

Charge, heat, and spin transport

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Requirements for theory of magnetoelectronics

Metals and insulators:

Fermi/screening wave length $O(\text{\AA})$; disorder; sharp interfaces

- Size quantization effects on transport negligible (exception: MgO|Fe|Cr).
- Many-body effects negligible (exception: Kondo effect).
- Weak spin-orbit interaction.
- Quantum mechanics at the interfaces.

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Overview first two lectures

- Elementary transport theory**
 - (a) Linear response theory of transport
 - (b) Scattering theory of transport
 - (c) Semiclassical transport
 - (d) Thermoelectricity and Onsager symmetry
 - (e) Collinear spin transport

G.D. Mahan, *Many-Particle Physics*, (Springer, 2000).
S. Doniach, E. H. Sondheimer, *Green's Functions for Solid State Physicists* (Imperial, 1998)
- DC magnetoelectronic circuit theory**
 - (a) Transport in non-collinear magnetization textures, non-collinear spin valves
 - (b) Spin transfer torque and spin mixing conductance
 - (c) Spintronic Kirchhoff Laws

A. Brataas et al., *Physics Reports* **427**, 157 (2006)
- AC magnetoelectronic circuit theory**
 - (a) Current-induced magnetization dynamics
 - (b) Spin pumping and enhanced Gilbert damping
 - (c) DC and AC spin pumping

Y. Tserkovnyak et al., *Rev. Mod. Phys.*, **77** 1375 (2005).

Not: domain walls, tunnel junctions, (spin-orbit interaction)

Ohm's Law

$$I = \frac{\Delta V}{R} = G \Delta V = \mathcal{A} \frac{G L}{\mathcal{A} L} \Delta V$$

$$j = \frac{I}{\mathcal{A}} = \frac{G L}{\mathcal{A} L} \Delta V = \sigma E = \frac{E}{\rho}$$

$$P = I \Delta V = R^2 I^2$$

$$[G] = \left[\frac{e^2}{h} \right] = S = \frac{1}{\Omega}$$

Linear response of heat and mass transport: Fourier/Fick Laws

Perturbation theory of transport

Perturbation theory of transport

Perturbation theory

Applied electric field \mathbf{E} generates current $\langle \mathbf{j} \rangle$ in a system H_0 :

$$H = H_0 + H' \text{ where } H' = -e\mathbf{r} \cdot \mathbf{E} \quad H_0 |\varphi_i\rangle = \varepsilon_i |\varphi_i\rangle$$

$$|\psi_i\rangle = |\varphi_i\rangle + |\varphi_i'\rangle \text{ where } |\varphi_i'\rangle = \sum_{j \neq i} \frac{\langle \varphi_j | H' | \varphi_i \rangle}{\varepsilon_i - \varepsilon_j} |\varphi_j\rangle$$

$$\langle \mathbf{j} \rangle = \sum_i f_i \langle \psi_i | \mathbf{j} | \psi_i \rangle = \sum_i f_i \left[\langle \varphi_i | \mathbf{j} | \psi_i \rangle + \text{h.c.} \right] \quad f_i \text{ occupation number}$$

$$= \sum_i f_i \sum_{j \neq i} \left[e \frac{\langle \varphi_i | \mathbf{j} | \varphi_j \rangle \langle \varphi_j | \mathbf{r} | \varphi_i \rangle}{\varepsilon_i - \varepsilon_j} + \text{h.c.} \right] \cdot \mathbf{E} = \boldsymbol{\sigma} \cdot \mathbf{E}$$

$$\langle \varphi_i | \mathbf{j} | \varphi_j \rangle = \frac{e\hbar}{2mi} (\varphi_i^* \nabla \varphi_j - \text{h.c.}) \quad \boldsymbol{\sigma} \text{ conductance tensor}$$

But $\langle \varphi_j | \mathbf{r} | \varphi_i \rangle$ is problematic for large systems.

Kubo formula

$$H = \frac{1}{2m} [\mathbf{p} - e\mathbf{A}]^2 + U = \frac{p^2}{2m} + U + \mathbf{j} \cdot \mathbf{A} + \frac{eA^2}{2m}$$

$$\left(\nabla \cdot \mathbf{A} = 0; \quad \mathbf{E} = -\frac{\partial \mathbf{A}}{\partial t} \right) \quad \mathbf{A}(t) = \mathbf{A}_0 e^{-i\omega t} \rightarrow \mathbf{E} = i \frac{\mathbf{A}_0}{\omega}$$

$H' = \mathbf{j}(\mathbf{r}) \cdot \mathbf{A}(t)$ by time-dependent perturbation theory

$$\langle \sigma \rangle_{ij}(\mathbf{r}, \mathbf{r}') = \lim_{\omega \rightarrow 0} \left\{ i \frac{ne^2}{m\omega} \delta_{ij} + \frac{1}{\hbar\omega\Omega} \int_{-\infty}^{\infty} dt e^{i\omega t} \langle \Psi_0 | [j_i(\mathbf{r}, t), j_j(\mathbf{r}', 0)] | \Psi_0 \rangle \right\}$$

$|\Psi_0\rangle$ ground state wavefunction (no field)

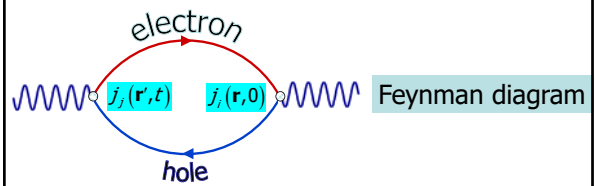
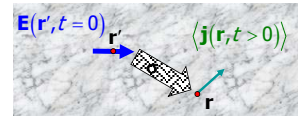
$j_i(\mathbf{r}, t)$ current operator in Heisenberg picture

$[a, b] = ab - ba$ commutator

Fluctuation-dissipation theorem

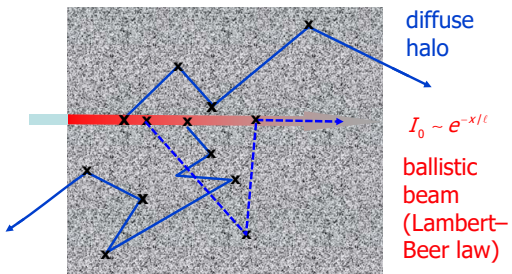
Linear response (Kubo) formalism

$$\langle \mathbf{j}(\mathbf{r}) \rangle = \int_V d\mathbf{r}' \sigma(\mathbf{r}, \mathbf{r}') \cdot \mathbf{E}(\mathbf{r}')$$



Disorder

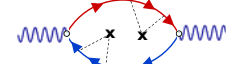
mean free path $\ell = V_F \tau$



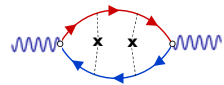
Impurity scattering (short-range)



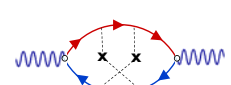
ballistic: $\sigma = \infty$



Drude: $\sigma_0 = \frac{ne^2\tau}{m}$
 $\tau^{-1} \sim nV_x^2$



diffuse scattering (ladder)



interference (cross)

$\Delta\sigma < 0$ weak localization

Scattering theory of transport

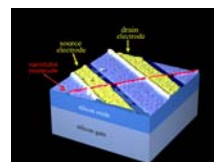
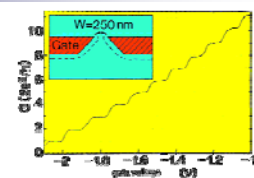
Joseph McElhenny, 2006
The Last Scattering Surface



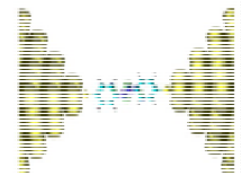
Nanostructures



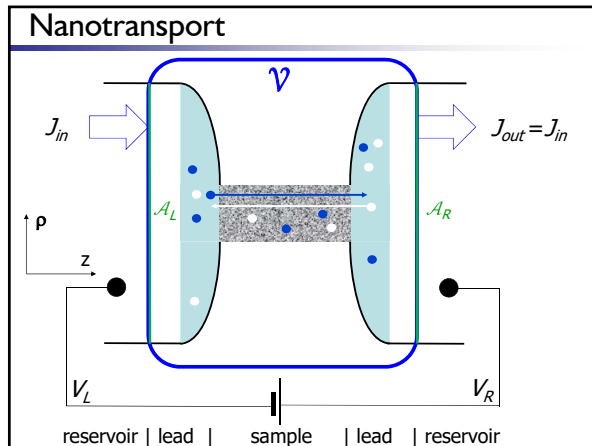
quantum point contacts



quantum wires



molecules



Fisher-Lee theory

Phys. Rev. B 23, 6851 (1981)

$$J_{out} = \int_{A_R} \mathbf{j}(\mathbf{r}, z) d\mathbf{p} = \int_{A_R} d\mathbf{p} \int_V d\mathbf{r}' \hat{\mathbf{z}} \cdot \boldsymbol{\sigma}(\mathbf{r}, \mathbf{r}') \cdot \mathbf{E}(\mathbf{r}')$$

$$e\mathbf{E}(\mathbf{r}) = \nabla\mu(\mathbf{r}) \quad \text{In the leads: } \mathbf{E}(\mathbf{r}) = 0$$

Divergence theorem and current conservation ($\nabla \cdot \mathbf{j}(\mathbf{r}) = 0$):

$$\int_V d\mathbf{r}' \hat{\mathbf{z}} \cdot \boldsymbol{\sigma}(\mathbf{r}, \mathbf{r}') \cdot \mathbf{E}(\mathbf{r}') \cdot \nabla\mu(\mathbf{r}') = \int_{A_L} d\mathbf{p}' \hat{\mathbf{z}} \cdot \boldsymbol{\sigma}(\mathbf{r}, \mathbf{r}') \mu(\mathbf{r}')$$

$$eJ = (\mu_R - \mu_L) \int_{A_L} d\mathbf{p}' \int_{A_R} d\mathbf{p} (\boldsymbol{\sigma})_{zz}(\mathbf{r}, \mathbf{r}') = G\Delta\mu \quad \text{independent of electric field distribution}$$

Landauer-Büttiker formula

$$G = \int_{A_L} d\mathbf{p} \int_{A_R} d\mathbf{p}' (\boldsymbol{\sigma})_{zz}(\mathbf{r}, \mathbf{r}')$$

Expansion into eigenstates i, j of the leads at Fermi energy

$$G = \frac{e^2}{h} \sum_i^{k_i^{(L)} > 0, \mu} \sum_j^{k_j^{(R)} > 0, \mu} |t_{ij}|^2 = \frac{e^2}{h} \sum_{ij} |t_{ij}|^2 = \frac{e^2}{h} \sum_{ij} T_{ij}$$

t_{ij} transmission coefficient (probability amplitude)

$T_{ij} = |t_{ij}|^2$ transmission probability

Semiclassics

Interference and semiclassical approximation

$$\langle \mathbf{j}(\mathbf{r}) \rangle = \int_V d\mathbf{r}' \mathbf{G}(\mathbf{r}, \mathbf{r}') \cdot \mathbf{j}(\mathbf{r}, \mathbf{r}')$$

Wigner representation:

$$\mathbf{G}(\mathbf{r}, \mathbf{r}') \Rightarrow \mathbf{G}\left(\frac{\mathbf{r} + \mathbf{r}'}{2}, \mathbf{r} - \mathbf{r}'\right)$$

$$\mathbf{G}(\mathbf{R}, \mathbf{k}) = \int d(\mathbf{r} - \mathbf{r}') \mathbf{G}(\mathbf{R}, \mathbf{k}) e^{i\mathbf{k}(\mathbf{r} - \mathbf{r}')}$$

Semiclassical approximation holds for disordered metals:

$$\mathbf{j}(\mathbf{R}) = \sum_{\mathbf{k}} \mathbf{G}(\mathbf{R}, \mathbf{k}) \cdot \mathbf{j}_{\mathbf{k}} \rightarrow \sum_{\mathbf{k}} f_{\mathbf{k}}(\mathbf{R}) \cdot \mathbf{j}_{\mathbf{k}}$$

$$\mathbf{j}_{\mathbf{k}} = e\mathbf{v}_{\mathbf{k}} = \frac{e\partial\epsilon_{\mathbf{k}}}{\partial\mathbf{k}} \rightarrow \frac{e\hbar}{m^*} \mathbf{k} \quad f_{\mathbf{k}}(\mathbf{R}) > 0$$

Distribution functions

$$f_{\mathbf{k}}(\mathbf{R}, \delta t) = f_{\mathbf{k} + \frac{e\mathbf{E}}{\hbar}\delta t}(\mathbf{R} - \mathbf{v}_{\mathbf{k}}\delta t) \quad \text{electron distribution function}$$

$$\frac{df}{dt} = \left(\mathbf{v}_{\mathbf{k}} \cdot \frac{\partial}{\partial \mathbf{R}} + \frac{e\mathbf{E}}{\hbar} \cdot \frac{\partial}{\partial \mathbf{k}} \right) f_{\mathbf{k}}(\mathbf{R}) - \left(\frac{\partial f}{\partial t} \right)_{\text{scatt}} = 0 \quad \text{steady state Boltzmann equation}$$

$$f_{\mathbf{k}}(\mathbf{R}) \approx f_0(\epsilon, \mathbf{R}) \Big|_{\epsilon=\epsilon_{\mathbf{k}}} + \frac{\partial f_0(\epsilon, \mathbf{R})}{\partial \epsilon} g_{\mathbf{k}}(\mathbf{R}) \quad \text{linearization}$$

$$f_0(\epsilon, \mathbf{R}) = f_0^{(FD)}(\epsilon, \mathbf{R}) \Big|_{\epsilon=\epsilon_{\mathbf{k}}} = (2\pi)^{-3} \int d\Omega_{\mathbf{k}} \frac{1}{e^{-(\epsilon_{\mathbf{k}} - \mu(\mathbf{R})) / kT} - 1} \quad \text{Fermi-Dirac distribution}$$

$$\frac{\partial f_0(\epsilon, \mathbf{R})}{\partial \epsilon} \xrightarrow{kT \ll \mu} -\delta(\epsilon - \mu(\mathbf{R})) \quad \text{Fermi energy}$$

$$g_{\mathbf{k}}(\mathbf{R}) \quad \text{deformation due to perturbation}$$

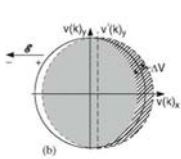
Diffusion approximation

$$\left(\frac{\partial f}{\partial t}\right)_{\text{scatt}} = -\frac{g_{\mathbf{k}}(\mathbf{R})}{\tau_{\mathbf{k}}} + \sum_{\mathbf{k}'} W_{\mathbf{k}\mathbf{k}'} g_{\mathbf{k}'}(\mathbf{R}) \rightarrow -\frac{g_{\mathbf{k}}(\mathbf{R})}{\tau} + W \sum_{\mathbf{k}'} g_{\mathbf{k}'}(\mathbf{R}) = 0$$

$\tau_{\mathbf{k}} \approx \tau$ relaxation time approximation
 $W_{\mathbf{k}\mathbf{k}'} \approx W$ (short range impurity scattering)

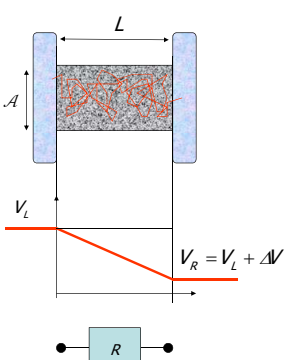
$$\mathbf{v}_{\mathbf{k}} \cdot \left[\nabla_{\mathbf{R}} - e\mathbf{E} \frac{\partial}{\partial \varepsilon} \right] f_0(\varepsilon, \mathbf{R}) + \frac{\partial f_0(\varepsilon, \mathbf{R})}{\partial \varepsilon} \frac{g_{\mathbf{k}}(\mathbf{R})}{\tau} = 0$$

$$g_{\mathbf{k}}(\mathbf{R}) \approx -\tau \mathbf{v}_{\mathbf{k}} \cdot \left[\nabla_{\mathbf{R}} - e\mathbf{E} \right] f_0(\varepsilon, \mathbf{R})$$

$$g_{\mathbf{k}} \rightarrow e\tau v_{\mathbf{k}} E \cos \theta_{\mathbf{k}}$$


$$\sigma \equiv \frac{e^2 \tau}{3l^2} \sum_{\mathbf{k}} v_{\mathbf{k}}^2 \left(-\frac{\partial f_0}{\partial \varepsilon_{\mathbf{k}}} \right) \rightarrow \frac{ne^2 \tau}{m^*}$$

Diffusion in bulk 3D metal



Ohm's Law

$$\frac{\partial V(x)}{\partial x} = E = \rho j$$


$$\rho = \frac{m^*}{ne^2 \tau} \quad \text{resistivity}$$

$$R = \frac{\rho L}{A} \quad \text{resistance}$$

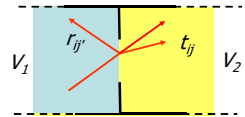
Current conservation

$$\frac{\partial}{\partial x} \frac{\partial \mu(x)}{\rho \partial x} = 0 \rightarrow \frac{eE}{\rho} = \text{const.}$$

Interfaces



Interfaces



$I = G_{LB}^I (V_1 - V_2)$
 $G_{LB}^I = \frac{e^2}{h} \sum_{ij} \delta_{\varepsilon_i = \varepsilon_j = E_F} |t_{ij}|^2 = \frac{e^2}{h} \sum_{k=1}^N T_k$ Landauer-Büttiker formula

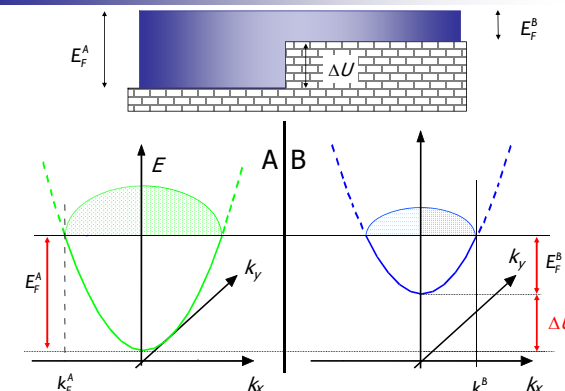
Ballistic point contact:

$$G_{LB} \xrightarrow{2 \rightarrow 1} G_{\text{Sharvin}} = \frac{2e^2}{h} \sum_{ij} \delta_{\varepsilon_i = \varepsilon_j = E_F} \delta_{ij} = \frac{2e^2}{h} \frac{A}{(2\pi)^2} \int d\mathbf{k}_{\parallel} = \frac{2e^2}{h} \frac{A k_F^2}{4\pi}$$

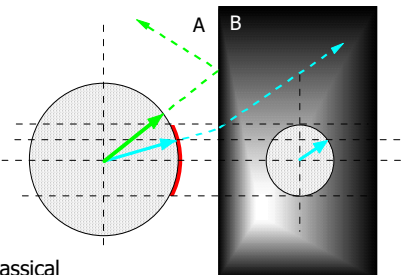
Sharvin conductance

$$= \frac{2e^2}{h} N$$

Metallic interface



Specular metallic interface

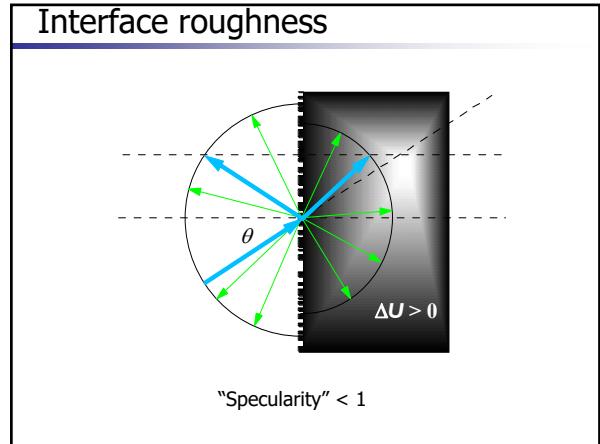
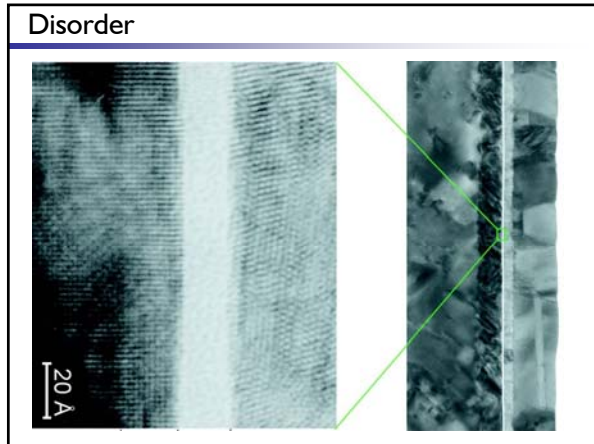


semiclassical approximation:

$$T_{\mathbf{k}_i, \mathbf{k}_i'} \approx \delta_{\mathbf{k}_i, \mathbf{k}_i'} \begin{cases} 1 & \text{for } E_{k_x} > \Delta U \\ 0 & \text{for } E_{k_x} \leq \Delta U \end{cases}$$

$$G = \frac{2e^2}{h} \frac{A (k_F^2)^2}{4\pi} \left(1 - \frac{\Delta U}{E_F^A} \right)$$

A interface area



Series resistor model

$$\frac{\partial V_{L/R}(x)}{\partial x} = E_{L/R} = -j \rho_{L/R}$$

$$j = -\frac{G_I \Delta \mu_I}{\mathcal{A} e}$$

G_I interface conductance

$$(G^I)^{-1} = (G_{LB}^I)^{-1} - \frac{1}{2} \left((G_{Sh}^A)^{-1} + (G_{Sh}^B)^{-1} \right)$$

equivalent circuit

Power Generation Mode

Refrigeration Mode

Thermoelectrics and Onsager

Heat and charge transport in metals

Seebeck coefficient $S = \left(\frac{\partial V}{\partial T} \right)_{J_e=0}$

$$\lim_{T \rightarrow 0} S = - \frac{e L_0 T}{g(\epsilon_F)} \left. \frac{\partial g(\epsilon)}{\partial \epsilon} \right|_{\epsilon_F} < 0$$

Lars Onsager Memorial at NTNU Trondheim

The Nobel Prize in Chemistry 1968:
 "for the discovery of the reciprocal relations bearing his name, which are fundamental for the thermodynamics of irreversible processes"

Onsager symmetry (1931)

$i = \{\text{mass, charge, energy, volume, (angular) momentum, ...}\}$

X_i generalized forces
 J_i generalized currents

$J_m = \sum_n L_{mn} X_n$ linear response

If: $\dot{S} = \sum_i X_i J_i$ entropy creation rate

then: $L_{ij} = L_{ji}$ **Onsager relations**

When time reversal symmetry is broken:

$L_{ij}(\mathbf{m}, \mathbf{H}_{ext}) = \varepsilon_i \varepsilon_j L_{ji}(-\mathbf{m}, -\mathbf{H}_{ext})$

$\varepsilon_i = \begin{cases} 1 & \text{when variable } i \text{ even (charge)} \\ -1 & \text{odd (spin)} \end{cases}$

1st and 2nd Law of Thermodynamics

$dU_n = dQ_n + dW_n = T_n dS_n + \mu_n dN_n$

$dS_n = \frac{dU_n}{T_n} - \frac{\mu_n}{T_n} dN_n$

$dU_1 = -dU_2 \equiv dU; \quad dN_1 = -dN_2 \equiv dN$

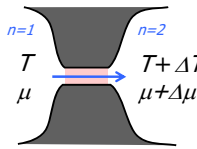
$J_U = -\frac{dU}{dt}; \quad J_N = -\frac{dN}{dt}$

$dS = dS_1 + dS_2; \quad T_1 = T; \quad T_2 = T + \Delta T$

$\frac{dS}{dt} = \left(\frac{1}{T} - \frac{1}{T+\Delta T}\right) J_U + \left(\frac{\mu}{T} - \frac{\mu+\Delta\mu}{T+\Delta T}\right) J_N$

$T \frac{dS}{dt} \approx (J_U - \mu J_N) \left(-\frac{\Delta T}{T}\right) - J_N \Delta\mu$ **conjugate currents and forces identified!**

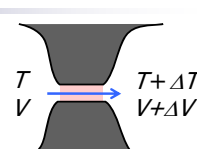
$= J_Q \left(-\frac{\Delta T}{T}\right) + J_N (-\Delta\mu) = \sum_i J_i X_i \geq 0$



Thermoelectrics

$\begin{pmatrix} J_c \\ J_Q \end{pmatrix} = \begin{pmatrix} L_{11} & L_{21} \\ L_{12} & L_{22} \end{pmatrix} \begin{pmatrix} \Delta V \\ -\frac{\Delta T}{T} \end{pmatrix}$

$L_{12} = L_{21}$ Onsager reciprocity

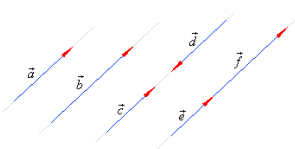


$\begin{pmatrix} \Delta V \\ J_Q \end{pmatrix} = \begin{pmatrix} R & S \\ \Pi & K \end{pmatrix} \begin{pmatrix} J_c \\ -\Delta T \end{pmatrix}$

$R = 1/G$ electrical resistance
 K thermal conductance
 S Seebeck coefficient
 $\Pi = ST$ Peltier coefficient

$\Pi = ST$ **Onsager-Thomson (Kelvin) relation**

Collinear spin transport



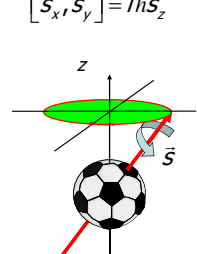
Electron spin and quantum mechanics

$[S_x, S_y] = i\hbar S_z$

$S_z = \frac{\hbar}{2}$ $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ $\begin{pmatrix} \uparrow \end{pmatrix}$

$S_z = -\frac{\hbar}{2}$ $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ $\begin{pmatrix} \downarrow \end{pmatrix}$

$S = \sqrt{S^2} = \frac{\sqrt{3}}{2} \hbar$



Electron spin vector operator

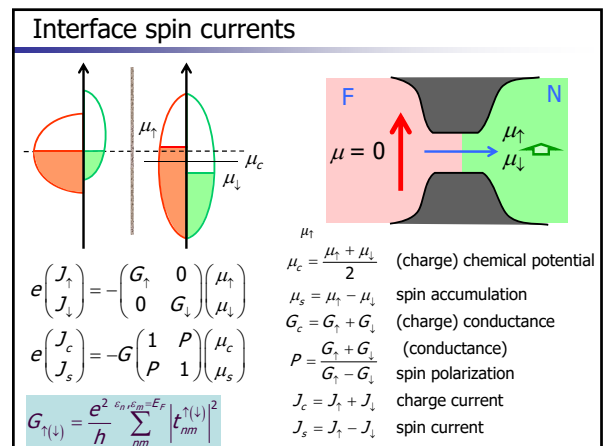
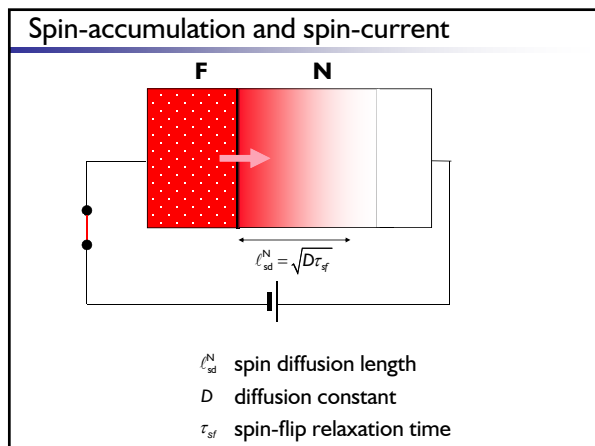
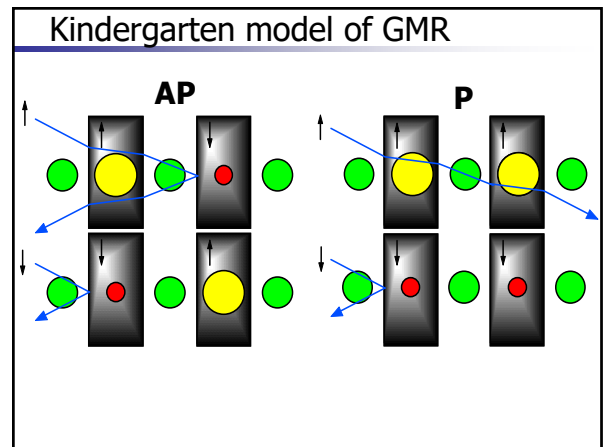
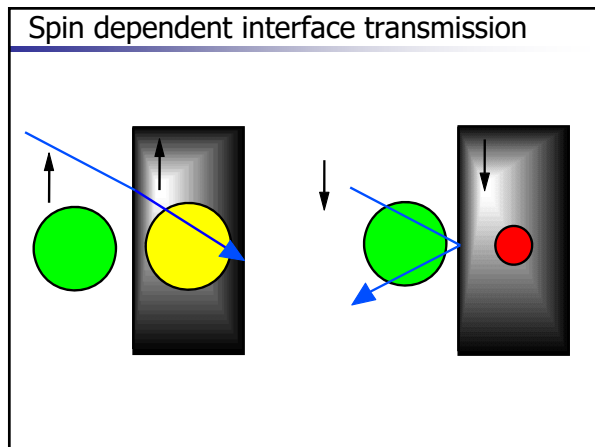
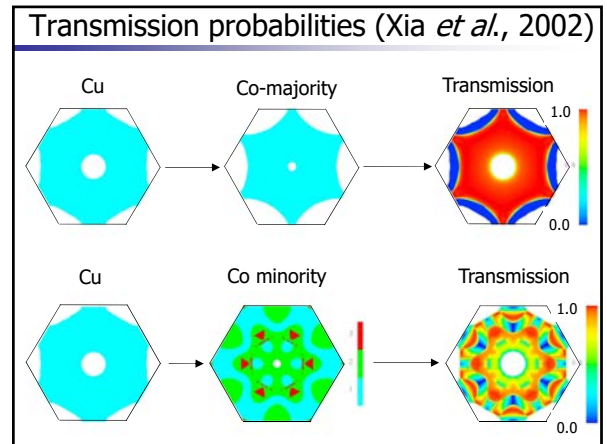
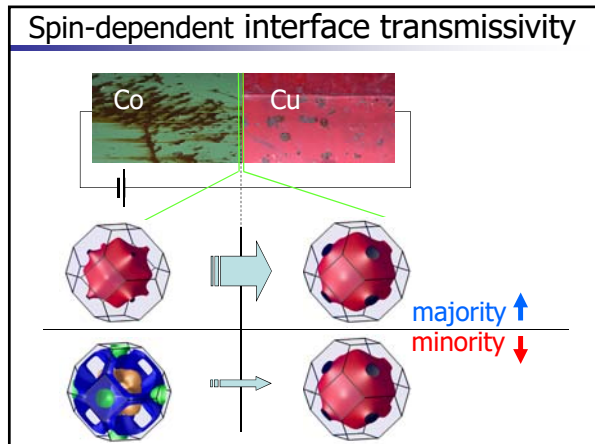
$\boldsymbol{\mu} = g_e \frac{-e\hbar}{2m} \mathbf{s} = -\gamma \mathbf{s} = -g_e \mu_B \frac{\boldsymbol{\sigma}}{2}$ $\mu_B = \frac{e\hbar}{2m}$ Bohr magneton

$\mathbf{s} = \frac{\hbar}{2} \boldsymbol{\sigma}$ $\gamma = g_e \frac{\mu_B}{\hbar}$

$\boldsymbol{\sigma} = \left\{ \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right\}$ Pauli matrices

$\mathcal{H} = -\mathbf{B} \cdot \boldsymbol{\mu} \xrightarrow{\text{Field } \hat{z}} -B_0 \mu_z = -\frac{g_e \mu_B B_0}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

Field on $m_s = +1/2$
 $\mathbf{g} \cdot \boldsymbol{\mu} B_0 = \hbar \omega_0$ $\mathcal{H} \left| m_s = \pm \frac{1}{2} \right\rangle = \pm \hbar \omega_0 \left| m_s = \pm \frac{1}{2} \right\rangle$
 Field off $m_s = -1/2$



Spin diffusion in bulk metal (Valet-Fert)

Ohm's Law

$$j_s = -\sigma \frac{\partial \mu_s(x)}{\partial x}, \quad s = \{\uparrow, \downarrow\}$$

spin relaxation

$$\frac{\partial(j_\uparrow - j_\downarrow)}{\partial x} = \frac{e(n_\uparrow - n_\downarrow)}{\tau_{sf}}$$

spin-flip diffusion

$$\frac{\partial^2(\mu_\uparrow - \mu_\downarrow)(x)}{\partial x^2} = \frac{(\mu_\uparrow - \mu_\downarrow)(x)}{\ell_{sd}^2}$$

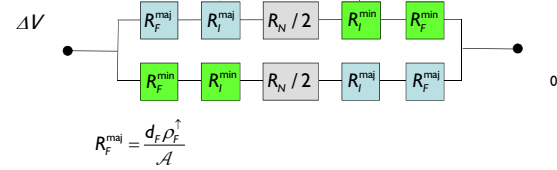
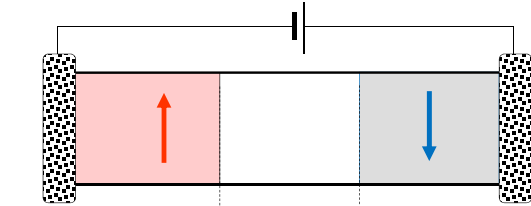
$$\ell_{sd} = \sqrt{D\tau_{sf}}$$

spin diffusion length

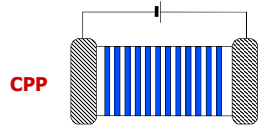
$$D = \frac{1}{3} v_F^2 \tau$$

averaged diffusion constant

Two-channel series resistor model



Two-channel series resistor model



$$AR_s^{\uparrow} = N_{bl} \left(\rho_s^{(F)} d_F + \frac{\rho_s^{(N)}}{2} d_N + 2AR_s^{(F/N)} \right)$$

\mathcal{A} cross section of sample
 N_{bl} number of bilayers
 $\rho_s^{(F)}$ spin-up resistivity of F
 $R_s^{(F/N)}$ spin-up interface resistance

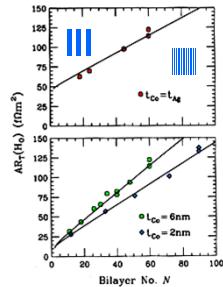
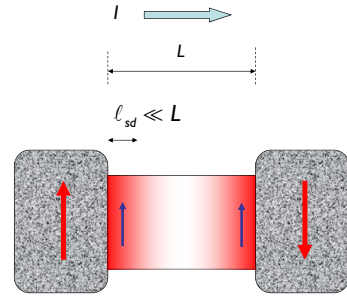


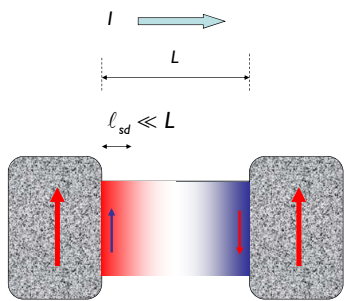
Fig. 2. $AR_s(H_0)$ versus bilayer number N for three different sets of Co/Ag multilayers, all with fixed total thickness $t = 720$ nm. The curves shown are fits to the two-channel model!

MSU group in the 90's

F|N|F spin valves



F|N|F spin valves



F|N|F spin valves

