Modelling and Simulation:
a physicist's point of view

Part 1

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Kavli Institute of NanoScience, TU Delft

I want you (to talk about Modelling and Simulation)

What is simulation

Simulant (German) = Malingerer

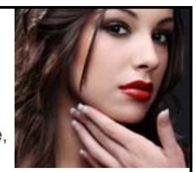
History: Horse simulator (Wikipedia)

Simulation is the imitation of the operation of a real-world process or system over time.

The act of simulating something requires a **model**.

Model

Occupation



A model, is a person with a role either to promote, display, or advertise commercial products or to serve as a visual aide for people who are creating works of art. Wikipedia

Median pay (annual): 18,750 USD (2012)

Median pay (hourly): 9.02 USD (2012)

Entry level education: Less than high school

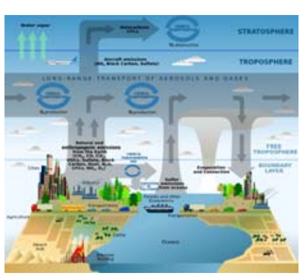
Projected 10-year growth: 15% (2012)

Number of jobs: 4,800 (2012)

Similar professions: Child Actor, Fashion Designers

Modelling (Wikipedia)

Modelling: A scientific activity, the aim of which is to make a particular part or feature of the world easier to understand, define, quantify, visualize, or simulate by referencing it to existing and usually commonly accepted knowledge



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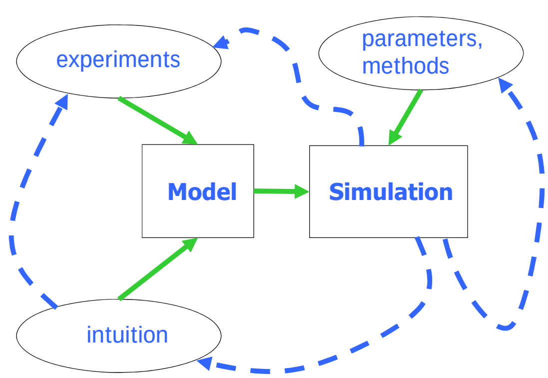
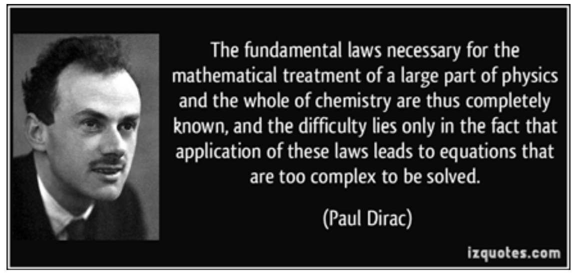
Philosophy



Our model

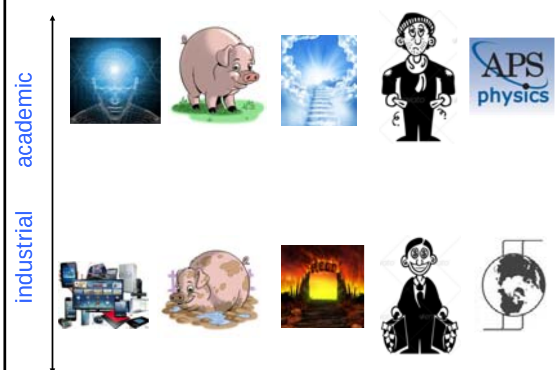
$$\left(i\gamma^{\mu}\left(\partial_{\mu}+ieA_{\mu}\right)-m\right)\psi=0$$

Modeling and simulation



All of condensed matter theory
is modelling and simulation!

The fundamental–applied divide



Contents

- **Modelling and simulation: a physicists point of view**

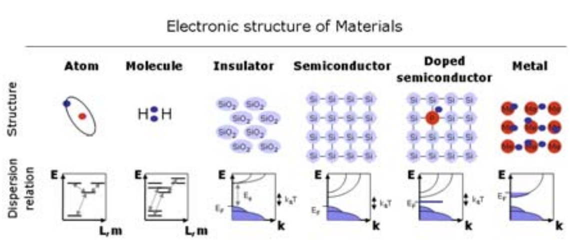
Part 1

I. M&S of electronic structure
II. M&S of magnetization
III. M&S of spin and charge transport
IV. M&S of MRAM elements

Part 2

- Case study: heterostructures with magnetic insulators

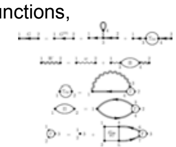
I. M&S of electronic structure

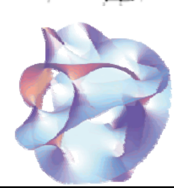


Many-body problem

- Exact solutions (hydrogen molecule, 1D systems, 2D Ising model)
- Many-body perturbation theory, Green's functions, diagrammatic methods (also for alloys)
- Configuration interaction (chemistry)
- Coupled cluster expansions (chemistry)
- Quantum Monte-Carlo approaches
- **Density functional theory**
- Lattice gauge theory
- Quantum tensor network theory
- Numerical renormalization group
- AdS-CFT (string theory)

⋮





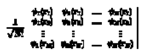
"Mean-field" theory

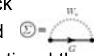
Models

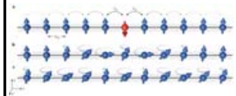
- Dirac Hamiltonian
- Pauli spin (non rel.)
- tight-binding models
- Hubbard models
- spin models

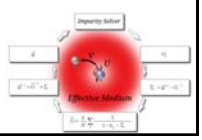
Simulation methods

- Hartree-Fock
- GW-method
- Density functional theory
  - Local density approximation
  - Corrections: LDA+U, LDA+C
- Dynamic mean-field theory









Density functional theory

The ground state energy $E[\rho]$ is a functional of the electron (spin) density $\rho(\mathbf{r})$ (Hohenberg & Kohn, 1964):

Constrained search:
$$E[\rho] = \min_{\Psi_\rho} \langle \Psi_\rho | T | \Psi_\rho \rangle + E_H[\rho]$$
$$E_0[\rho_0] = \min_{\rho} E[\rho]$$

Kohn-Sham non-interacting auxiliary particles:

$$\Psi_\rho^{KS} = \frac{1}{\sqrt{N}} \left| \varphi_1(\mathbf{r}_1), \cdots, \varphi_N(\mathbf{r}_N) \right|$$
$$\int |\varphi_i(\mathbf{r})|^2 d\mathbf{r} = 1 \qquad \rho(\mathbf{r}) = \sum_{i=1}^{N} |\varphi_i(\mathbf{r})|^2$$
$$E[\rho] = \min_{\Psi_\rho^{KS}} \langle \Psi_\rho | T | \Psi_\rho \rangle + E_H[\rho] + E_{xc}[\rho]$$

Kohn-Sham equations

Variational principle: ground state energy is minimal for the ground state density.

The variation under particle number constraint $N = \int \rho(\mathbf{r}) d\mathbf{r}$ is stationary:

$$\frac{\delta(E[\rho] - \mu N)}{\delta \rho(\mathbf{r})} = 0 \Rightarrow \frac{\delta E[\rho]}{\delta \rho(\mathbf{r})} = \mu \qquad \mu \text{ chemical potential}$$

$$\frac{\delta\left(E[\{\varphi_i^*\}] - \varepsilon_i N_i\right)}{\delta \varphi_i^*(\mathbf{r})} = 0 \Rightarrow H_{KS}\varphi_i(\mathbf{r}) = \varepsilon_i \varphi_i(\mathbf{r})$$

$$H_{KS} = -\frac{\hbar^2\nabla^2}{2m} + V_H(\mathbf{r}) + V_{xc}[\rho](\mathbf{r}) \qquad V_{xc}[\rho](\mathbf{r}) = \frac{\delta E_{xc}[\rho]}{\delta \rho(\mathbf{r})}$$

$$E_{xc}^{LDA}[\rho] = \int \varepsilon_{xc}(\rho(\mathbf{r})) d\mathbf{r} \qquad \text{local density approximation}$$

Spin density-functional theory

Spin-polarized Kohn-Sham equations:

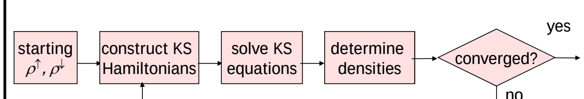
$$\rho_\uparrow(\mathbf{r}) = \sum_i^{occ} \left|\varphi_i^{(\uparrow)}(\mathbf{r})\right|^2$$

$$H_{KS}^{(\uparrow)}[\rho_\uparrow, \rho_\downarrow]\varphi_i^{(\uparrow)}(\mathbf{r}) = \varepsilon_i^{(\uparrow)}\varphi_i^{(\uparrow)}(\mathbf{r})$$
$$H_{KS}^{(\downarrow)}[\rho_\uparrow, \rho_\downarrow]\varphi_i^{(\downarrow)}(\mathbf{r}) = \varepsilon_i^{(\downarrow)}\varphi_i^{(\downarrow)}(\mathbf{r})$$

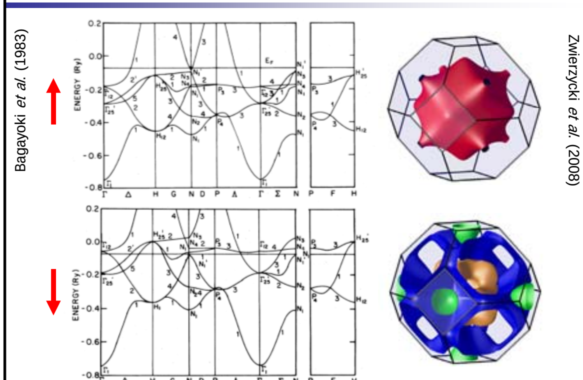
$$H_{KS}^{(\sigma)}[\rho_\uparrow, \rho_\downarrow] = -\frac{\hbar^2\nabla^2}{2m} + V_{nucl}(\vec{r}) + V_C[\rho](\vec{r}) + V_{xc}^{(\sigma)}[\rho_\uparrow, \rho_\downarrow](\vec{r})$$

Hartree Hamiltonian — exchange (-correlation) potentials

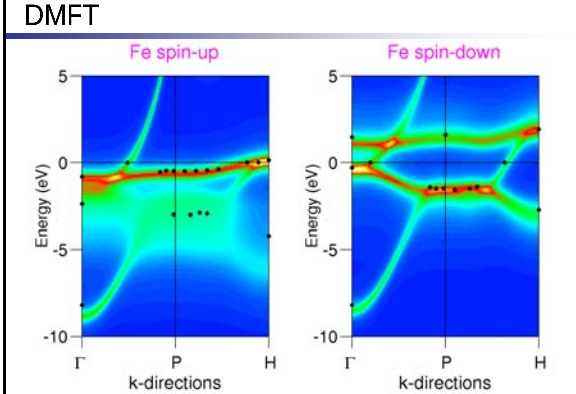
Self-consistency cycle:



Band structure and Fermi surfaces of Co

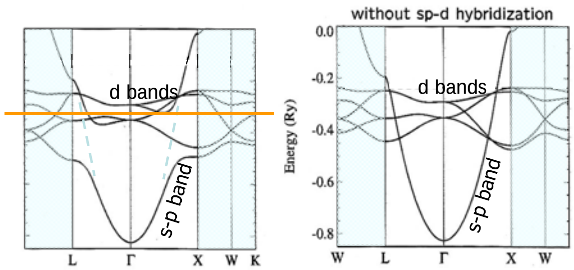


DMFT



Lichtenstein et al. (2001)

Transition metals and s-d hybridization



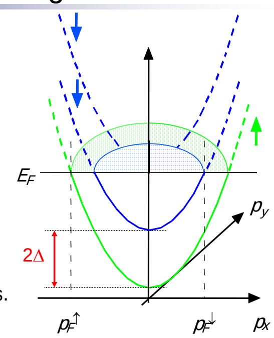
$$\Delta E_{sd} \sim 10\,eV \Leftrightarrow \Delta t_{sd} \sim \frac{\hbar}{\Delta E_{sd}} \sim fs$$

sp and d- electrons are strongly hybridized and cannot be distinguished on electron transport time scales.

Stoner metallic ferromagnet

$$\hat{H}_{\uparrow(\downarrow)} = -\frac{\hbar^2}{2m}\vec{\nabla}^2 - (+)\Delta$$

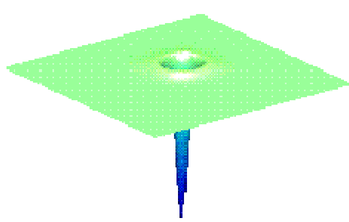
Δ: exchange(-correlation) potential that reflects the energy splitting between majory and minority spin states.



Spin-dependent densities, Fermi momenta, and mobilities

Halfmetallic ferromagnet

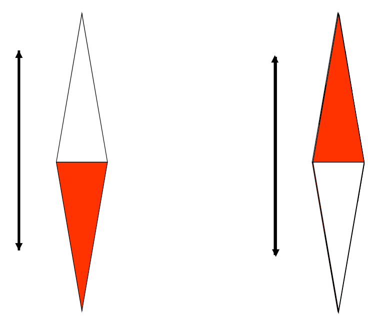
II. **M&S of magnetization (dynamics)**



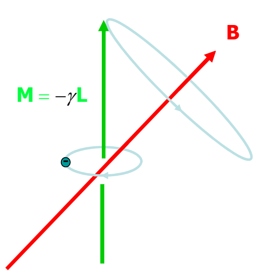
Simulated magnetic vortex switching

© G. Schütz

Magnetization dynamics



Magnetic dipole in a magnetic field



$U = -\mathbf{M}\cdot\mathbf{B}$ Energy

$\mathbf{F} = (\mathbf{M}\cdot\nabla)\mathbf{B}$ Force

$\frac{d\mathbf{L}}{dt} = \mathbf{T} = \mathbf{M}\times\mathbf{B}$ Torque

$$\frac{d\mathbf{M}}{dt} = -\gamma\frac{d\mathbf{L}}{dt} = -\gamma\mathbf{T} = -\gamma\mathbf{M}\times\mathbf{B}$$

Spin equation of motion

Heisenberg spin-operator equation of motion:

$$\frac{d}{dt}\mathbf{s} = \frac{i}{\hbar}[\mathbf{s},H] = -\frac{i}{\hbar}\gamma\sum_i B_i[\mathbf{s},s_i] \qquad [s_x,s_y] = i\hbar s_z$$

$$= -\gamma\mathbf{s}\times\vec{B}$$

$$\langle\mathbf{s}\rangle = \langle\psi|\mathbf{s}|\psi\rangle = (\langle s_x\rangle,\langle s_y\rangle,\langle s_z\rangle)$$

$$\mathbf{m} = -\gamma\langle\mathbf{s}\rangle$$

Spin-vector (Landau-Lifshitz) equation of motion:

$$\frac{d}{dt}\mathbf{m} = -\gamma\mathbf{m}\times\mathbf{B}$$

Magnetism, statics and dynamics

Quantum	Classical
Quantum spin models	First principles methods
Heisenberg	(Car-Parinello)
Ising	Classical spin models
X-Y	Landau-Lifshitz-Bloch
....	Landau-Lifshitz-Gilbert
Magnons	Spin waves

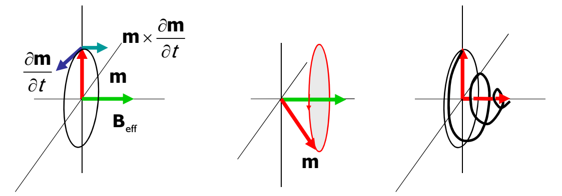
Landau-Lifshitz-Gilbert equation

$$\frac{d\mathbf{m}(t)}{dt} = -\gamma \mathbf{m} \times \left(\mathbf{B}_{\text{eff}}(t) - \frac{\alpha}{\gamma} \frac{d\mathbf{m}(t)}{dt} \right)$$

$$\mathbf{m} = \frac{\mathbf{M}}{M_s}; \quad M_s = |\mathbf{M}|$$

$$\mathbf{B}_{\text{eff}} = \frac{\partial F(\mathbf{m})}{M_s \partial \mathbf{m}}$$

Landau-Lifshitz-Gilbert equation; Gilbert damping constant α



Landau-Lifshitz-Gilbert equation

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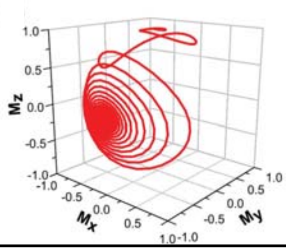


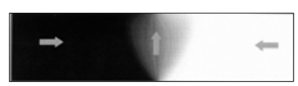
Micromagnetism (static)

Course grain minimization of magnetostatic energy with $\dot{\mathbf{M}} = 0$:

$$F[\mathbf{M}] = \int \left[-\mathbf{M}(\mathbf{r}) \cdot \mathbf{B}_{eff}[\mathbf{M}](\mathbf{r}) + \frac{C}{2} |\nabla \mathbf{M}(\mathbf{r})|^2 \right] d\mathbf{r}$$

$$\mathbf{B}_{eff}(\vec{r}) = \mathbf{B}_{appl} + \frac{1}{2} \mathbf{B}_{dipolar}[\vec{M}] + \frac{\mathbf{B}_{anisot.}}{2M_s}$$

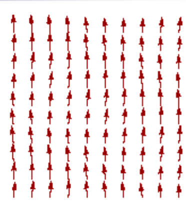
C spin-wave stiffness

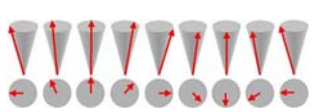


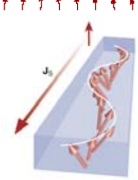
transverse magnetic
head-to-head
domain wall

Spin waves or magnons

Plane wave solution of LL equation:







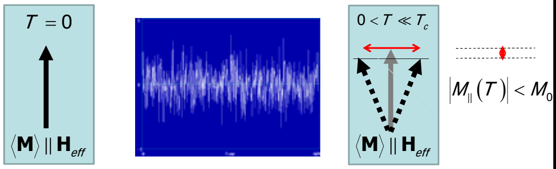
William Fuller Brown, Jr. (1904–1983)

FATHER OF MICROMAGNETICS

Thermal Fluctuations of a Single-Domain Particle
William Fuller Brown, Jr.
Phys. Rev. **130**, 1677 –
Published 1 June 1963

The Center for Micromagnetics and Information Technologies (MINT)

Thermal magnetization noise



Thermal equilibrium: $M(T) = M_0 \int f_{MB}(\mathbf{\Omega}) d\mathbf{\Omega} \rightarrow M_0 \left(1 - \frac{kT}{2\mu_B H_{eff}}\right)$

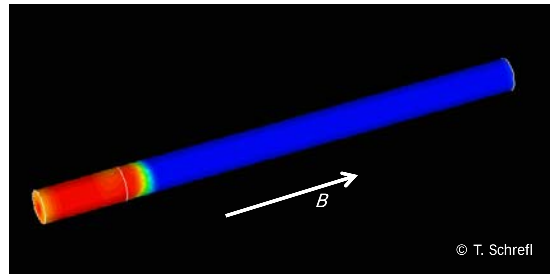
Stochastic field: $\dot{\mathbf{m}} = \mathbf{m} \times \left(-\gamma\left(\mathbf{H}_{eff} + \mathbf{h}(t)\right) + \alpha \dot{\mathbf{m}}\right)$

Fluctuation-dissipation theorem: $\langle h_i(t) h_j(t') \rangle = \frac{2\alpha k_B T}{\gamma M_0} \delta(t - t') \delta_{ij}$

⇨ Fokker-Planck equation for probability distribution function $P(\mathbf{m}, t)$

Magnetic domain walls

Moving domain walls by magnetic fields:

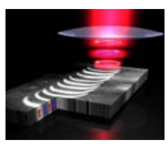


LL(Gilbert) vs. LLB(loch)

Garanin (1997)

LLG: $M_s = |\mathbf{M}| = const.$

LLB: $|\mathbf{M}| = M_s(T)$



transverse dynamics

$$\frac{d\mathbf{m}}{\gamma dt} = -\mathbf{m} \times \mathbf{B}_{\text{eff}} - \alpha_{\perp} \mathbf{m} \times \left(\mathbf{m} \times \left(\mathbf{B}_{\text{eff}} + \mathbf{b}_{\perp}(t)\right)\right) + \alpha_{\parallel} \mathbf{m}\left(\mathbf{m} \cdot \mathbf{B}_{\text{eff}}\right) + \mathbf{b}_{\parallel}(t)$$

longitudinal dynamics

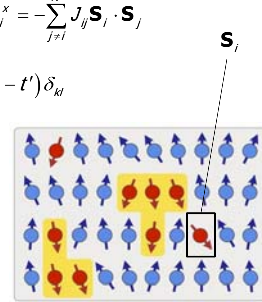
+ FD theorem

Atomistic spin simulations for localized spins

$$\dot{\mathbf{S}}_i = -\gamma \mathbf{S}_i \times \mathbf{B}_i^{eff} + \alpha_i \mathbf{S}_i \times \dot{\mathbf{S}}_i$$

$$\mathbf{B}_i^{eff} = -\frac{\partial E_i}{\partial \mathbf{S}_i} + \mathbf{b}_i(t) \qquad E_i^x = -\sum_{j \neq i}^{N} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$$

$$\langle b_k(t) b_l(t') \rangle_i = \frac{2 k_B T \alpha_i}{\gamma M_i} \delta(t - t') \delta_{kl}$$

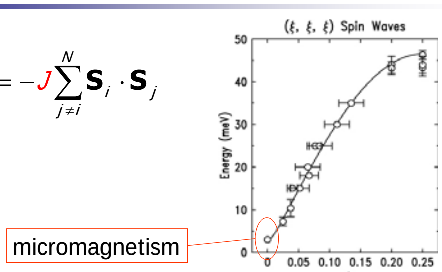


Ellis et al., arXiv:1505.07367

© J. Barker

Parameters

$$E_i^x = -J \sum_{j \neq i}^{N} \mathbf{S}_i \cdot \mathbf{S}_j$$



Spin-wave dispersion in the (1, 1, 1) direction of the reciprocal space for $LaTiO_3$ measured by neutron-scattering experiment. The line is the fitting curve by using the Heisenberg model with isotropic J of 15.5 meV on the cubic lattice (Keimer *et al., 2000)*

III. Transport

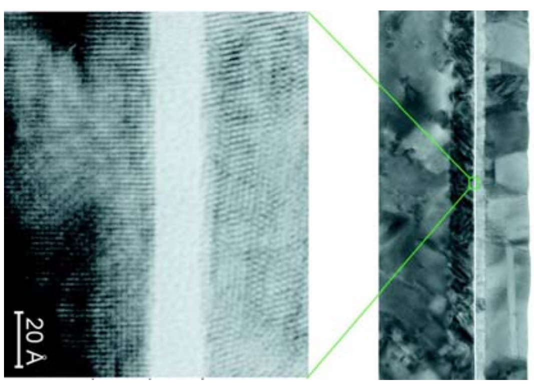
Charge and spin transport

- Green function methods
  - Diagrammatic, Kubo formula, Keldysh
- Scattering theory of transport
- Semiclassical methods
  - Kinetic, Boltzmann, diffusion (Valet-Fert)
- Numerical (first principles and model)
  - Recursive GF, Kwant
- Hybrid methods
  - circuit theory, Continuous-RMT

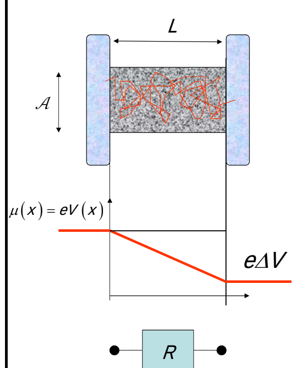
Regimes dictate the models and methods

Linear vs. non-linear transport	Ohm's Law
Ballistic vs. diffuse transport	Disorder
Bulk vs. interfaces	Multilayers
Zero vs. finite temperature	Noise
Relativistic vs. non-relativistic	Spin Hall effect
Metals vs. insulators	YIG
Qualititative vs. predictive	material design

Atomic scale interfaces + disorder



Diffusion in bulk 3D metal



no quantum interference effects such as weak localization: **semiclassical diffusion**

Ohm's Law

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

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

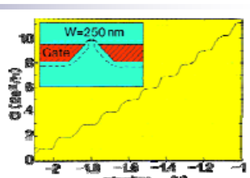
$$R = \frac{\rho L}{\mathcal{A}}$$ resistance

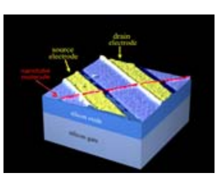
Current conservation

$$\frac{\partial}{\partial x} j = 0 \rightarrow \frac{eE}{\rho} = const.$$

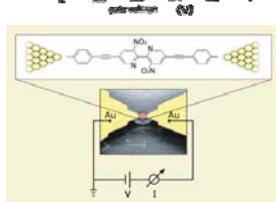
Mesoscopic physics

quantum point contacts



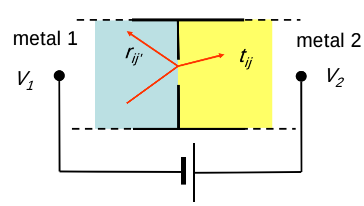


quantum wires



break junctions

Interface conductance



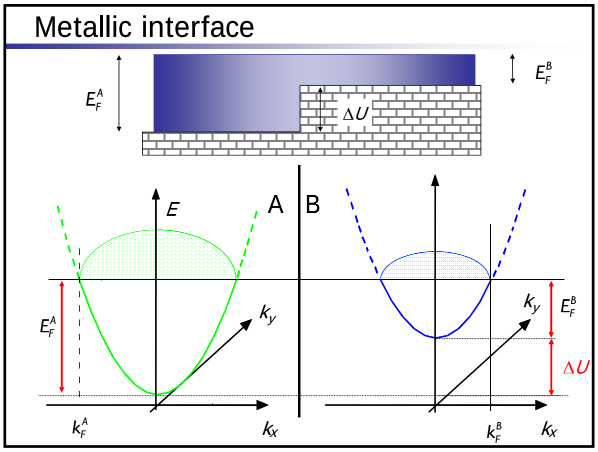
$$I = G'_{LB}(V_1 - V_2)$$

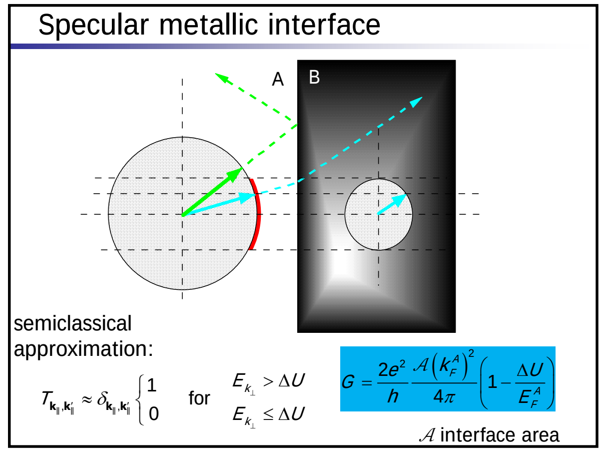
Landauer-Büttiker formula

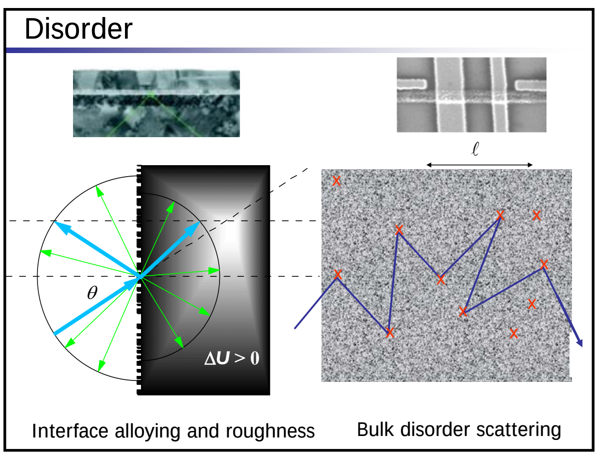
$$G'_{LB} = \frac{e^2}{h}\sum_{ij}^{\varepsilon_i=\varepsilon_j=E_F} |t_{ij}|^2 = \frac{e^2}{h}\sum_{k=1}^{N} T_k$$

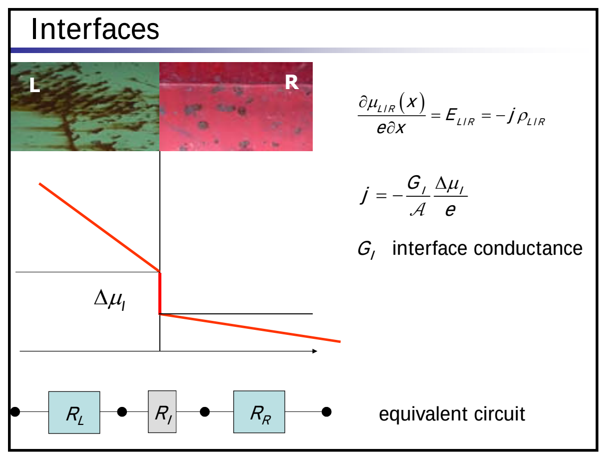
$$G_{LB} \xrightarrow{2=1} G_{Sharvin} = \frac{e^2}{h}\sum_{ij}^{\varepsilon_i=\varepsilon_j=E_F} 1 = \frac{e^2}{h}N$$

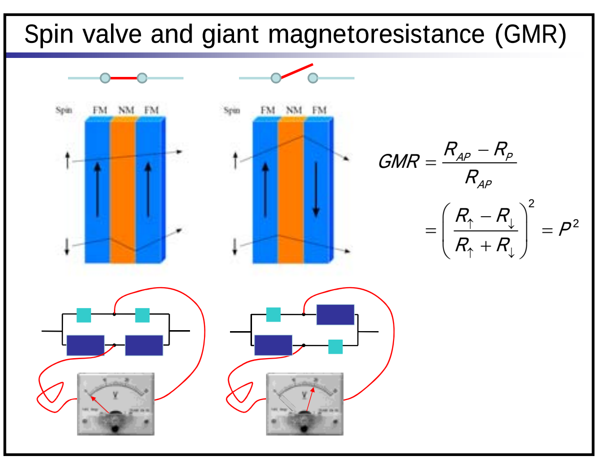
Sharvin conductance

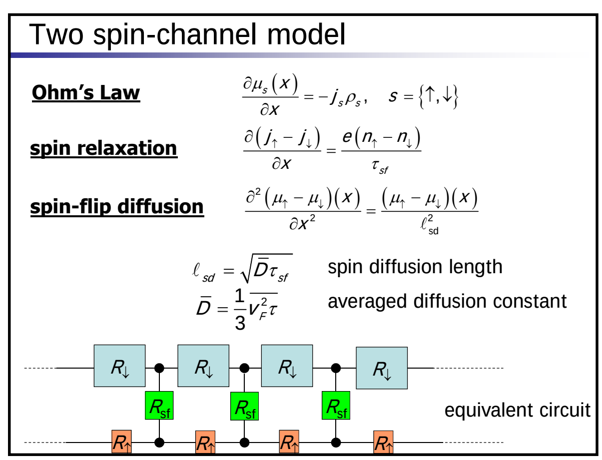

Metallic interface
E_F^A
ΔU
E_F^B
E
A
B
k_y
E_F^A
k_F^A
k_x
k_y
E_F^B
ΔU
k_F^B
k_x


Specular metallic interface
A
B
semiclassical
approximation:
$T_{\mathbf{k}_\parallel,\mathbf{k}'_\parallel} \approx \delta_{\mathbf{k}_\parallel,\mathbf{k}'_\parallel} \begin{cases} 1 & \text{for } E_{k_\perp} > \Delta U \\ 0 & E_{k_\perp} \le \Delta U \end{cases}$
$G = \frac{2e^2}{h} \frac{\mathcal{A}\left(k_F^A\right)^2}{4\pi}\left(1 - \frac{\Delta U}{E_F^A}\right)$
$\mathcal{A}$ interface area

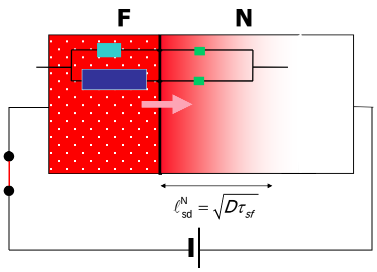

Disorder
ℓ
θ
$\Delta U > 0$
Interface alloying and roughness
Bulk disorder scattering


Interfaces
L
R
$\frac{\partial \mu_{L/R}(x)}{e\partial x} = E_{L/R} = -j\rho_{L/R}$
$j = -\frac{G_I}{\mathcal{A}} \frac{\Delta \mu_I}{e}$
G_I interface conductance
$\Delta \mu_I$
R_L
R_I
R_R
equivalent circuit


Spin valve and giant magnetoresistance (GMR)
Spin FM NM FM
Spin FM NM FM
$GMR = \frac{R_{AP} - R_P}{R_{AP}}$
$= \left(\frac{R_\uparrow - R_\downarrow}{R_\uparrow + R_\downarrow}\right)^2 = P^2$

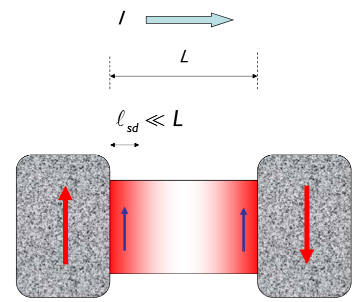

Two spin-channel model
Ohm's Law
$\frac{\partial \mu_s(x)}{\partial x} = -j_s \rho_s, \quad s = \{\uparrow,\downarrow\}$
spin relaxation
$\frac{\partial (j_\uparrow - j_\downarrow)}{\partial x} = \frac{e(n_\uparrow - n_\downarrow)}{\tau_{sf}}$
spin-flip diffusion
$\frac{\partial^2 (\mu_\uparrow - \mu_\downarrow)(x)}{\partial x^2} = \frac{(\mu_\uparrow - \mu_\downarrow)(x)}{\ell_{sd}^2}$
$\ell_{sd} = \sqrt{\bar{D}\tau_{sf}}$ spin diffusion length
$\bar{D} = \frac{1}{3}\overline{v_F^2}\tau$ averaged diffusion constant
$R_\downarrow$
R_{sf}
$R_\uparrow$
equivalent circuit

Spin accumulation and spin current

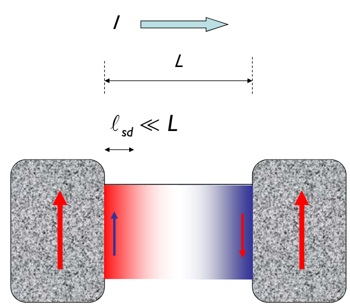


ℓ_{sd}^{N} spin-flip diffusion length
D diffusion constant
τ_{sf} spin-flip relaxation time

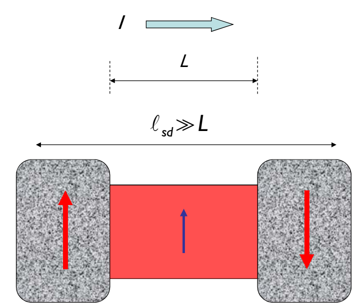
F|N|F spin valves



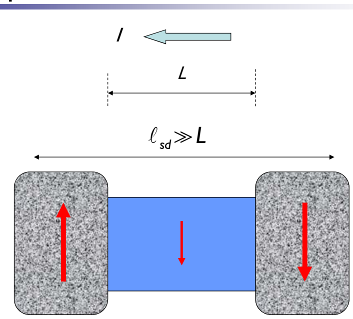
F|N|F spin valves



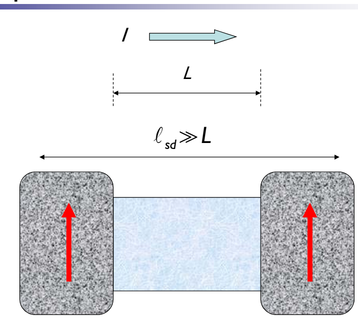
F|N|F spin valves



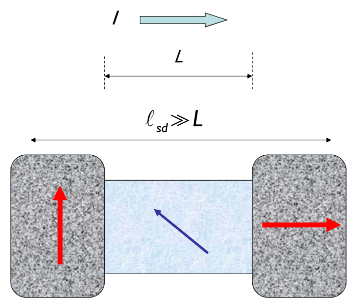
F|N|F spin valves



F|N|F spin valves



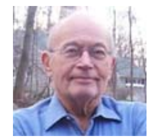
F|N|F spin valves: non-collinear



2013 Oliver E. Buckley Condensed Matter Physics Prize

Luc Berger
Carnegie Mellon University

John Slonczewski
IBM Research Staff Emeritus



Citation:
"*For predicting spin-transfer torque and opening the field of current-induced control over magnetic nanostructures.*"

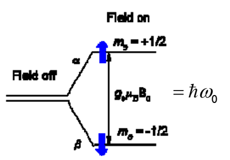
Electron spin vector operator

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

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

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

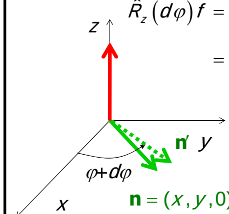
$$\mathcal{H} = -\mathbf{B}\cdot\boldsymbol{\mu} \xrightarrow{\mathbf{B}\parallel\hat{z}} -B_0\mu_z = -\frac{g_e\mu_B B_0}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$



$$\mathcal{H}\left|m_s = \pm\frac{1}{2}\right\rangle = \pm\hbar\omega_0\left|m_s = \pm\frac{1}{2}\right\rangle$$

When $\mathbf{B} \perp \mathbf{s}$ the system oscillates with Larmor frequency ω_0.

Rotation in quantum mechanics



$$\hat{R}_z(d\varphi) f = f(x+dx, y+dy) = f + \left(-y\frac{\partial}{\partial x} + x\frac{\partial}{\partial y}\right) f d\varphi = \left(1 + \frac{i}{\hbar}\hat{L}_z d\varphi\right) f$$

$\mathbf{n} = (x, y, 0)$

Finite rotation: $\varphi = \lim_{n\to\infty} n d\varphi$

$$\hat{R}_z(\varphi) = \lim_{n\to\infty}\left(1 + \frac{i}{\hbar}d\varphi\hat{L}_z\right)^n$$

$x' = x - y d\varphi$
$y' = y + x d\varphi$

$\log(1+x) \approx x \rightarrow \lim_{n\to\infty}\log(1+x)^n \approx \lim_{n\to\infty} nx$

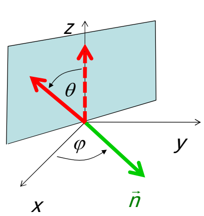
$$\log\hat{R}_z(\varphi) = \lim_{n\to\infty}\frac{i}{\hbar}(nd\varphi)\hat{L}_z = \frac{i}{\hbar}\varphi\hat{L}_z \rightarrow \hat{R}_z(\varphi) = e^{\frac{i}{\hbar}\varphi\hat{L}_z}$$

Rotation in quantum mechanics

Rotation of a state $|\Psi\rangle$ by an angle θ around an axis with unit vector $\mathbf{n}$: $\qquad |\Psi\rangle_R = \hat{R}_{\mathbf{n}}(\theta)|\Psi\rangle$

Rotation operator: $\hat{R}_{\mathbf{n}}(\theta) = \exp\left(i\theta\mathbf{n}\cdot\hat{\mathbf{L}}\right)$

Electron spin: $\hat{\mathbf{L}} = \mathbf{s} = \frac{\hbar}{2}\boldsymbol{\sigma}$ $\qquad \boxed{\hat{R}_{\mathbf{n}}(\theta) = e^{i\mathbf{n}\cdot\boldsymbol{\sigma}\theta/2}}$



With $\mathbf{n} = (\cos\varphi, \sin\varphi, 0)$

$$\psi(\varphi,\theta) = \mathbf{R}(\varphi,\theta)\begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

generates all possible spin states.
Example:

$$|\rightarrow\rangle_x = \mathbf{R}\left(\frac{\pi}{2},\frac{\pi}{2}\right)\begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

Spins on the Bloch sphere

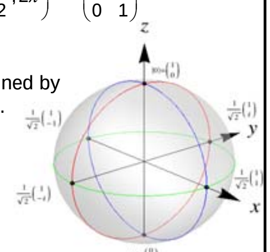
$$\mathbf{R}\left(\frac{\pi}{2},\theta\right) = e^{i\sigma_y\theta/2} = e^{\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}\theta/2} = \sum_{m=0}^{\infty}\frac{1}{m!}\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}^m \left(\frac{\theta}{2}\right)^m$$

$$= \begin{pmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix} \qquad \mathbf{R}\left(\frac{\pi}{2},2\pi\right) = -\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

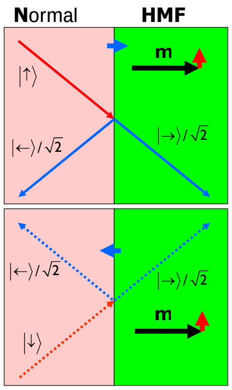
Spin-up state in *x*-direction is obtained by rotation about *y*-axis with $\theta = \pi/2$.

$$|\rightarrow\rangle_x = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

Check: ${}_x\langle\rightarrow|\mathbf{s}|\rightarrow\rangle_x = \frac{\hbar}{2}(1,0,0)$



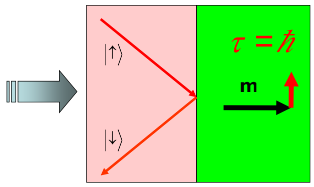
Slonczewski torque and Andreev reflection



$|\uparrow\rangle \Rightarrow (|\rightarrow\rangle + |\leftarrow\rangle)/\sqrt{2}$

longitudinal spin current

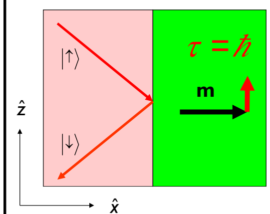
transverse spin current = torque



$$\left|\tau\left(\theta = \frac{\pi}{2}\right)\right| = \frac{Ne}{2\pi}(V_\uparrow - V_\downarrow)$$

N = number of incoming channels

Spin-mixing conductance



$$\tau(\mathbf{m} = \hat{x}) = \hat{z}\,\frac{\hbar}{e}\frac{e^2N}{h}(V_\uparrow - V_\downarrow)$$

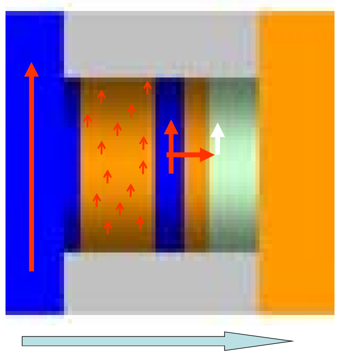
$$G_{\text{Sharvin}} = \frac{2e^2}{h}\sum_{\nu\vec{k}}^{E_F} 1 = \frac{2e^2}{h}N$$

$\vec{\mathbf{k}}$ incoming wave vector

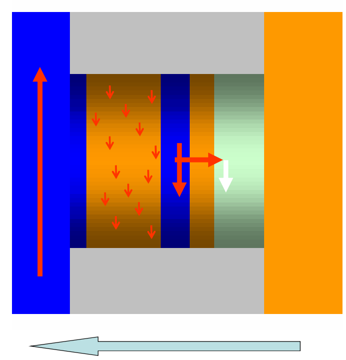
Scattering theory: $\tau(\mathbf{m} = \hat{x}) = \hat{z}\,\frac{\hbar}{e}(V_\uparrow - V_\downarrow)\,\mathrm{Re}\,G_{\uparrow\downarrow}$

Spin mixing conductance: $G_{\uparrow\downarrow} = \frac{e^2}{h}\sum_{\nu\vec{k}}^{E_F}\left(1 - r^\uparrow_{\nu\vec{k}}\left(r^\downarrow_{\nu\vec{k}}\right)^*\right) \approx \frac{e^2N}{h}$

Switching by spin transfer



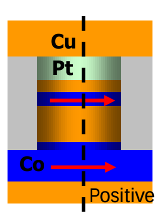
Switching by spin transfer

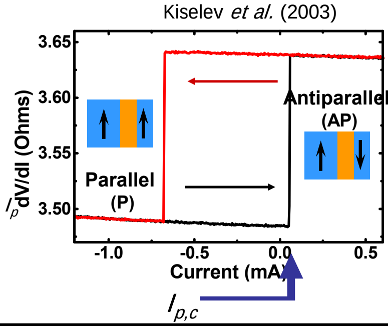


Current-induced magnetization reversal

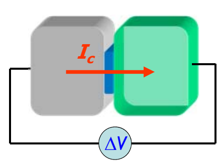
Electrical currents can controllably reverse the magnetization in small (< 200 nm) magnetic devices (Slonczewski, Berger):

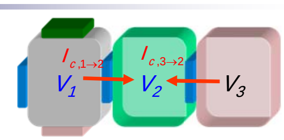
Kiselev *et al.* (2003)





Ohm's and Kirchhoff's Laws





charge conservation

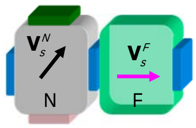
$$\sum_j I_{c,j\to i} = 0$$

Charge current:

$I_{c,1\to2} = G_{1\to2}(V_1 - V_2)$ — $G_{1\to2}$ conductance

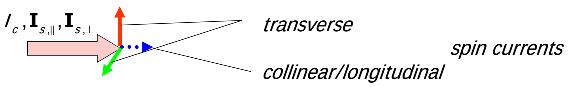
$G = \frac{e^2}{h}g = \frac{e^2}{h}\sum_{nm}|t_{nm}|^2$ — Landauer formula

Spin currents



$\mathbf{V}_s^N$ spin accumulation in N

$\mathbf{V}_s^F$ spin accumulation in F ∥ $\mathbf{m}$ magnetization direction

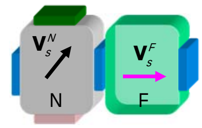


$$\mathbf{I}_{s,\perp} = 2\,\mathrm{Re}\,G_{\uparrow\downarrow}\left(\mathbf{m}\times\mathbf{V}_s^N\times\mathbf{m}\right) + 2\,\mathrm{Im}\,G_{\uparrow\downarrow}\left(\mathbf{V}_s^N\times\mathbf{m}\right)$$

in-plane — out-of-plane

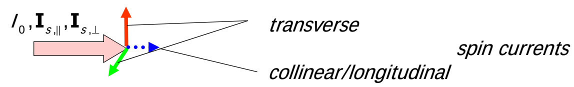
$$\tau = \frac{\hbar}{2e}\mathbf{I}_{s,\perp}$$

Spin currents



$\mathbf{V}_s^N$ spin accumulation in N

$\mathbf{V}_s^F$ spin accumulation in F ∥ $\mathbf{m}$ magnetization direction



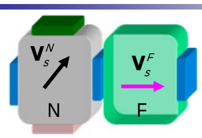
$$g_s = \sum_{nm}\left|t^s_{nm}\right|^2 = N - \sum_{nm}\left|r^s_{nm}\right|^2$$

$s=\uparrow,\downarrow$ spin-dependent Landauer conductances for charge and collinear spin current

$$g_{\uparrow\downarrow} = N - \sum_{nm} r^{\uparrow}_{nm}\left(r^{\downarrow}_{nm}\right)^*$$

complex spin-mixing conductance for transverse spin current (torque + exchange field)

Pauli matrix notation



$$\hat{X} = \begin{pmatrix} X_{\uparrow\uparrow} & X_{\uparrow\downarrow} \\ X^*_{\uparrow\downarrow} & X_{\downarrow\downarrow}\end{pmatrix} = X_c\hat{1} + \mathbf{X}_s\hat{\boldsymbol{\sigma}}$$

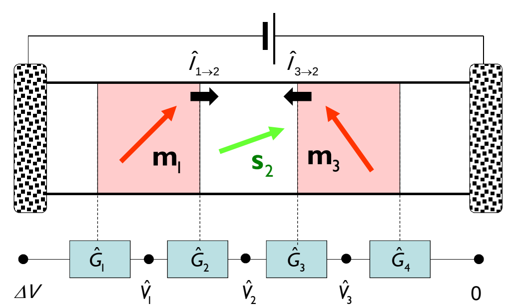
$$\hat{G} = \begin{pmatrix} G_{\uparrow} & G_{\uparrow\downarrow} \\ G^*_{\uparrow\downarrow} & G_{\downarrow}\end{pmatrix} \qquad \left(\hat{1},\hat{\boldsymbol{\sigma}}\right) = \left\{\begin{pmatrix}1&0\\0&1\end{pmatrix},\begin{pmatrix}0&1\\1&0\end{pmatrix},\begin{pmatrix}0&-i\\i&0\end{pmatrix},\begin{pmatrix}1&0\\0&-1\end{pmatrix}\right\}$$

$$\hat{V}^N = V_c^N\hat{1} + \mathbf{V}_s^N\cdot\hat{\boldsymbol{\sigma}}$$

$$\hat{V}^F = V_c^F\hat{1} + V_s^F\mathbf{m}\cdot\hat{\boldsymbol{\sigma}}$$

$$\hat{I} = I_c\hat{1} + \mathbf{I}_s\cdot\hat{\boldsymbol{\sigma}}$$

Circuit theory (Brataas *et al.*, 2000)

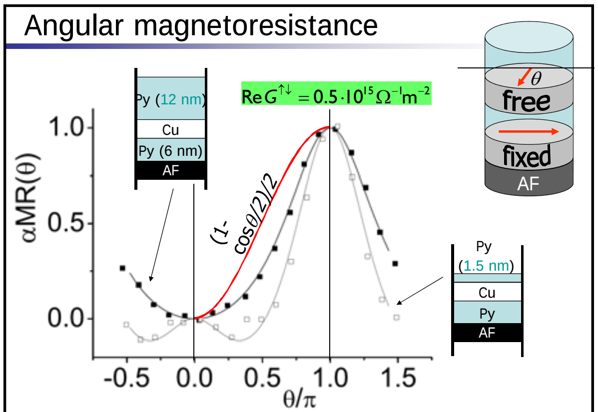


$$\hat{V}_1 = V_{c,1}\hat{1} + V_{s,1}\mathbf{m}_1\cdot\hat{\boldsymbol{\sigma}}$$

$$\hat{V}_2 = V_{c,2}\hat{1} + V_{s,2}\mathbf{s}_2\cdot\hat{\boldsymbol{\sigma}}$$

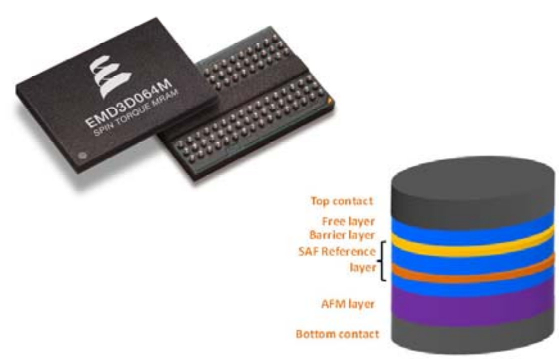
spin & charge conservation: $\hat{I}_{1\to2} + \hat{I}_{3\to2} = 0$

Angular magnetoresistance



Exp: S. Urazhdin *et al.* (2005)

III. M&S of MRAM elements



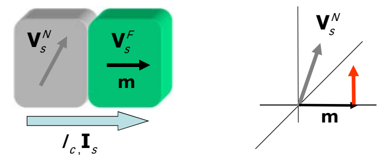
Spin torque and spin pumping

Onsager reciprocals (Brataas *et al.*, 2011) $\sim g^{\uparrow\downarrow}$

Spin currents cause magnetization motion (spin transfer torque, Slonczewski, 1996).

Magnetization motion causes spin currents (spin pumping, Tserkovnyak, 2002).

Dynamics of bilayers



$\mathrm{Re}\, g_{\uparrow\downarrow} = g_r$

$\mathrm{Im}\, g_{\uparrow\downarrow} \simeq 0$

Landau-Lifshitz-Gilbert equation with additional torque term:

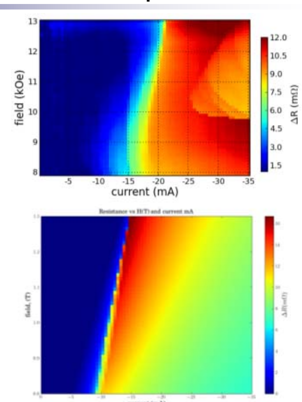
$$\frac{\partial \mathbf{m}}{\partial t} = -\gamma \mathbf{m}\times\mathbf{B} + \alpha_0 \mathbf{m}\times\frac{\partial \mathbf{m}}{\partial t} + \frac{\hbar\gamma}{4\pi M_s}\mathbf{m}\times\left(\mathbf{I}_s^{bias} + \mathbf{I}_s^{pump}\right)\times\mathbf{m}$$

$$= -\gamma \mathbf{m}\times\mathbf{B} + \left(\alpha_0 + \frac{\hbar\gamma g_r}{4\pi M_s}\right)\mathbf{m}\times\frac{\partial \mathbf{m}}{\partial t} + \frac{\hbar\gamma g_r}{4\pi M_s}\mathbf{m}\times\mathbf{V}_s^N\times\mathbf{m}$$

spin pumping   Slonczewski torque

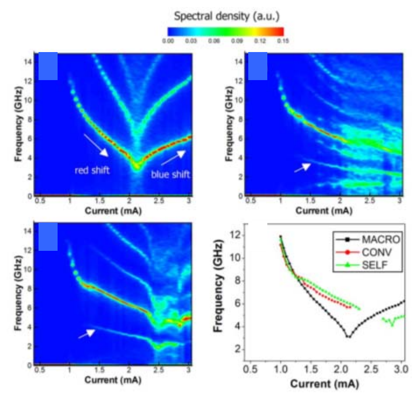
Macrospin simulation of nanopillar

Continuous random matrix theory [Waintal c.s.]



Borlenghi (2011)

Spin oscillators



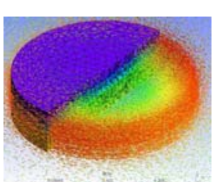
Kyung-Jin Lee *et al.* (2013)

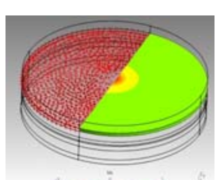
Exchange-only theory is **complete**

SpinFlow3D (Thierry Valet)

insilicio

- integration of current dynamics with micromagnetics (including Oersted fields)





Additional topics and challenges

- Current induces torques in magnetization textures (domain wall motion, emf due texture dynamics, topological Hall effect)
- Thermally induced spin currents (spin-dependent Seebeck effect, spin Seebeck effect)
- Spin Hall and related effects
- Spin orbit torques (field-like vs. damping-like)
- Magnetic insulators (YIG)
- Antiferromagnets
- Skyrmions


Give Us A Break