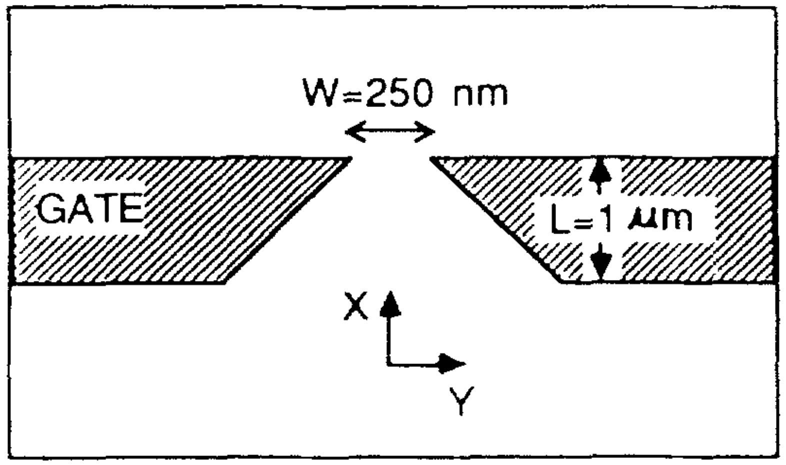


H. van Houten and C. W. J. Beenakker, Phys. Today, p 22, July 1996.

Conductance quantization in a 2DEG

AlGaAs/GaAs heteroestructure grown by MBE





Measurements at 0.6 K

B. van Wees et al., Phys. Rev. Lett. **60**, 848 (1988)

Conductance quantum

$$G_0 = \frac{2e^2}{h} = 7.748 \times 10^{-5}\,\mathrm{S}$$

Klaus von Klitzing (1943 -)

Nobel Prize in Physics 1985

Quantum Hall effect

von Klitzing's constant

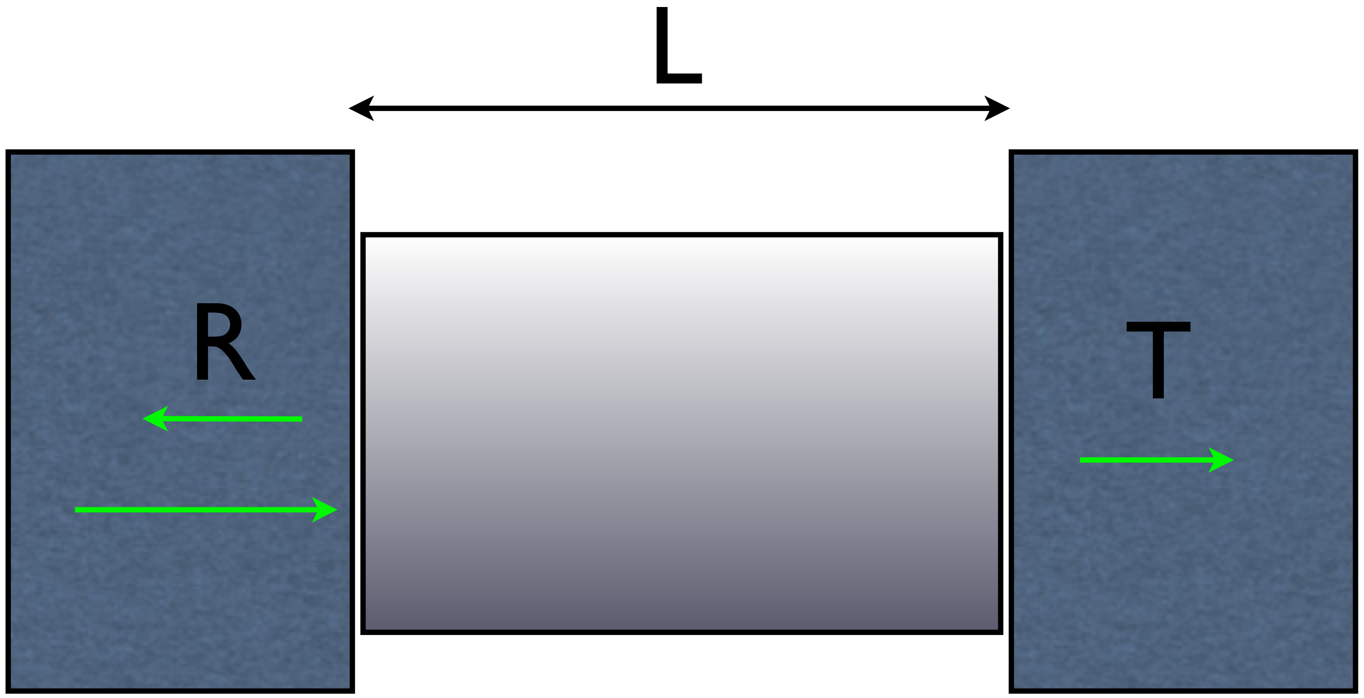
$$R_K = \frac{h}{e^2} = 25812.80745\,\Omega$$

Conductance as transmission

Rolf Landauer
(1927-1999)

Contacts with reflection

Landauer, 1957



T: transmission through the system

If $V \to 0$,

transmission takes place at the Fermi energy, $T(E_F)$

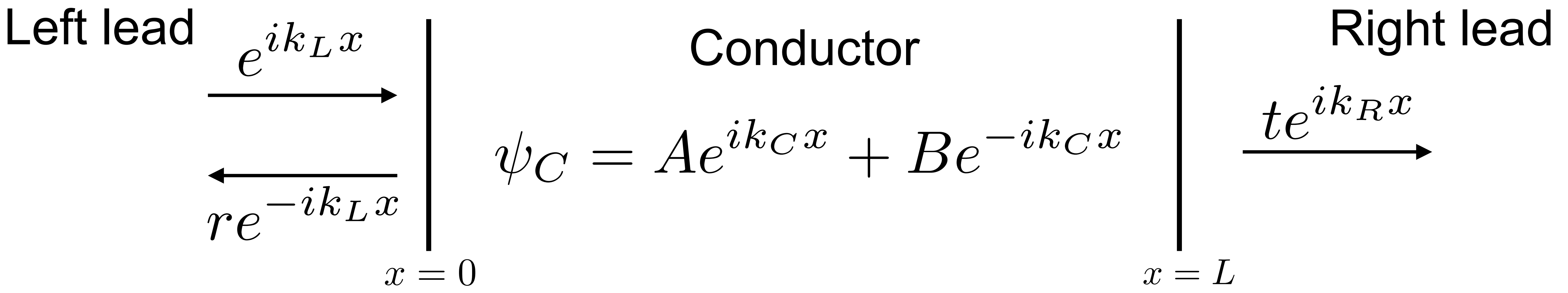
Landauer´s formula

$$G = \frac{2e^2}{h} T$$

Leads play a crucial role

One channel conductance

Incidence from the left lead:



Left lead

Conductor

Right lead

$e^{ik_L x}$

$re^{-ik_L x}$

$$\psi_C = Ae^{ik_C x} + Be^{-ik_C x}$$

$te^{ik_R x}$

$x = 0$

$x = L$

$$\psi_L = e^{ik_L x} + re^{-ik_L x} \qquad \psi_R = te^{ik_R x}$$

Boundary conditions: continuity of the wavefunction and the current (derivative) at the interfaces, 4 equations.

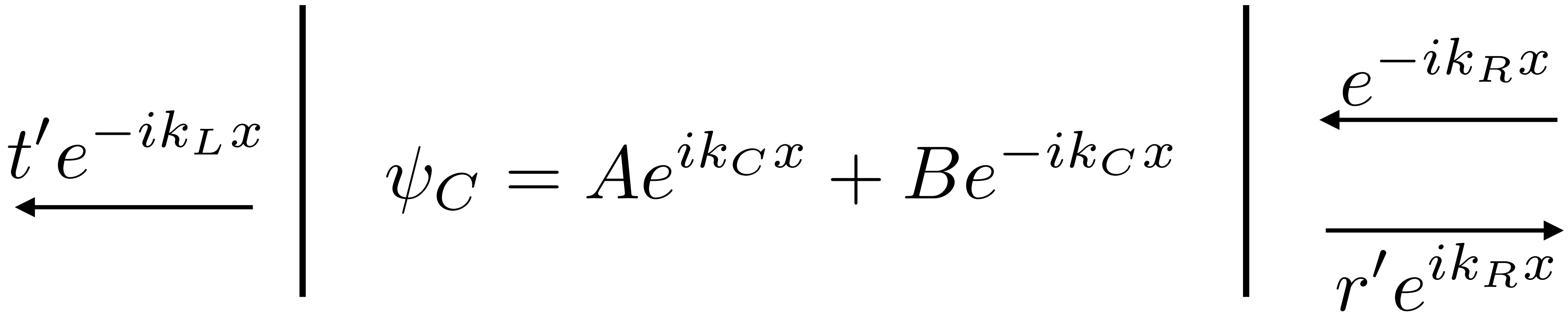
$\boxed{\text{Solve for } t}$ (transmission amplitude)

With the amplitude t the transmission T is just $\boxed{T = |t|^2}$

Of course, $R + T = 1$

One channel conductance

Incidence from the **right** lead:



$t'e^{-ik_Lx}$

$$\psi_C = Ae^{ik_Cx} + Be^{-ik_Cx}$$

e^{-ik_Rx}

$r'e^{ik_Rx}$

A general scattering matrix S from the system can be defined:

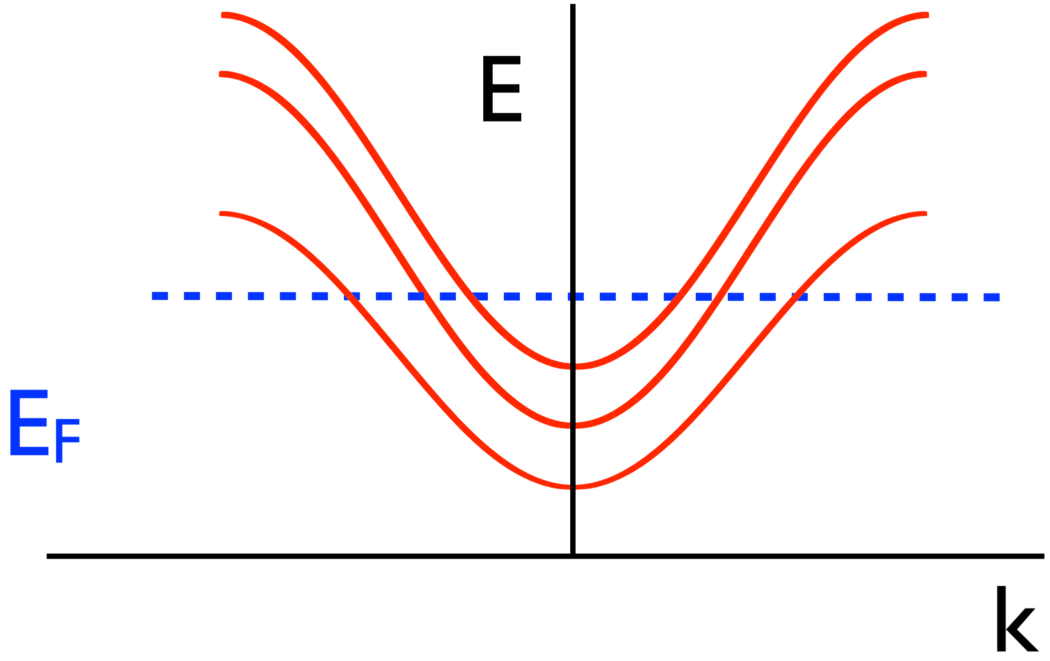
$$\begin{pmatrix} \psi_L^{out} \\ \psi_R^{out} \end{pmatrix} = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix} \begin{pmatrix} \psi_L^{in} \\ \psi_R^{in} \end{pmatrix} = \overbrace{\begin{pmatrix} s_{LL} & s_{LR} \\ s_{RL} & s_{RR} \end{pmatrix}}^{S} \begin{pmatrix} \psi_L^{in} \\ \psi_R^{in} \end{pmatrix}$$

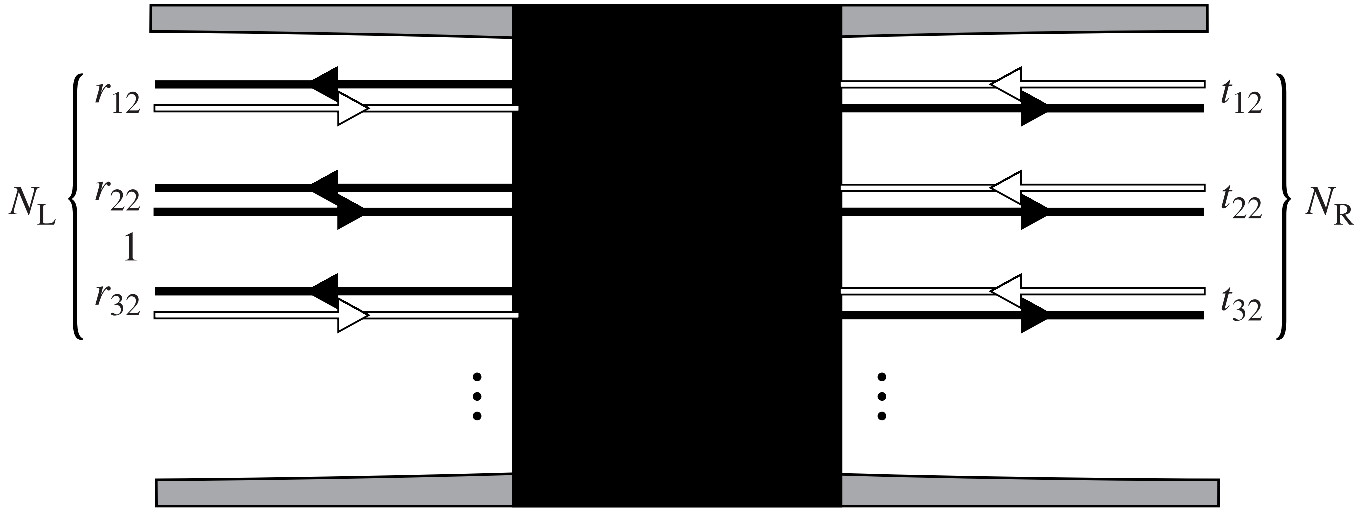
S is unitary, $\quad S^\dagger S = 1$

If time-reversal symmetry (TRS) holds, $\quad r = r'\,, \quad t = t'$

Conductance as transmission

Multichannel electrodes





$$\begin{pmatrix}\psi^{out}_L\,(N_L)\\ \psi^{out}_R\,(N_R)\end{pmatrix} = \begin{pmatrix} s_{LL}\,(N_L\times N_L) & s_{LR}\,(N_L\times N_R)\\ s_{RL}\,(N_R\times N_L) & s_{RR}\,(N_R\times N_R)\end{pmatrix}\begin{pmatrix}\psi^{in}_L\,(N_L)\\ \psi^{in}_R\,(N_R)\end{pmatrix}$$

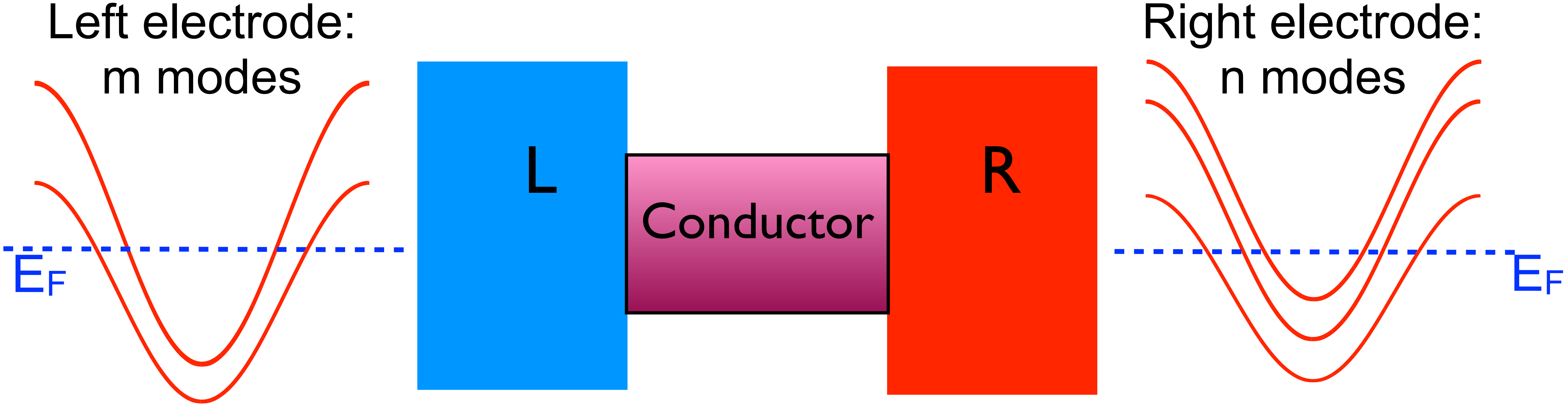
Matrix of transmission amplitudes t

$$\boxed{\mathrm{Tr}\left[t^\dagger t\right] = \sum_i^{N_L}\sum_j^{N_R}|t_{ij}|^2}$$

Nazarov & Blanter

Conductance as transmission

Multichannel electrodes

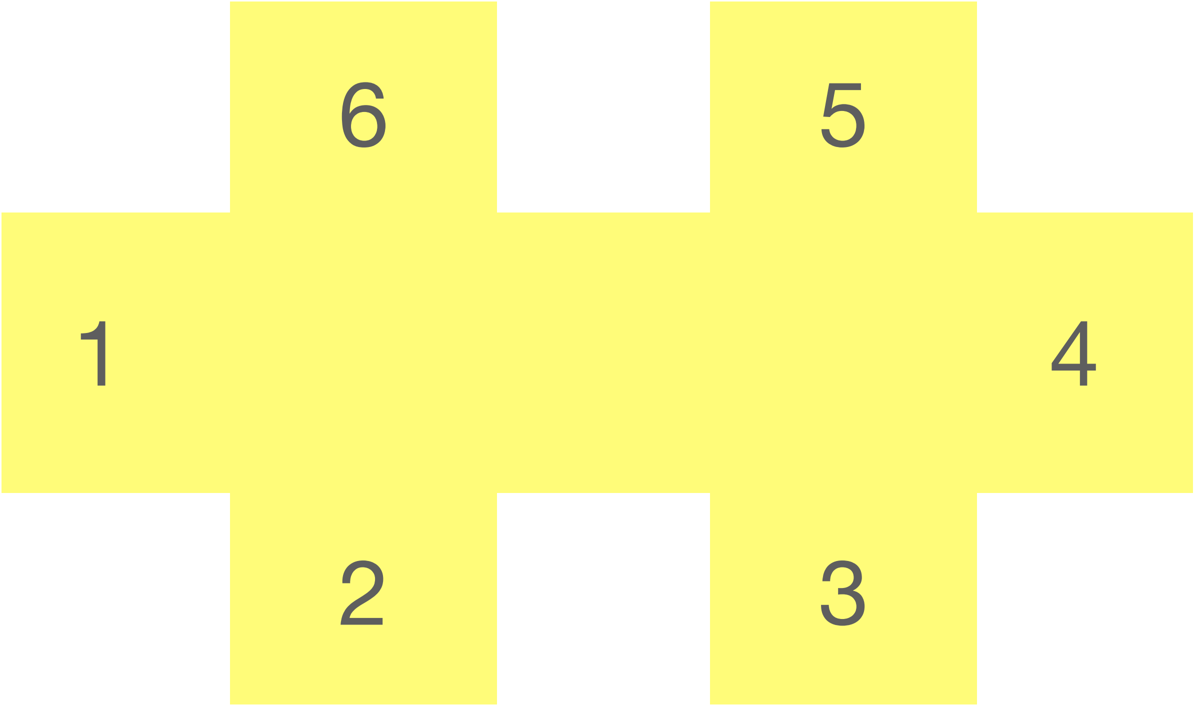


Multichannel Landauer formula

$$G(E_F) = \sum_{i=1}^{m} G_i(E_F) = \sum_{i=1}^{m} \sum_{j=1}^{n} G_{ij}(E_F)$$

$$G(E_F) = \frac{2e^2}{h} \sum_{i=1}^{m} T_i(E_F) = \frac{2e^2}{h} \sum_{i=1}^{m} \sum_{j=1}^{n} T_{ij}(E_F)$$

Multiterminal setups



At each terminal q the current I_q is measured

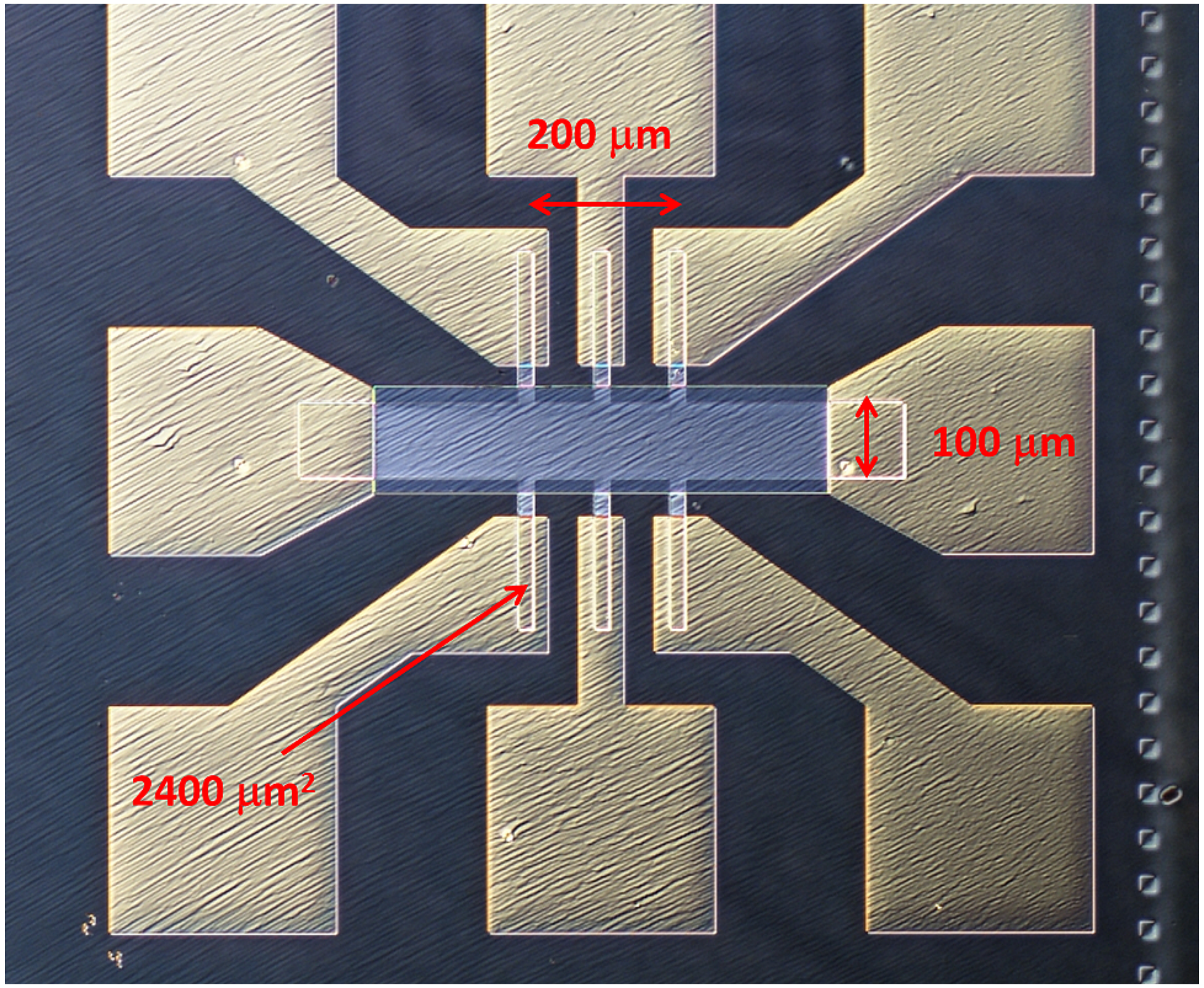
And it can be related to the potential differences between contacts:

$$I_q = \sum_q G_{pq}[V_p - V_q]$$

$$G_{pq} = \frac{2e^2}{h}\overline{T}_{pq}(E_F)$$

Experimental multiterminal setups

https://www.nist.gov/sites/default/files/images/pml/div684/grp05/bighallbar970.png



How to calculate the conductance?

The scattering matrix can be obtained by Green's function methods.

For the eigenvalue problem $(E - H)\phi = 0$

its Green's function (GF) G is defined as $(E - H)G = I$

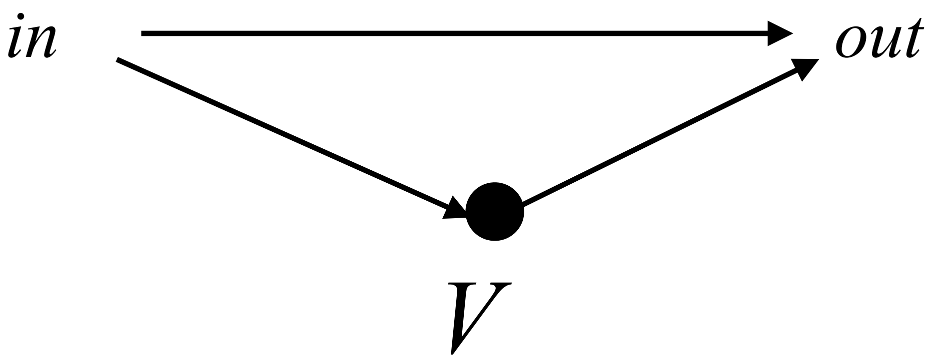
The eigenenergies are the poles of G: $G^{\pm} = \lim_{\eta \to 0^+} \frac{1}{E \pm i\eta - H}$

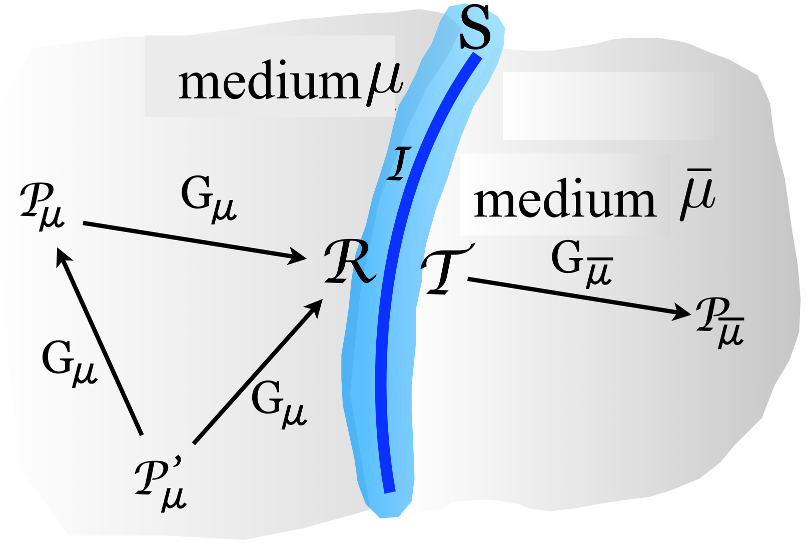
$+$ is also called the retarded or causal GF; $-$ is the advanced GF

In the coordinate representation, $\begin{cases} \langle \mathbf{r} | \mathbf{r}' \rangle = \delta(\mathbf{r} - \mathbf{r}') \\ \int d\mathbf{r} | \mathbf{r} \rangle \langle \mathbf{r} | = 1 \end{cases}$

$$[E + i\eta - H(\mathbf{r})] \, G^R(\mathbf{r}, \mathbf{r}', E) = \delta(\mathbf{r} - \mathbf{r}')$$

Green’s functions for the scattering matrix

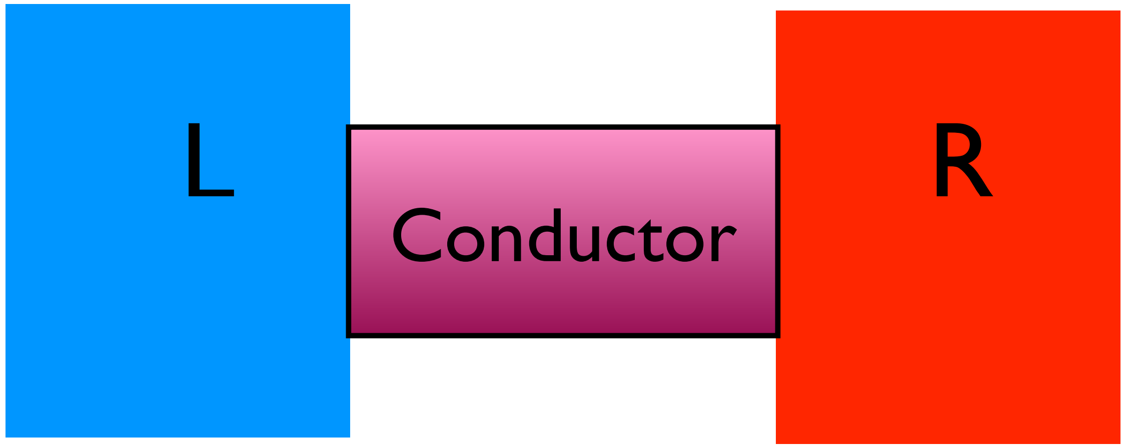




Lippmann-Schwinger equation:

$$\psi(\mathbf{r}) = \phi(\mathbf{r}) + \int d\mathbf{r}' G_0(\mathbf{r}, \mathbf{r}', E) V(\mathbf{r}') \phi(\mathbf{r}')$$

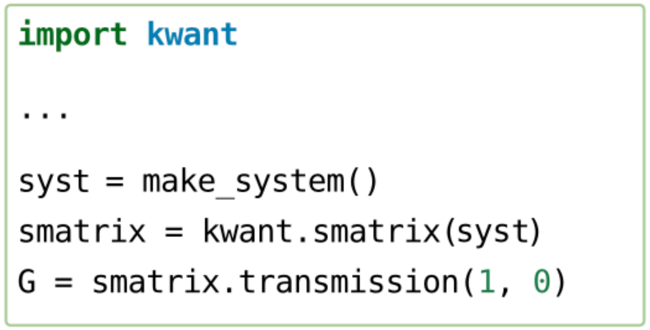
Approach used by tranSIESTA



Scattering matrix from wavefunctions

Open source program in Python for quantum transport

→

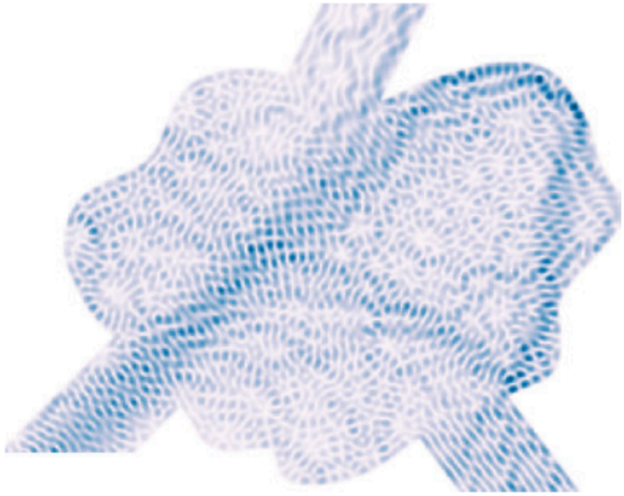


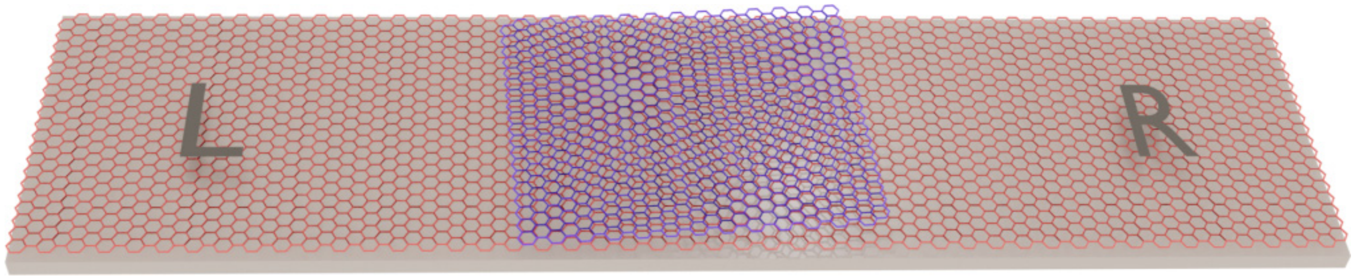
```
import kwant

...

syst = make_system()
smatrix = kwant.smatrix(syst)
G = smatrix.transmission(1, 0)
```

→





Moles Phys. Rev. B (2024)

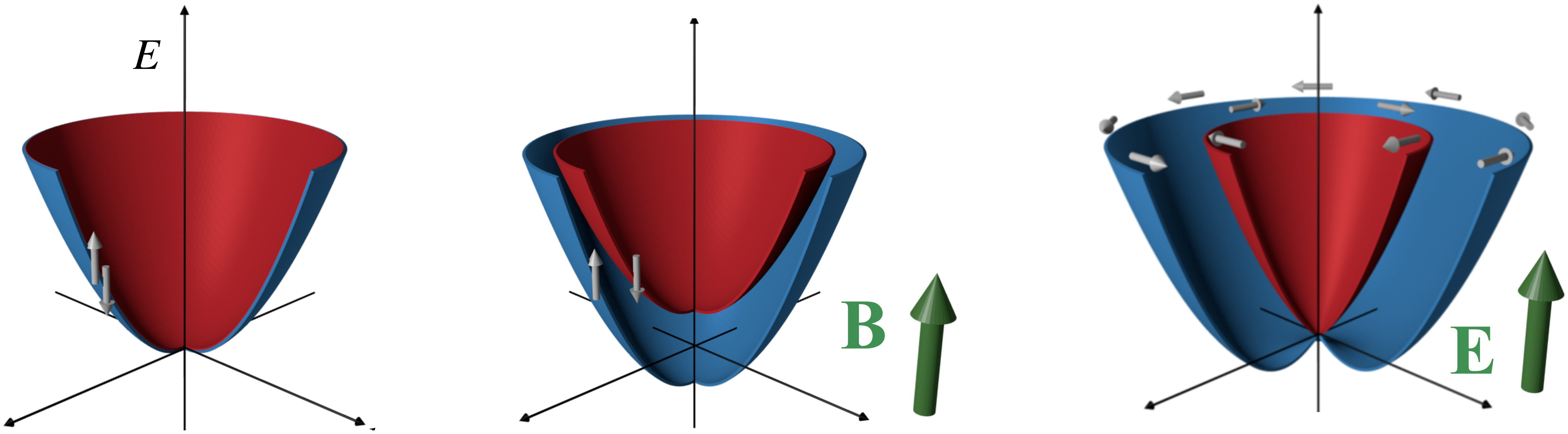
https://kwant-project.org/

C. W. Groth et al., New J. Phys. **14**, 063065 (2014)

Spin-dependent conductances

Multichannel electrodes

The leads and/or the conductor have spin-split states



No spin dependence

$$H_0 = \frac{\hbar^2 k^2}{2m^*}$$

Zeeman (B, FM)

Broken TRS

$$H_Z = -\vec{\mu}_e \cdot \vec{B}$$

Spin-orbit (Rashba)

Broken inversion sym.

$$H_{SO} = \frac{e\hbar}{4m^2c^2}(\nabla V \times \vec{p}) \cdot \vec{\sigma}$$

figure from S. Satpathy talk@correlated oxides 2014

Spin-orbit Hamiltonian

General spin-orbit Hamiltonian:

$$H_{SO} = \frac{e\hbar}{4m^2c^2}(\nabla V \times \vec{p}) \cdot \vec{\sigma}$$

In an atom, V is due to the nucleus, and it is spherically symmetric; this is the origin of the intrinsic spin-orbit term.

Near a surface, or with an applied electric field,
V is not spherically symmetric:

Inversion symmetry is broken

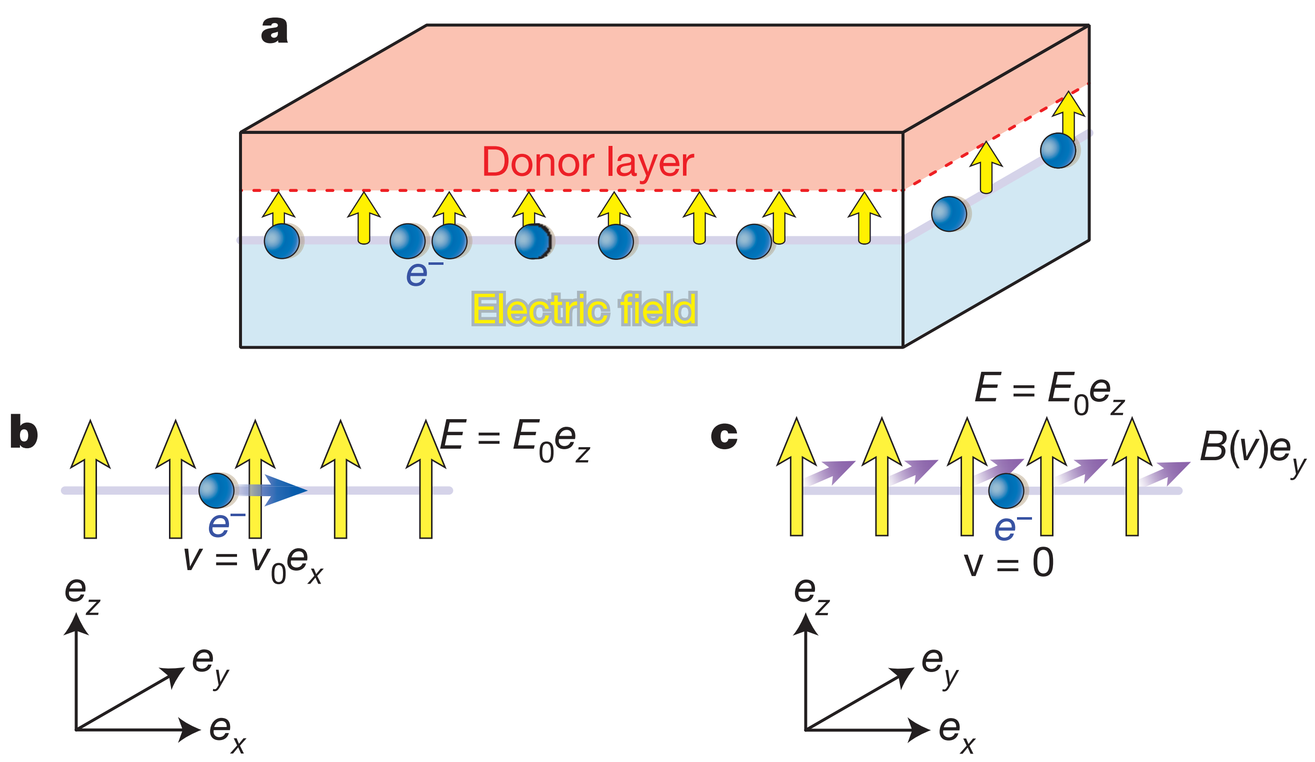
Since $\vec{E} = -\nabla V \quad \Rightarrow \qquad H_{SO} = \frac{e\hbar}{4m^2c^2}\left(\vec{p} \times \vec{E}\right) \cdot \vec{\sigma}$

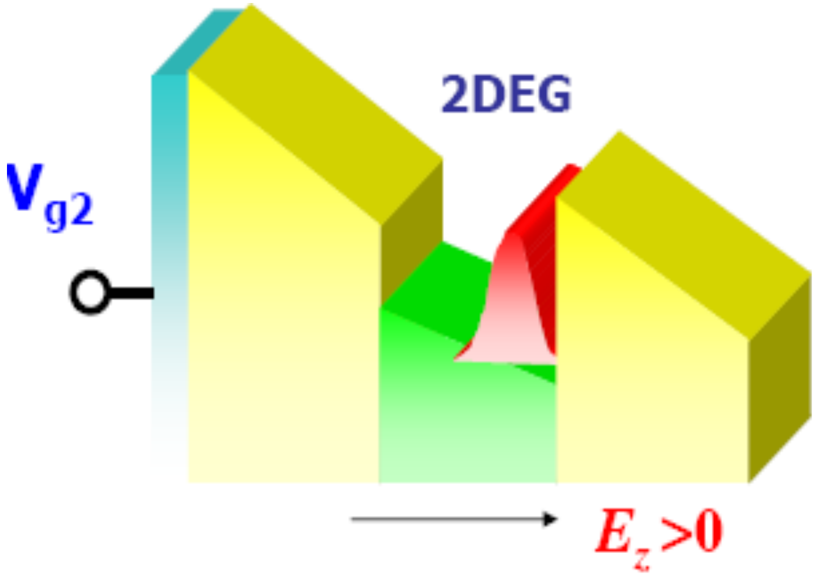
Rashba spin-orbit interaction

Spin-orbit interaction induced by an electric field

Initially conceived for a 2DEG at a surface (E.I. Rashba, 1960)

$$H_{SO} \propto (\boldsymbol{\sigma} \times \mathbf{p}) \cdot \mathbf{E}$$





Can be tuned by an external field!

figures from Suhagara & Nitta, Proc. IEEE (2010); Galitski & Spielman, Nature (2013)

Spin-dependent conductances

$$G = \boxed{\frac{e^2}{h}} \sum_{i=1}^{n} T_i = \boxed{\frac{e^2}{h}} \sum_{i=1}^{n} \sum_{j=1}^{m} T_{ij}$$

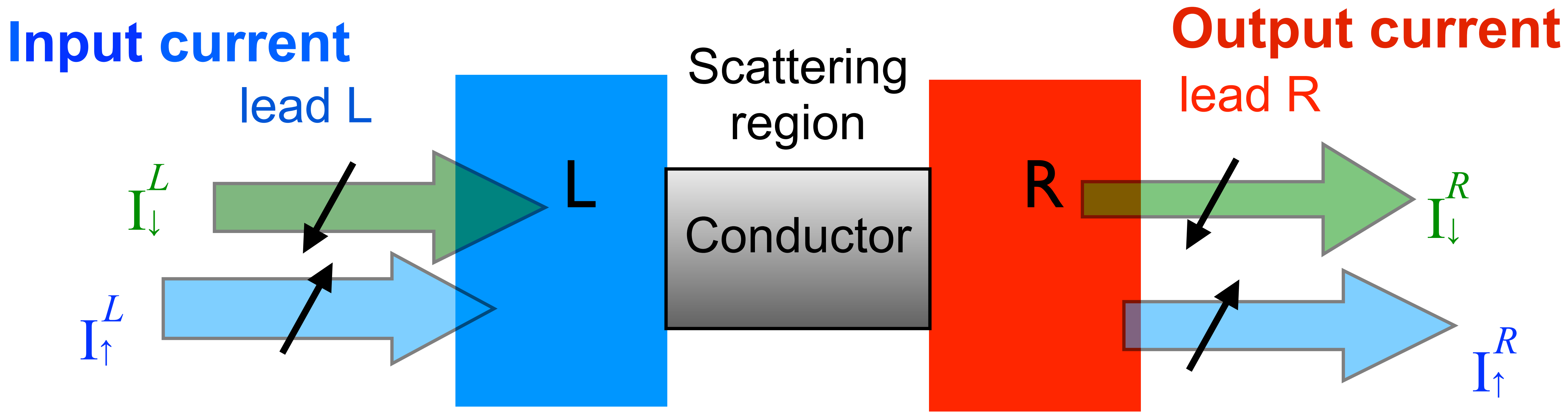
If TRS is broken, L ⇒ R is different from R ⇒ L

$G^{LR}_{\sigma\sigma'}$: probability for an electron in lead L with spin σ reaches electrode R with spin σ'

$$G^{LR} = G^{LR}_{\uparrow\uparrow} + G^{LR}_{\uparrow\downarrow} + G^{LR}_{\downarrow\downarrow} + G^{LR}_{\downarrow\uparrow}$$

Charge and spin currents

In a spin-dependent transport problem, we have to distinguish between charge and spin currents



$$I_\uparrow^R \propto G_{\uparrow\uparrow}^{LR} + G_{\downarrow\uparrow}^{LR}$$

Charge current I_c: $$I_c^R = I_\uparrow^R + I_\downarrow^R$$

Spin current I_s: $$I_s^R = I_\uparrow^R - I_\downarrow^R$$

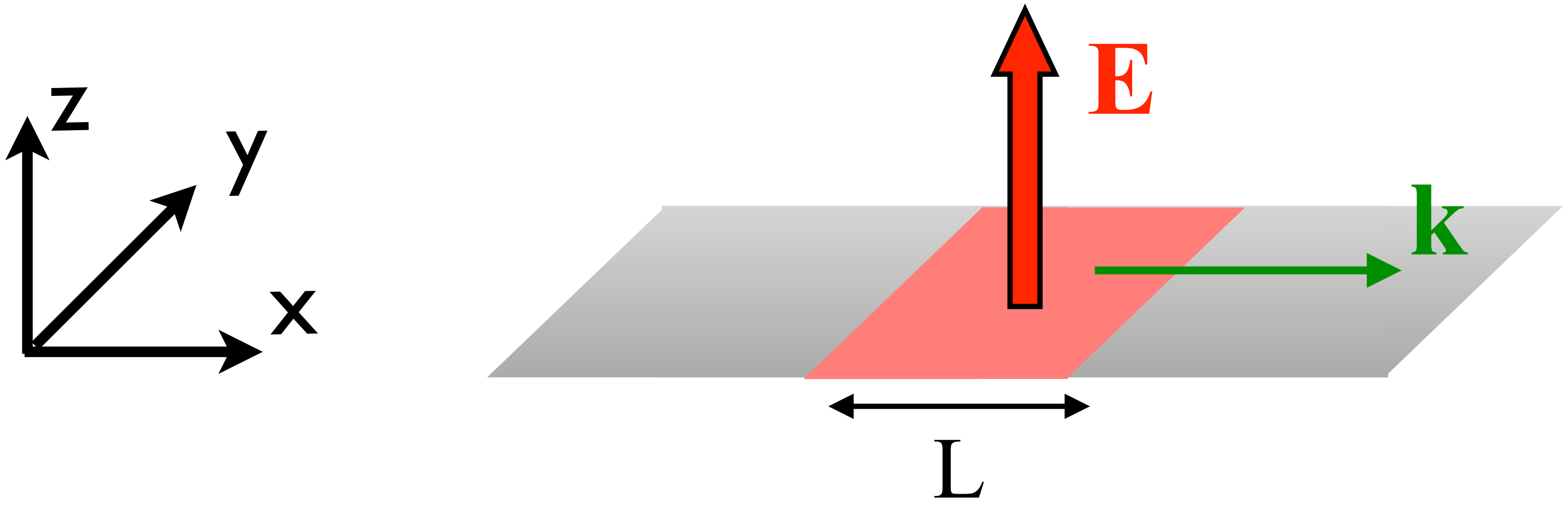
Case studies

1. FM leads, SO spin-dependent scatttering in the conductor: Datta-Das transistor
2. Unpolarized leads, SO spin-dependent scatttering in the conductor: all-electrical production of spin-polarized current

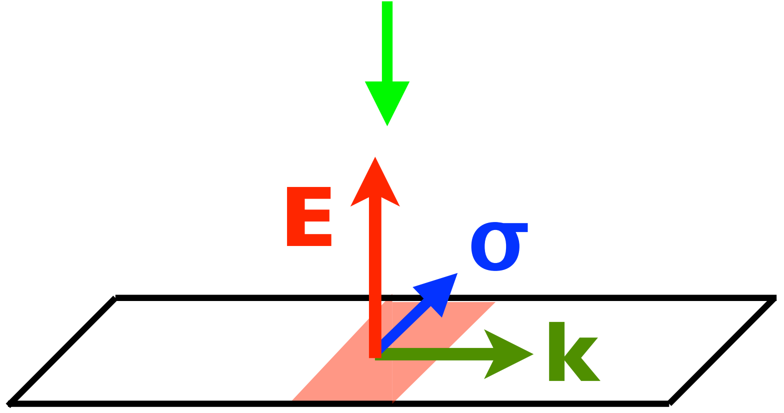
Notice that spin is well-defined in the leads - no SOC in the electrodes

1) FM leads, SO spin-dependent scattering in the conductor: Datta-Das transistor

1D conductor, current along *x*, E field along *z*



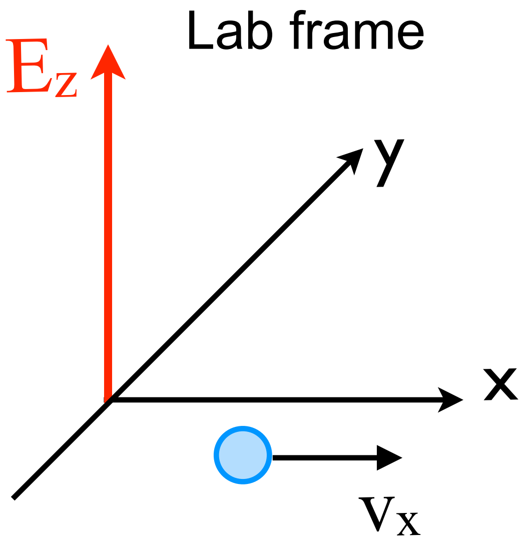
$$H_{SO} \propto (\boldsymbol{\sigma} \times \mathbf{k}) \cdot \mathbf{E} \quad \Longrightarrow \quad H_R = \alpha(k_y \sigma_x - k_x \sigma_y)$$

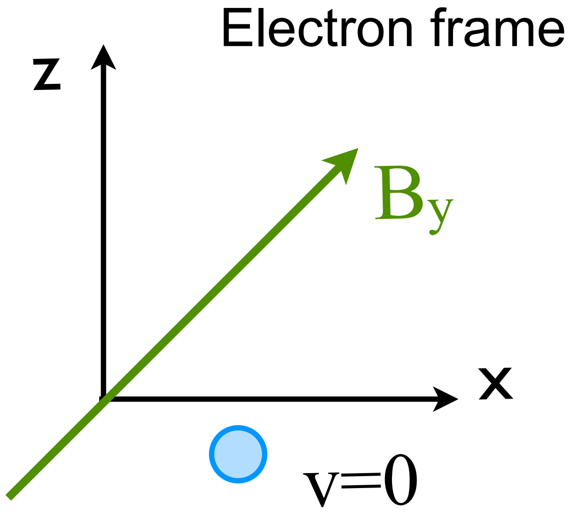


SO maximized for spin in the *y* direction

Rashba spin-orbit coupling

$$H_R = \alpha(k_y \sigma_x - k_x \sigma_y)$$





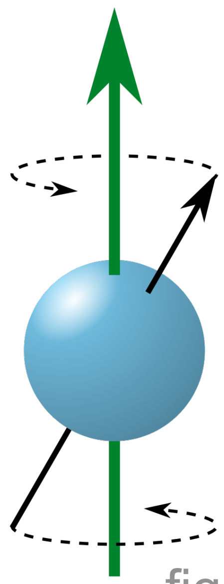


fig. from wikipedia

The precession frequency is given by

$$\omega = \frac{2\alpha k_x}{\hbar}$$

$$\Longrightarrow$$

The change of spin orientation along L is

$$\Delta\theta = \omega t = \frac{2m^* \alpha L}{\hbar^2}$$

Tuning Rashba SOC via V_{gate} allows for current control

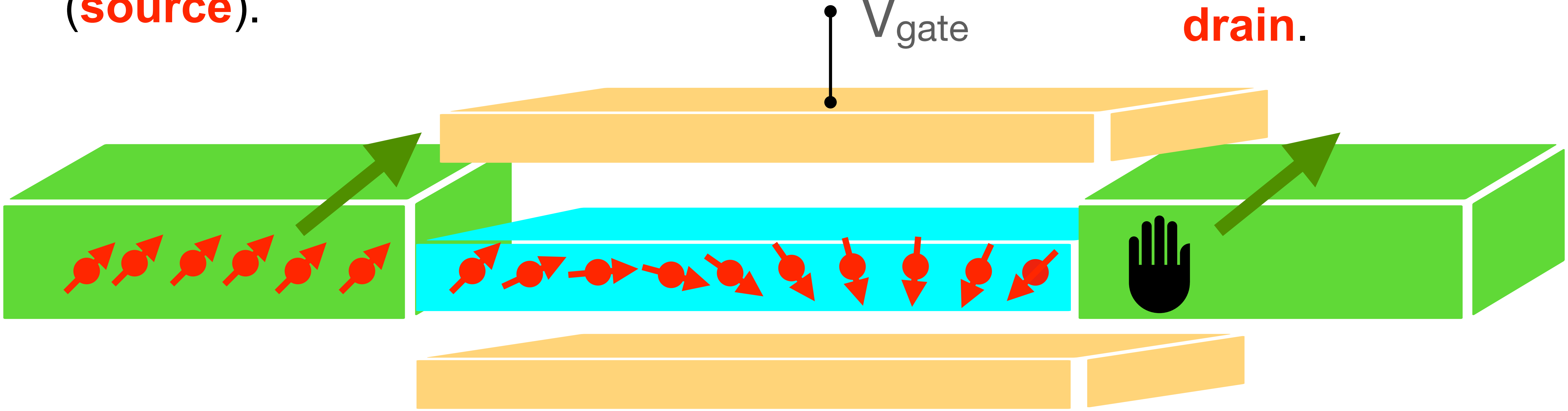
S. Datta and B. Das, Appl. Phys. Lett. **56**, 665 (1990)

1) FM leads, SO spin-dependent scattering in the conductor: Datta-Das transistor

A spin-polarized current is injected from the left lead (**source**).

A V_{gate} tunes the Rashba SOC in the conductor (**channel**).

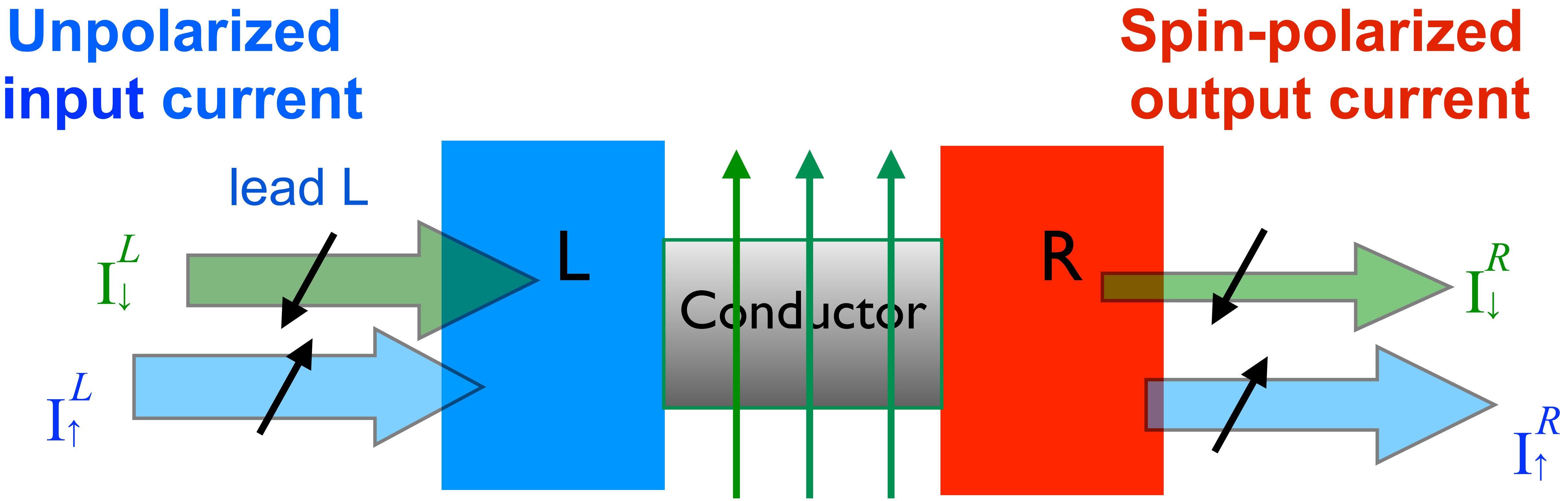
Depending on V_{gate}, we can have high or low current at the **drain**.



The spin in the conductor precesses.

S. Datta and B. Das, Appl. Phys. Lett. **56**, 665 (1990)

2) Unpolarized leads, Rashba SOC in the conductor: <u>all electrical production of spin-polarized currents</u>



Recall that $I_\uparrow^R \propto G_{\uparrow\uparrow}^{LR} + G_{\downarrow\uparrow}^{LR}$, so we can define the spin polarization of the current as

$$P_s = G_{\uparrow\uparrow}^{LR} + G_{\downarrow\uparrow}^{LR} - G_{\downarrow\downarrow}^{LR} - G_{\uparrow\downarrow}^{LR}$$

2) Unpolarized leads, Rashba SOC in the conductor: all electrical production of spin-polarized currents

Since spins with opposite directions precess in antiphase, there is no possible spin polarization for only one conduction channel in the out lead.

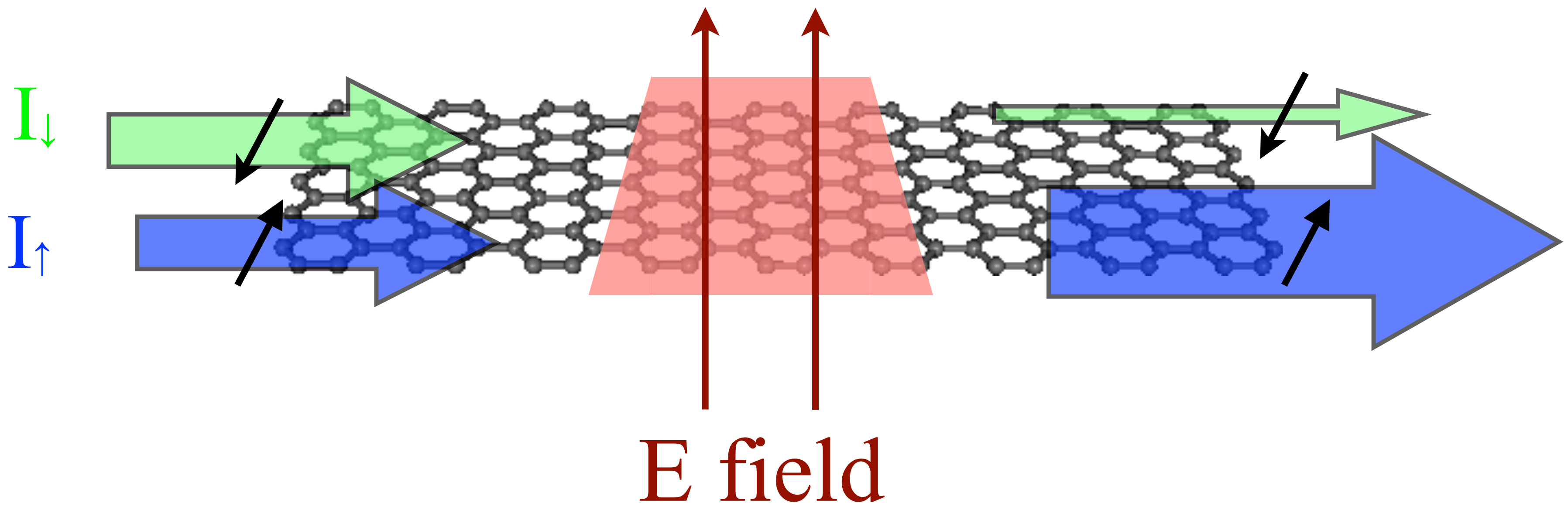
Symmetry of Spin Transport in Two-Terminal Waveguides with a Spin-Orbital Interaction and Magnetic Field Modulations, S. F. Zhai and H. Q. Xu, Phys. Rev. Lett. **94**, 246601 (2005).

But there is a way around if the lead has two or more conducting channels…

…symmetry permitting.

Goal:

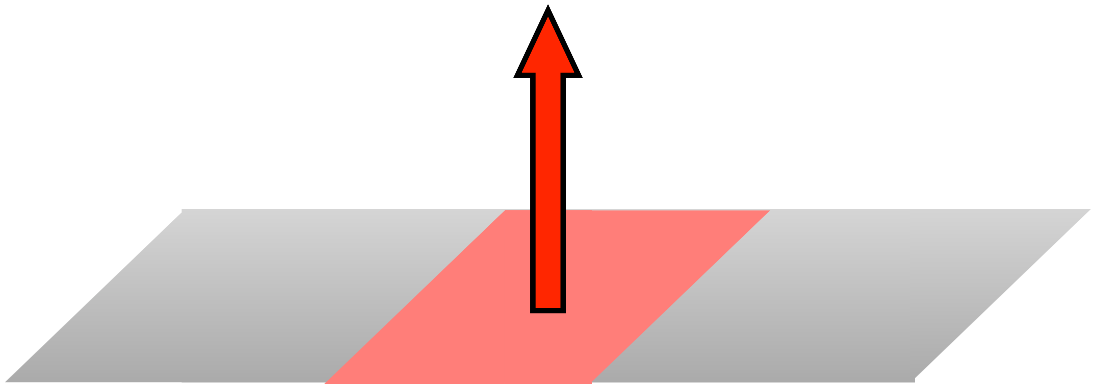
Obtain spin-polarized transport *in planar systems* without magnetic fields

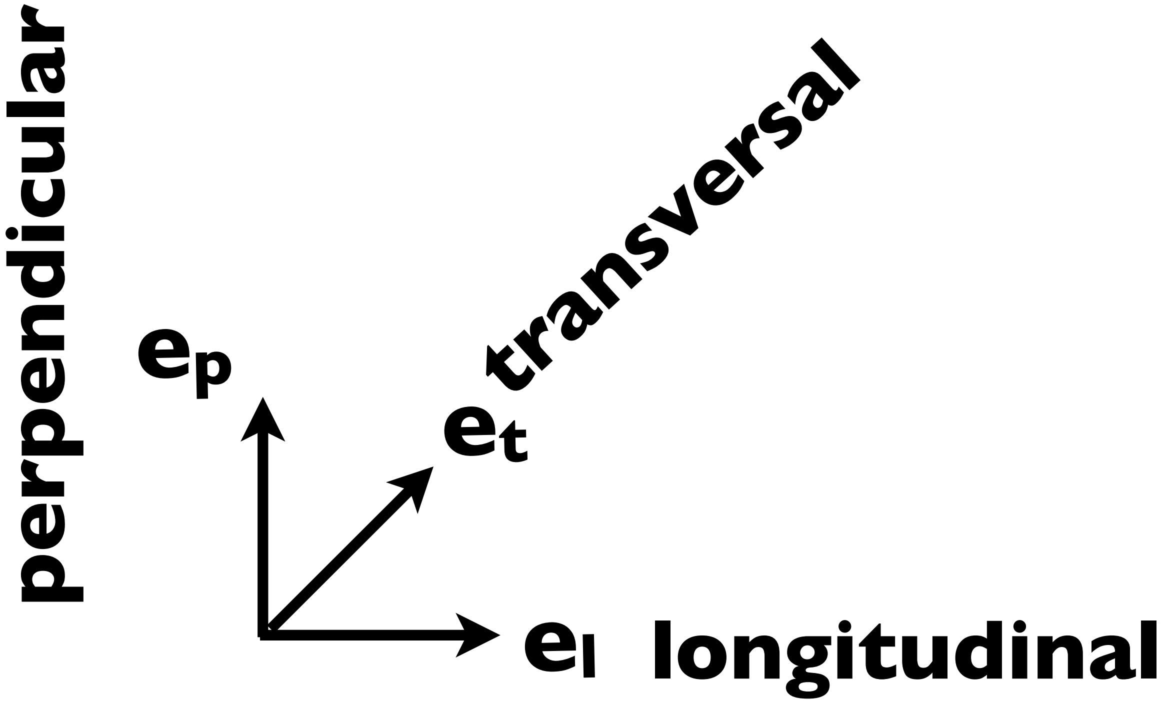


without magnetic fields or impurities - preserving time-reversal symmetry

Symmetries of planar systems in an external electric field

The symmetries of the conductance are those of the full Hamiltonian





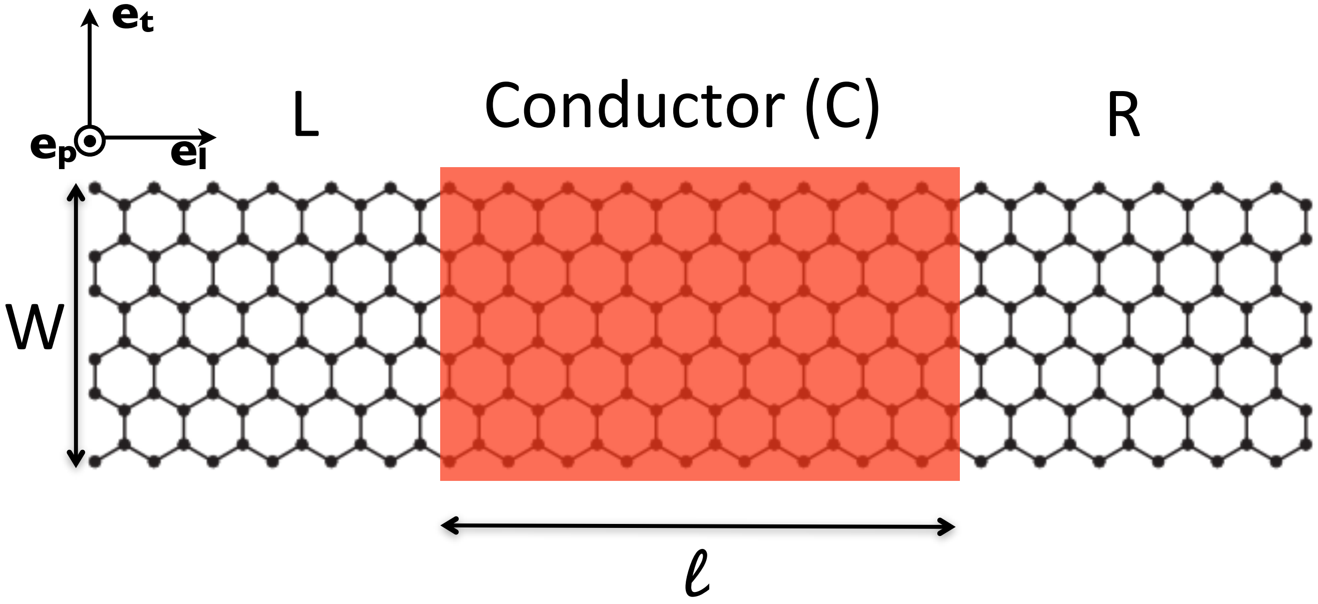
C_2 rotation

M_l, M_t mirror planes

Time reversal

Symmetries of planar systems in an external electric field

C_2 rotation



$$(e_l, e_t, e_p) \to (-e_l, -e_t, e_p)$$

$$(\sigma_l, \sigma_t, \sigma_p) \to (-\sigma_l, -\sigma_t, \sigma_p)$$

LR→RL

$$G^{LR}_{\sigma,\sigma'} = G^{RL}_{\bar{\sigma},\bar{\sigma}'} \quad \text{(l,t)}$$

$$G^{LR}_{\sigma,\sigma'} = G^{RL}_{\sigma,\sigma'} \quad \text{(p)}$$

Symmetries of planar systems in an external electric field

time-reversal

$t \to -t$

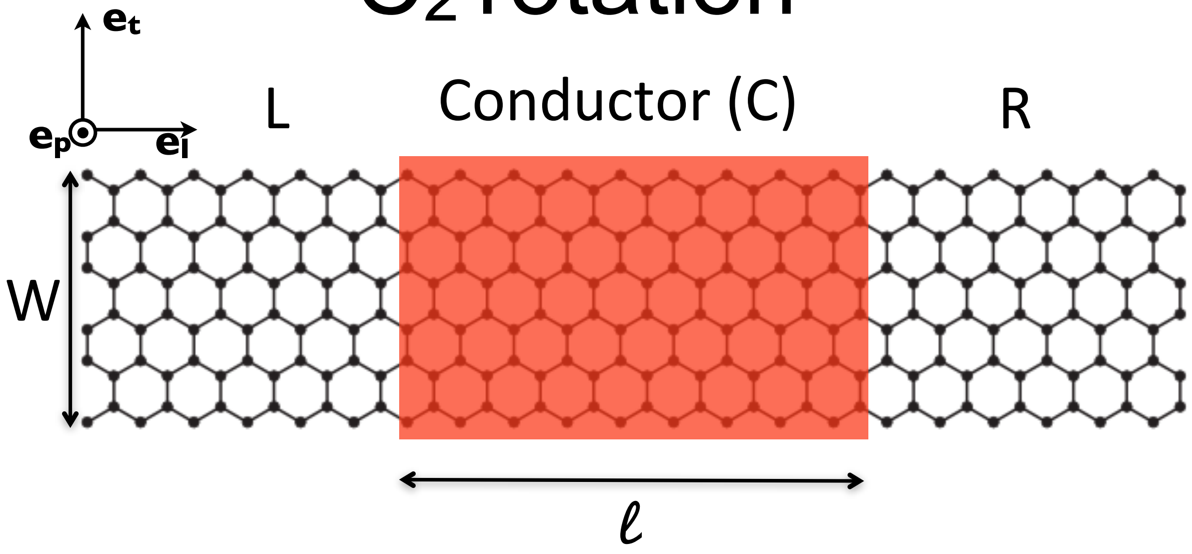
$$\boxed{\begin{array}{c} \mathbf{r} \to \mathbf{r} \\ \mathbf{p} \to -\mathbf{p} \\ \boldsymbol{\sigma} \to -\boldsymbol{\sigma} \end{array}} \quad \Rightarrow \quad G^{LR}_{\sigma,\sigma'} = G^{RL}_{\bar{\sigma}',\bar{\sigma}}$$

In graphene, electron-hole (charge conjugation)

$$\boxed{\begin{array}{c} q \to -q \\ E \to -E \end{array}} \quad \Rightarrow \quad G^{LR}_{\sigma,\sigma'}(E) = G^{RL}_{\sigma',\sigma}(-E)$$

Symmetries of planar systems in an external electric field

C$_2$ rotation



$$\left.\begin{array}{c} G^{LR}_{\sigma,\sigma'} = G^{RL}_{\bar{\sigma},\bar{\sigma}'} \text{ (t)} \\ + \\ G^{LR}_{\sigma,\sigma'} = G^{RL}_{\bar{\sigma}',\bar{\sigma}} \text{ (TR)} \end{array}\right\} \begin{array}{c} \nearrow \\ \\ \searrow \end{array}$$

$$G^{LR}_{\uparrow\uparrow} = G^{RL}_{\downarrow\downarrow}$$

$$G^{RL}_{\downarrow\downarrow} = G^{LR}_{\uparrow\uparrow}$$

$$G^{LR}_{\uparrow\uparrow} = G^{LR}_{\uparrow\uparrow}$$

tautology

$$G^{LR}_{\uparrow\downarrow} = G^{RL}_{\downarrow\uparrow}$$

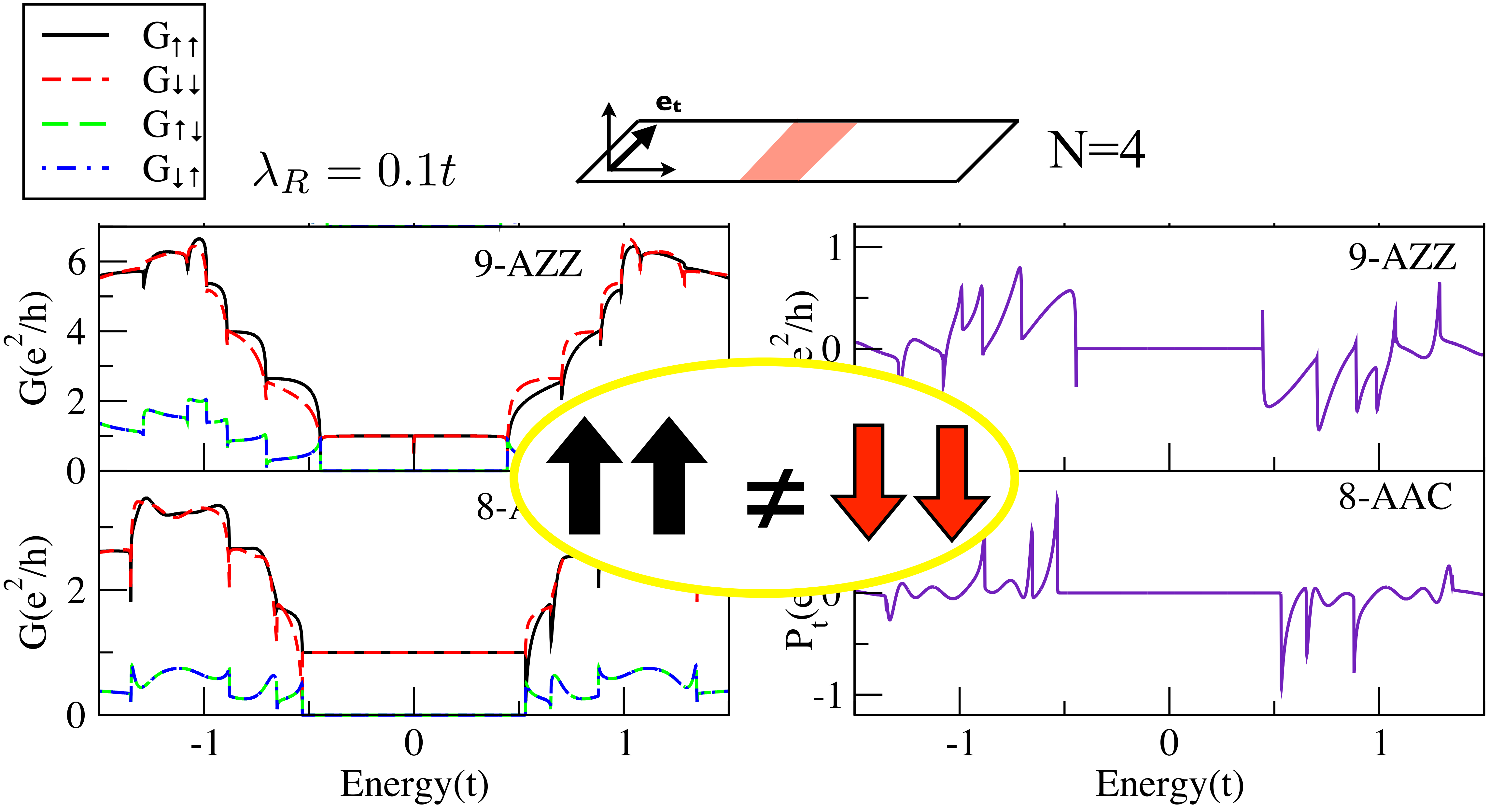
$$G^{RL}_{\downarrow\uparrow} = G^{LR}_{\downarrow\uparrow}$$

$$G^{LR}_{\downarrow\uparrow} = G^{LR}_{\downarrow\uparrow}$$

spin-flip conductances
are equal

$$P_s = G^{LR}_{\uparrow\uparrow} + \cancel{G^{LR}_{\downarrow\uparrow}} - G^{LR}_{\downarrow\downarrow} - \cancel{G^{LR}_{\uparrow\downarrow}}$$

Spin-resolved conductances and ...current polarization



L. Chico, A. Latgé, L. Brey, Phys. Chem. Chem. Phys. **17**, 16469 (2015)

Summary

- We have reviewed the fundamentals of quantum transport and its extension to spin-dependent problems

- We have studied two cases in which SOC plays a fundamental role in transport:

    1. Datta-Das transistor
    2. All-electrical production of spin-polarized currents (Rashba)

- Symmetry reasoning allows us to analyze the the existence of spin-polarized currents - **symmetry as a guiding principle**

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