Spintronics

- In collaboration with : McGill U. (Hong Guo, Derek Waldron)

Group meeting 9/27/06

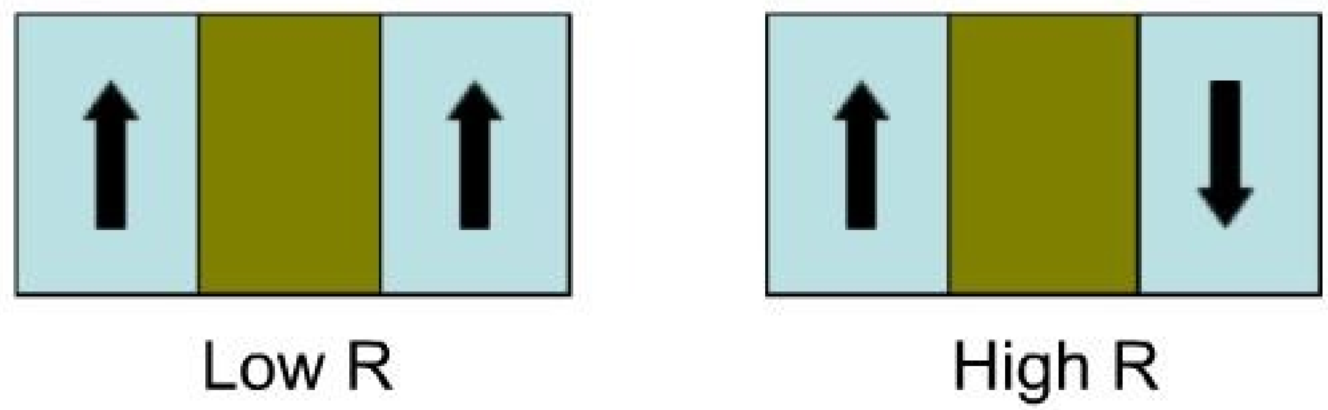
Thanks to TACC, etc

Contents:

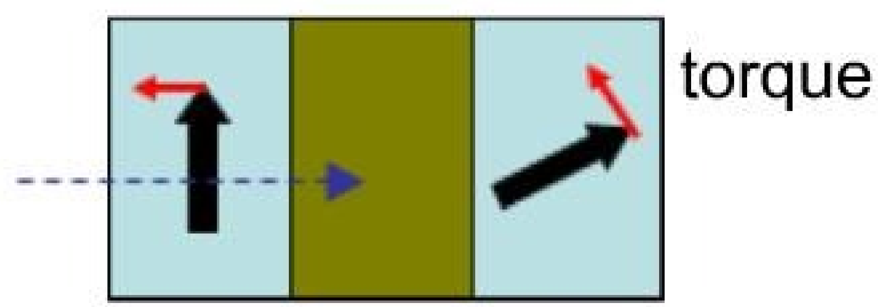
- Toy model vs. realistic model for GMR □ what do we learn from realistic models?
- A realistic (the 1st)(?) calculation of spin transfer
- Toy models of spin transfer – how do we decrease the switching current?

Practical spintronics = GMR, spin transfer

1. GMR:



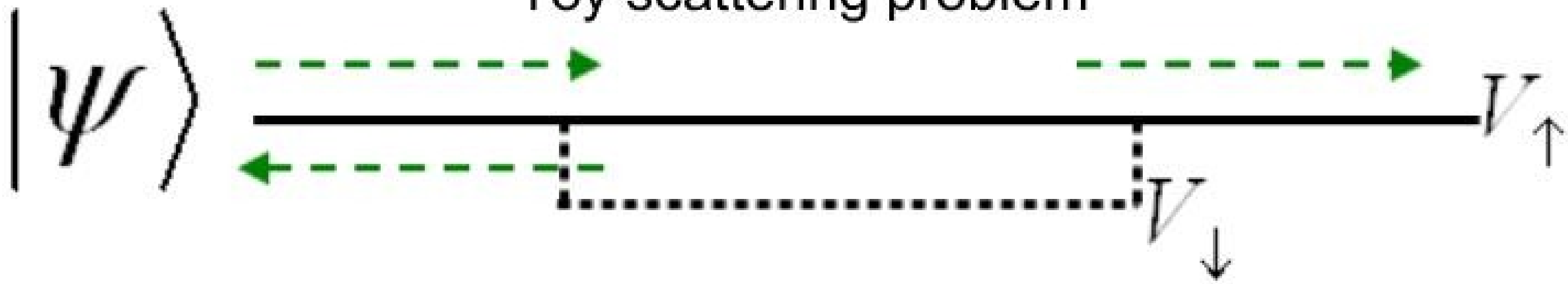
2. Spin transfer:



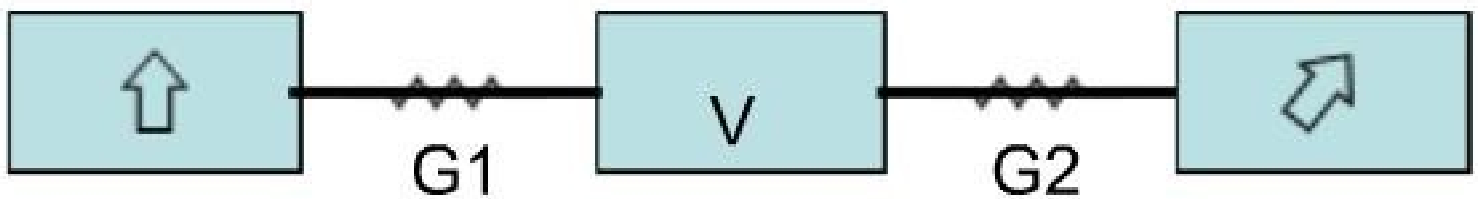
Effects rely on transport + spin.

Practical physics requires realistic calculations.

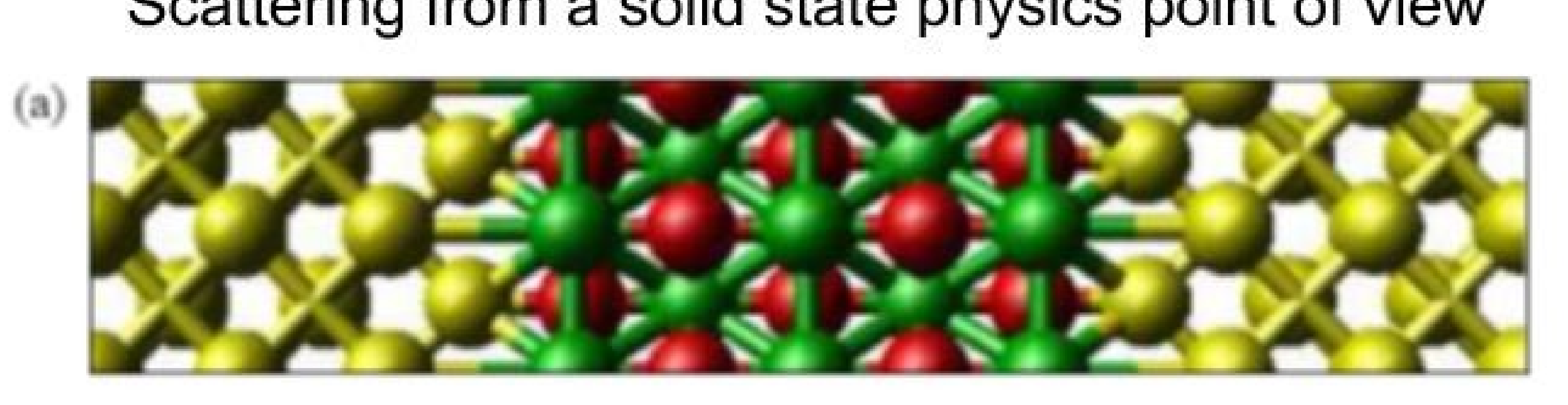
Toy scattering problem



Spin dependent circuit theory

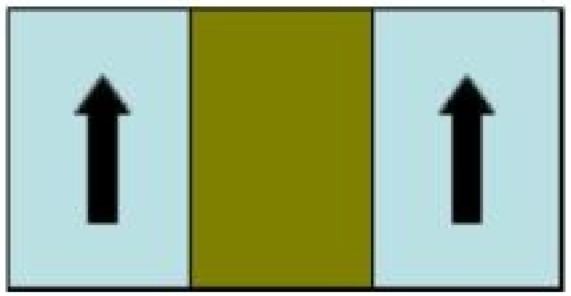


Scattering from a solid state physics point of view

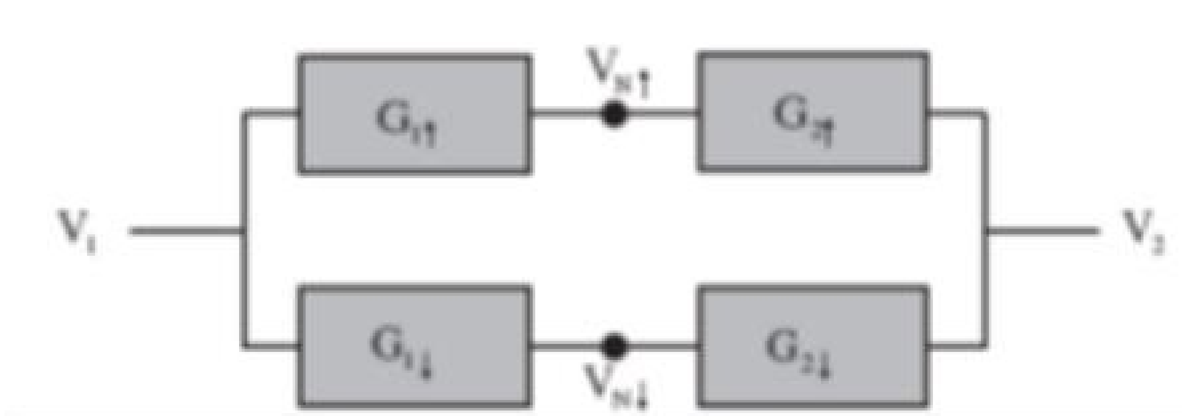


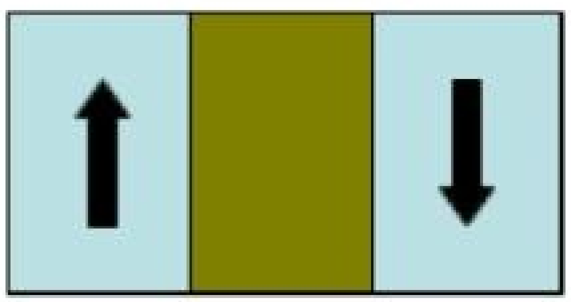
Consider the difference between the 2 approaches with GMR,
And get a sense of how electronic structure plays a role…

Toy model of GMR

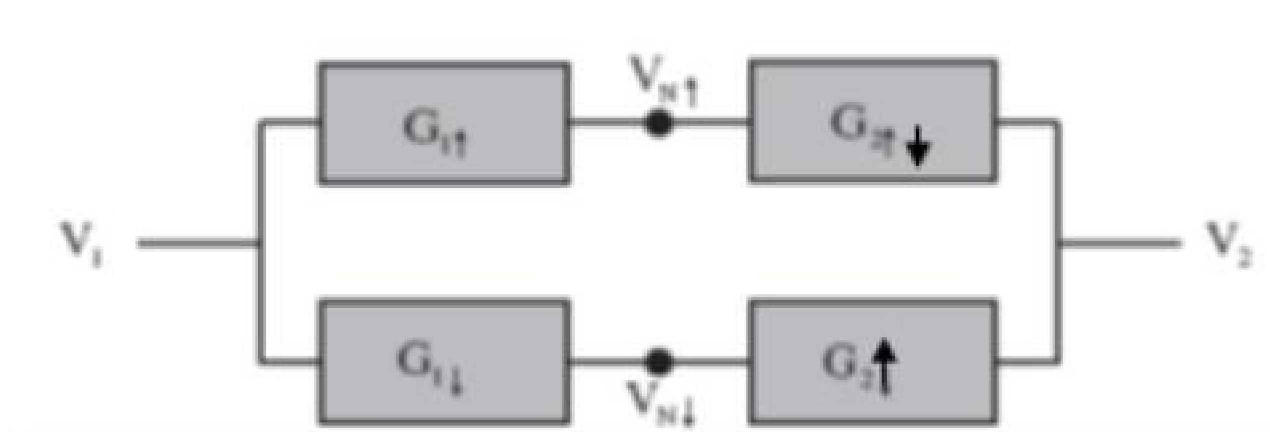


P





AP

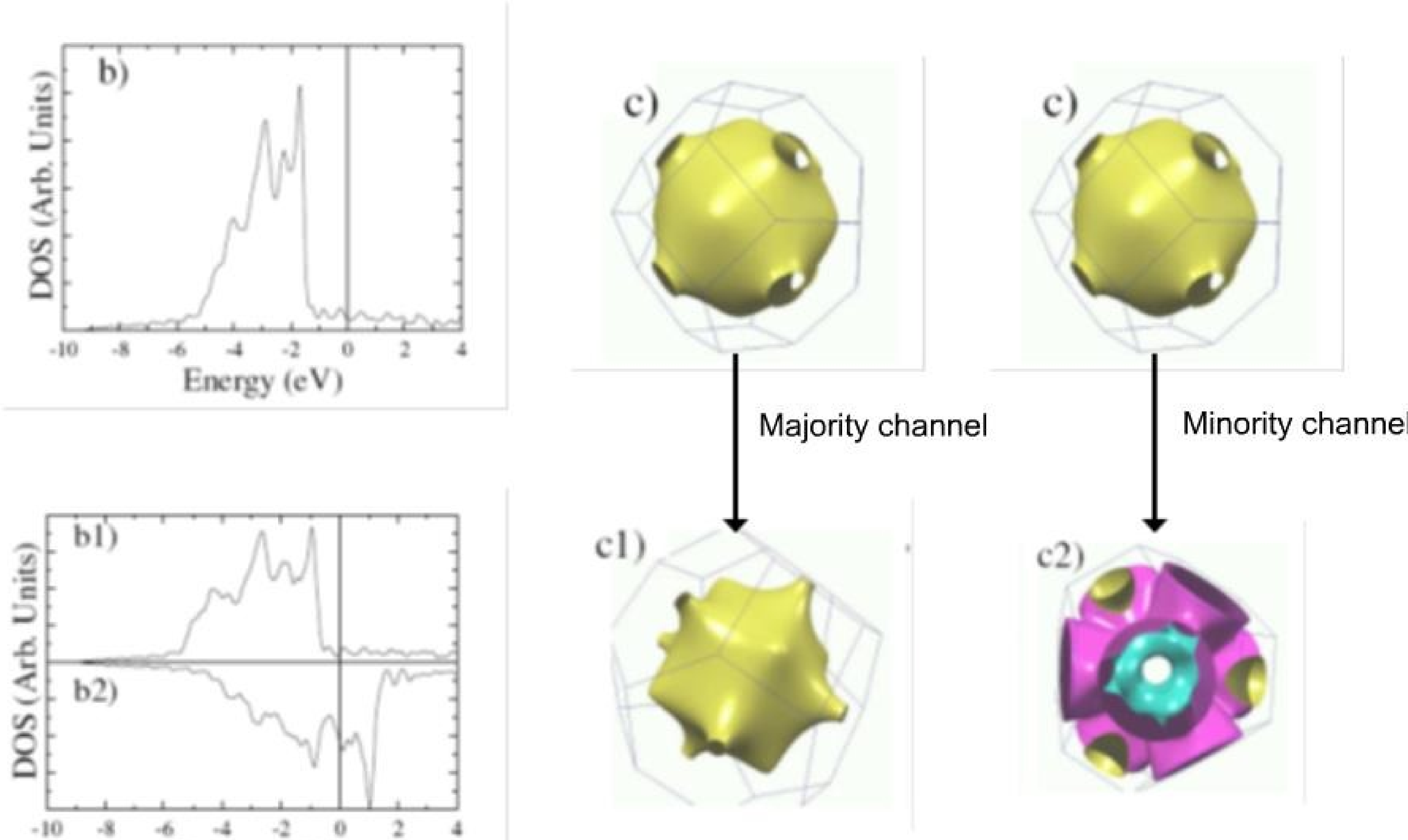


$$\mathrm{MR} \equiv \frac{I_C^{\mathrm{p}} - I_C^{\mathrm{ap}}}{I_C^{\mathrm{p}}} = P^2.$$

$$P = \frac{G_\uparrow - G_\downarrow}{G_\uparrow + G_\downarrow}$$

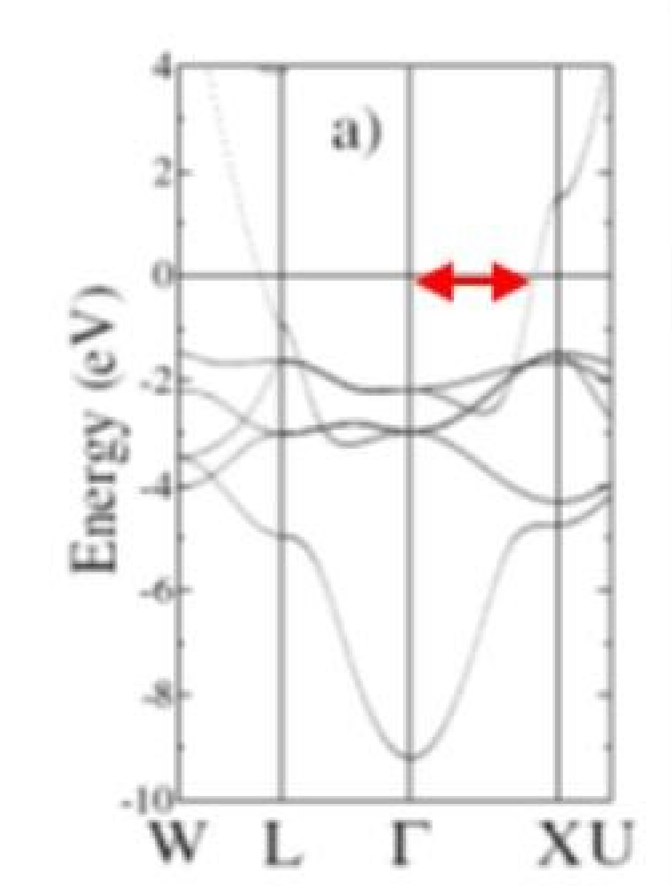
To maximize GMR, maximize polarization

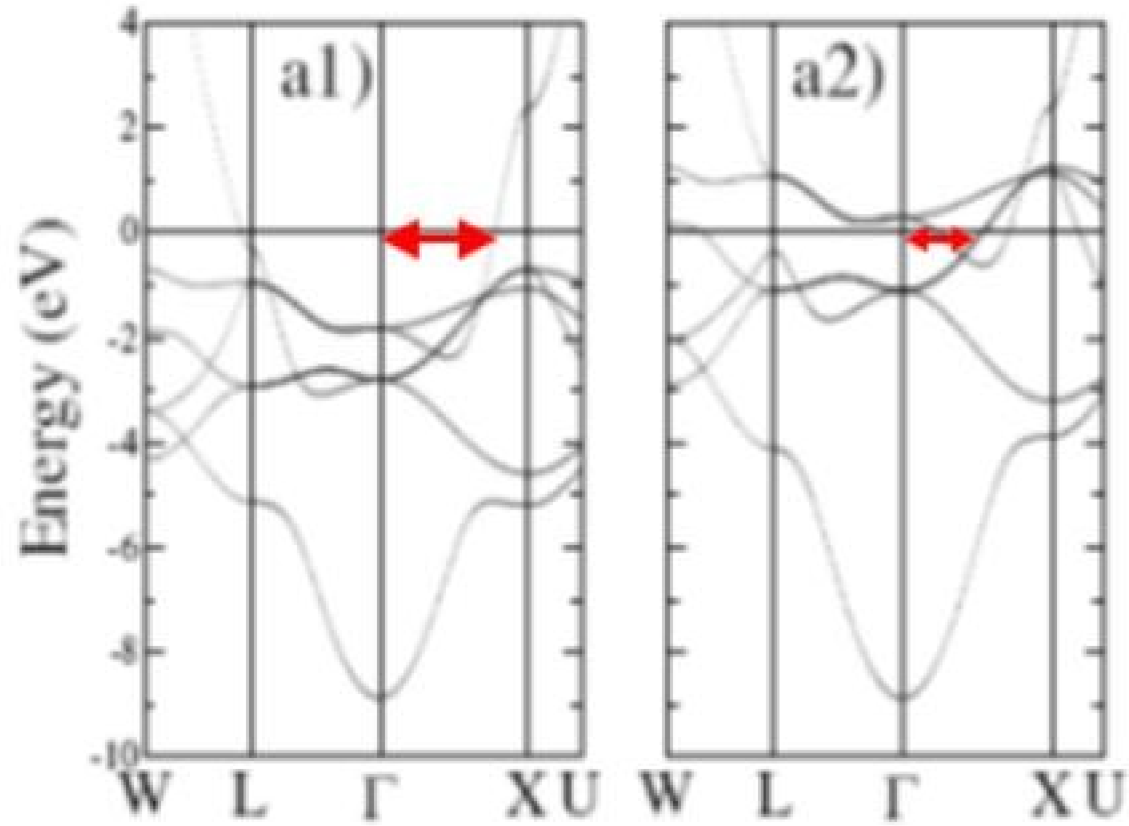
Co-Cu electronic structure explains GMR effect.

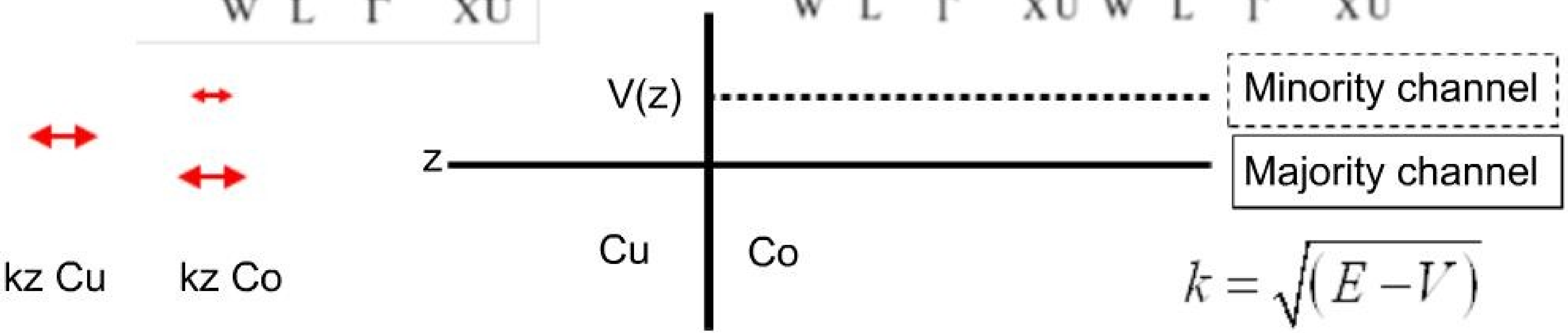


Explain match

Example of how to think about quantum transport – Co,Cu

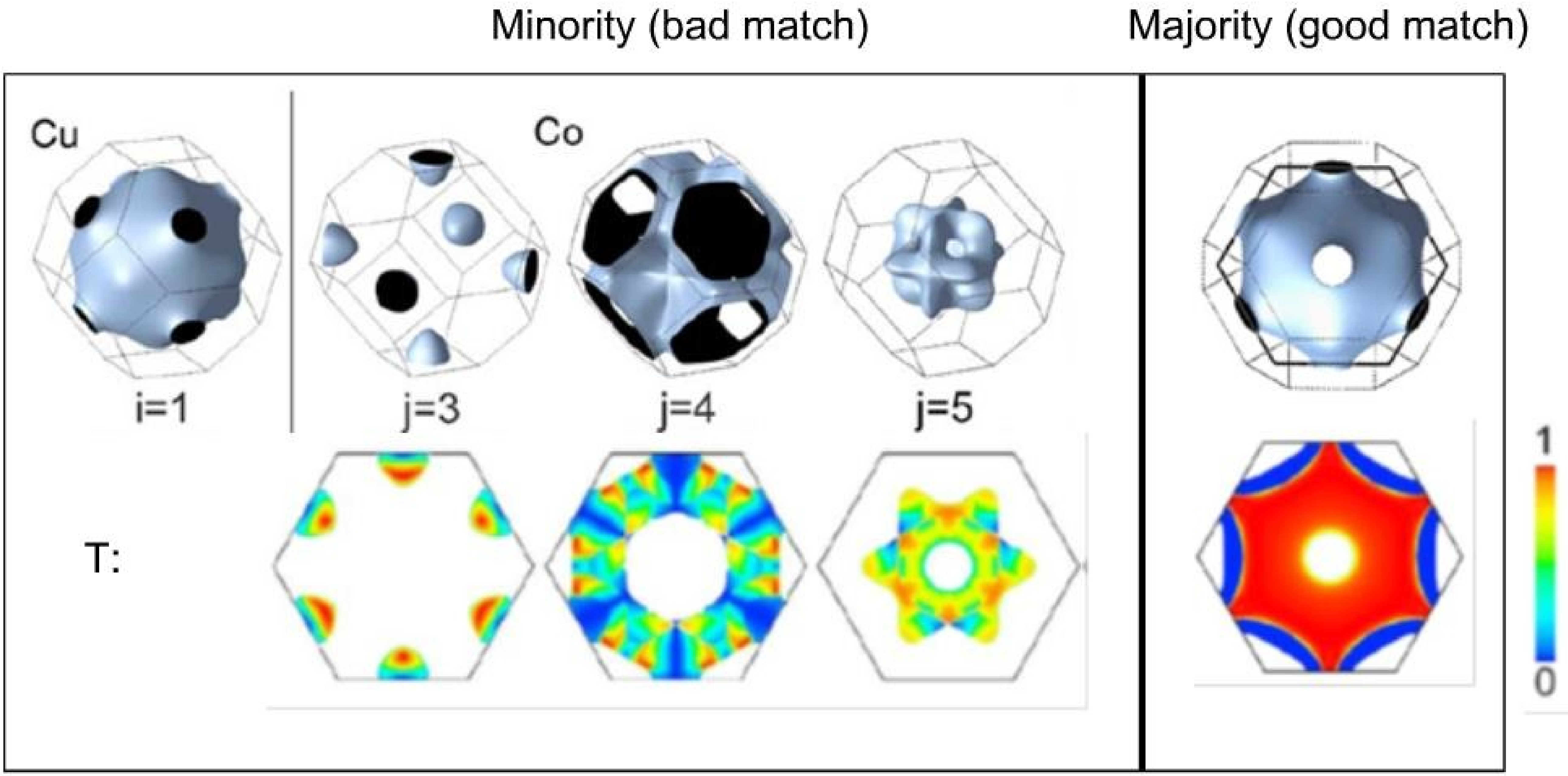






$$k=\sqrt{(E-V)}$$

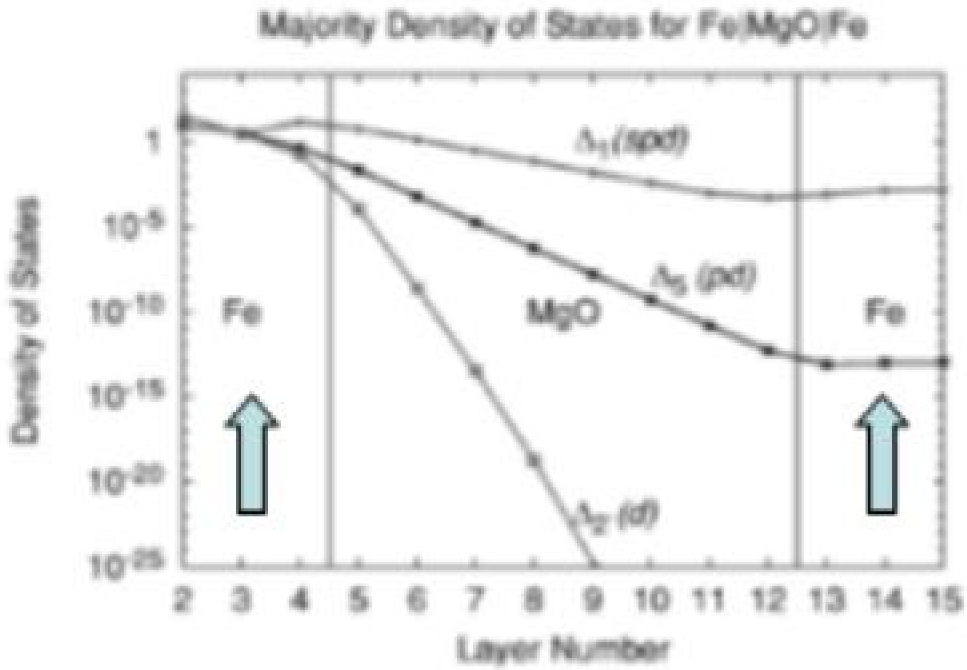
More Co-Cu GMR details



Predicted GMR =

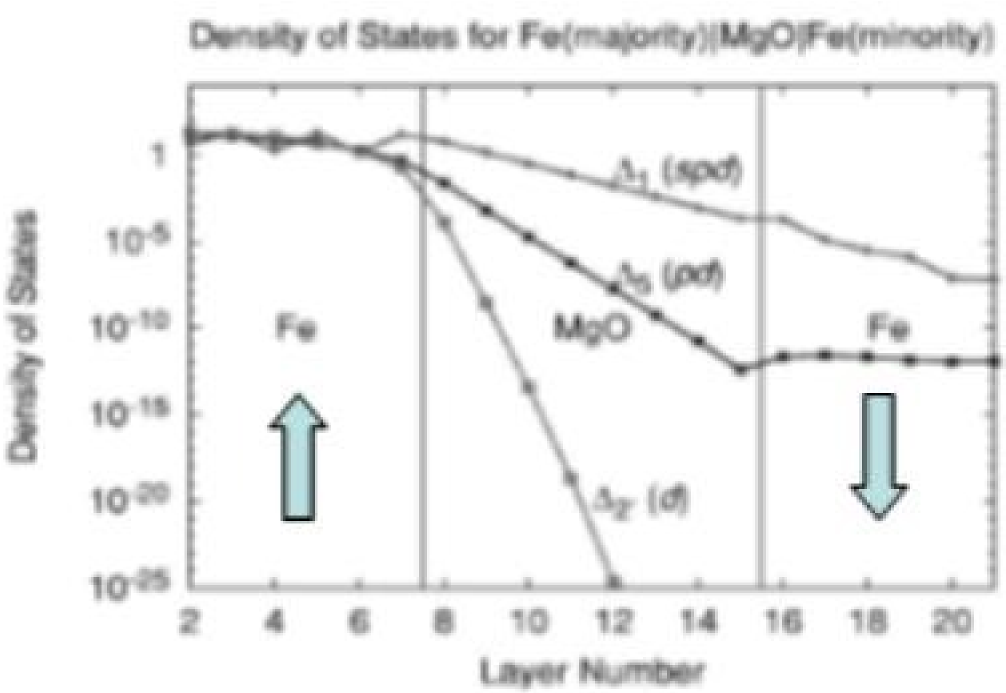
Compare to P^2?

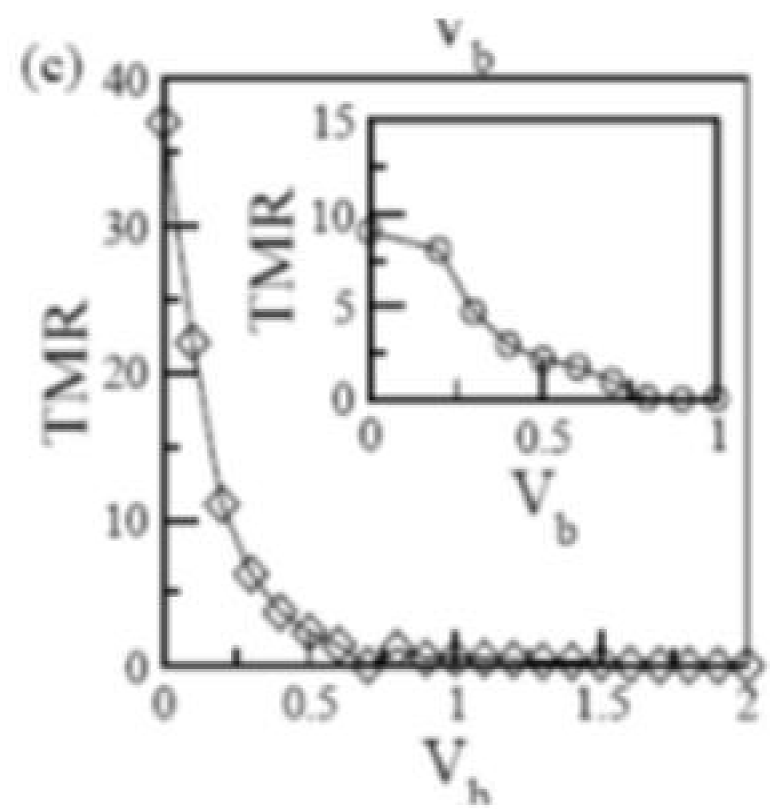
MgO – TMR from symmetry

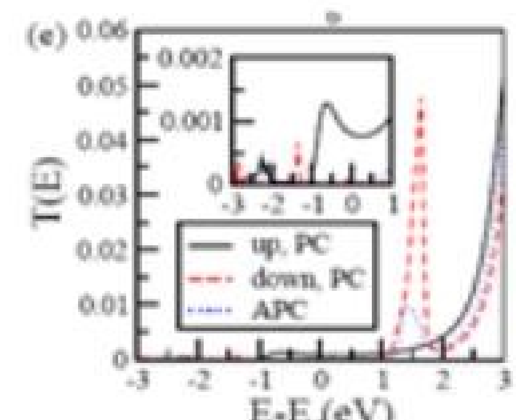


Fe majority □ Δ1, Δ5, Δ2’
Fe minority □ Δ2, Δ5, Δ2’

MgO lets through Δ1 mostly





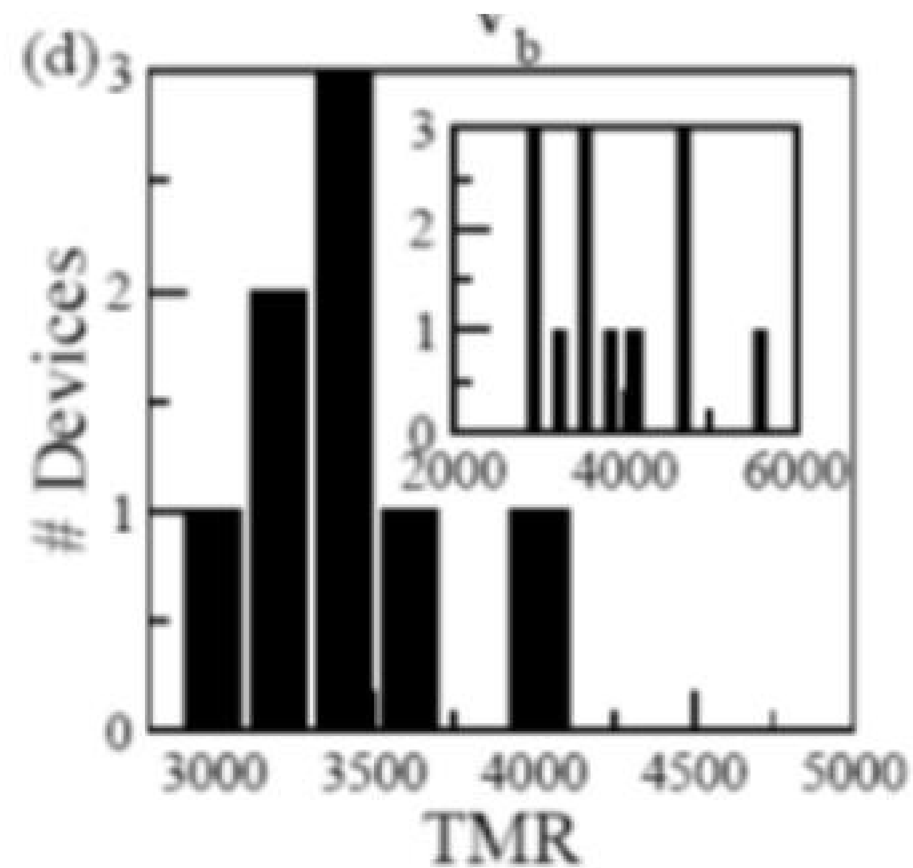


Ab-initio methods → include the key physics and then slowly remove it

For MgO – large TMR relies on Symmetry of Bloch bands

☐ Break symmetry and see if effect remains

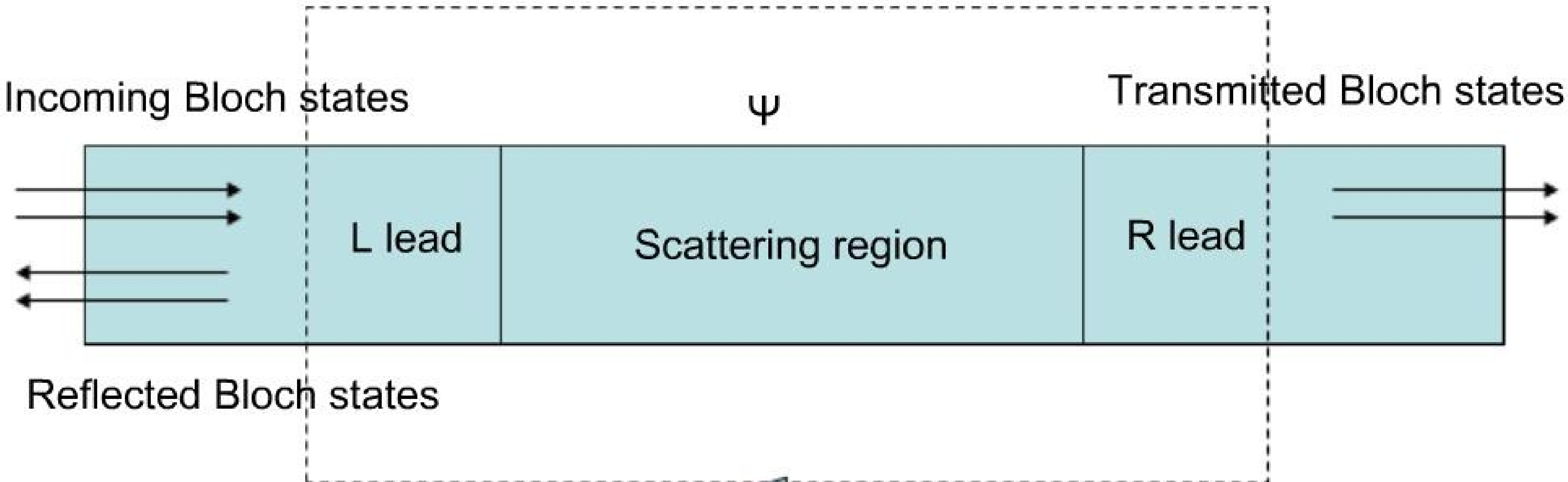
Displace Mg and O atoms randomly by 1%, see if TMR is ruined ☐ it is not.



How do we do realistic calculations?

- Need to include electronic structure □ need tight binding or density functional theory.
- Need to calculate transport properties □ Calculate conductance, or solve scattering problem exactly.
- Non-equilibrium Green's Functions are a convenient, powerful choice.

Physical explanation for NEGF



The wave function |ψ> in the scattering region defines a density matrix A= |ψ> <ψ|. The G< in NEGF is identical to this A.

Landauer formula for ballistic conductance: $G = \frac{e}{h}\sum_{nm} T_{nm}$

Density Functional Theory

- **Hohenberg-Kohn theorem - maps ground state of a many-body problem to a single particle, mean field equation (Kohn Sham equation).**
- **The basis used in our calculation = Local Combination of Atomic Orbitals (LCAO) - H retains tight-binding form.**

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + U(r) + \int d\bar{r}\,'\frac{n(\bar{r}\,')}{|\bar{r}-\bar{r}\,'|} + \frac{\partial \varepsilon_{cx}}{\partial n}\right]\psi_l(\bar{r}) = \varepsilon_l \psi_l(\bar{r})$$

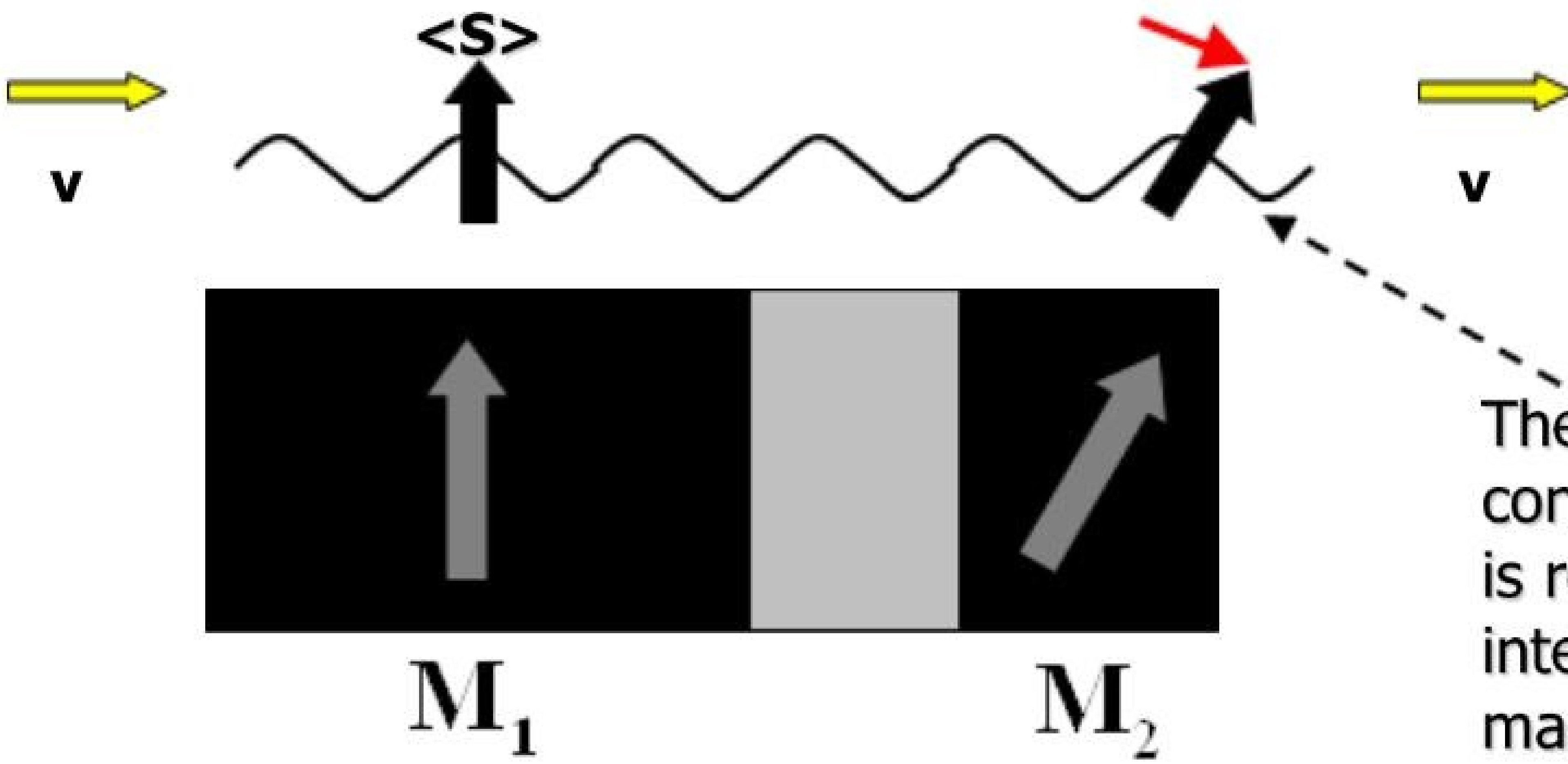
$$n(\bar{r}) = \sum_l |\psi_l(\bar{r})|^2 f(\varepsilon_l - \mu)$$

$$\varepsilon_{xc}(r) = \varepsilon_{xc}^{\text{homogeneous gas}}\left[n(\bar{r})\right] \text{ (LDA)}$$

All of the many-body physics is encoded here. This is the only approximation. In time-dependent DFT, this becomes non-local in time.

Realistic calculations of spin transfer torque

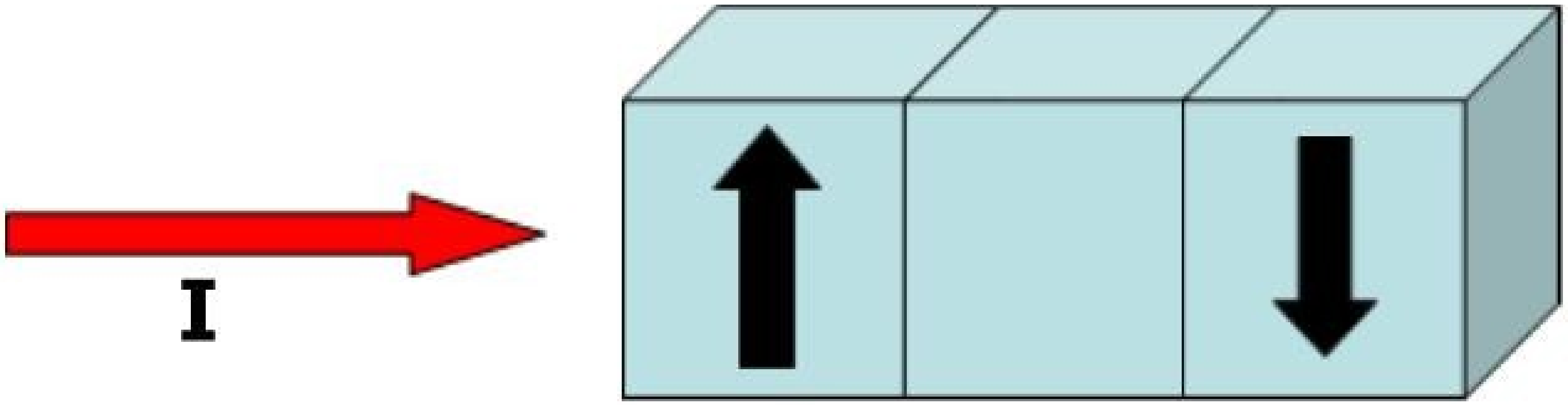
Spin Transfer Torque Cartoon



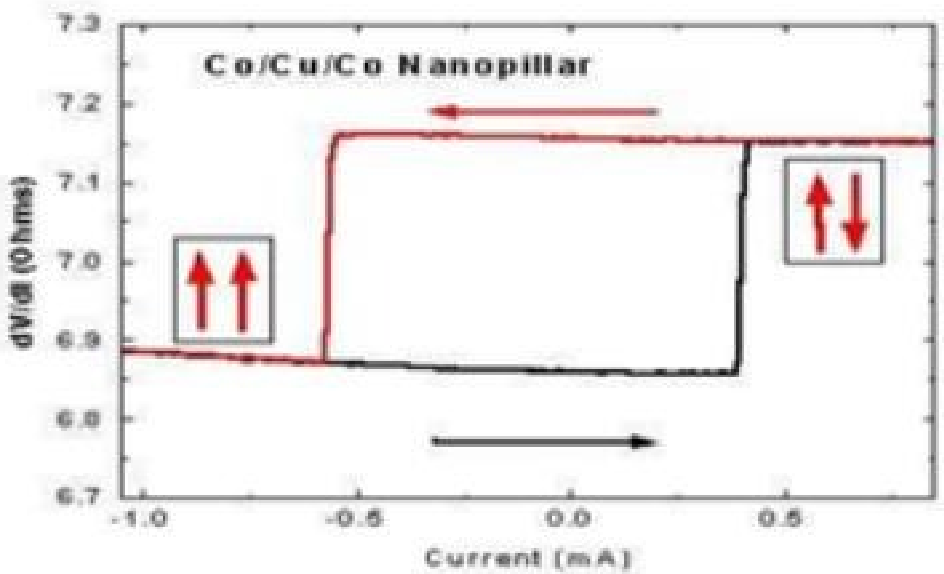
The spin of the conduction electron is rotated by its interaction with the magnetization.

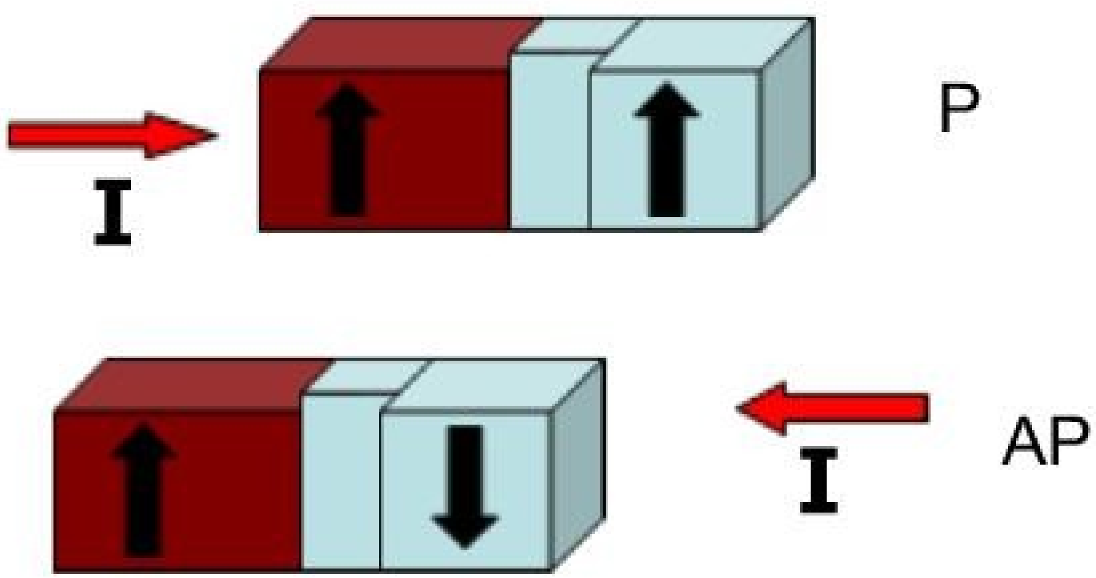
This implies the magnetization exerts a torque on the spin. By Conservation of angular momentum, the spin exerts an equal and Opposite torque on the magnetization.

Experimental Evidence of Spin Transfer

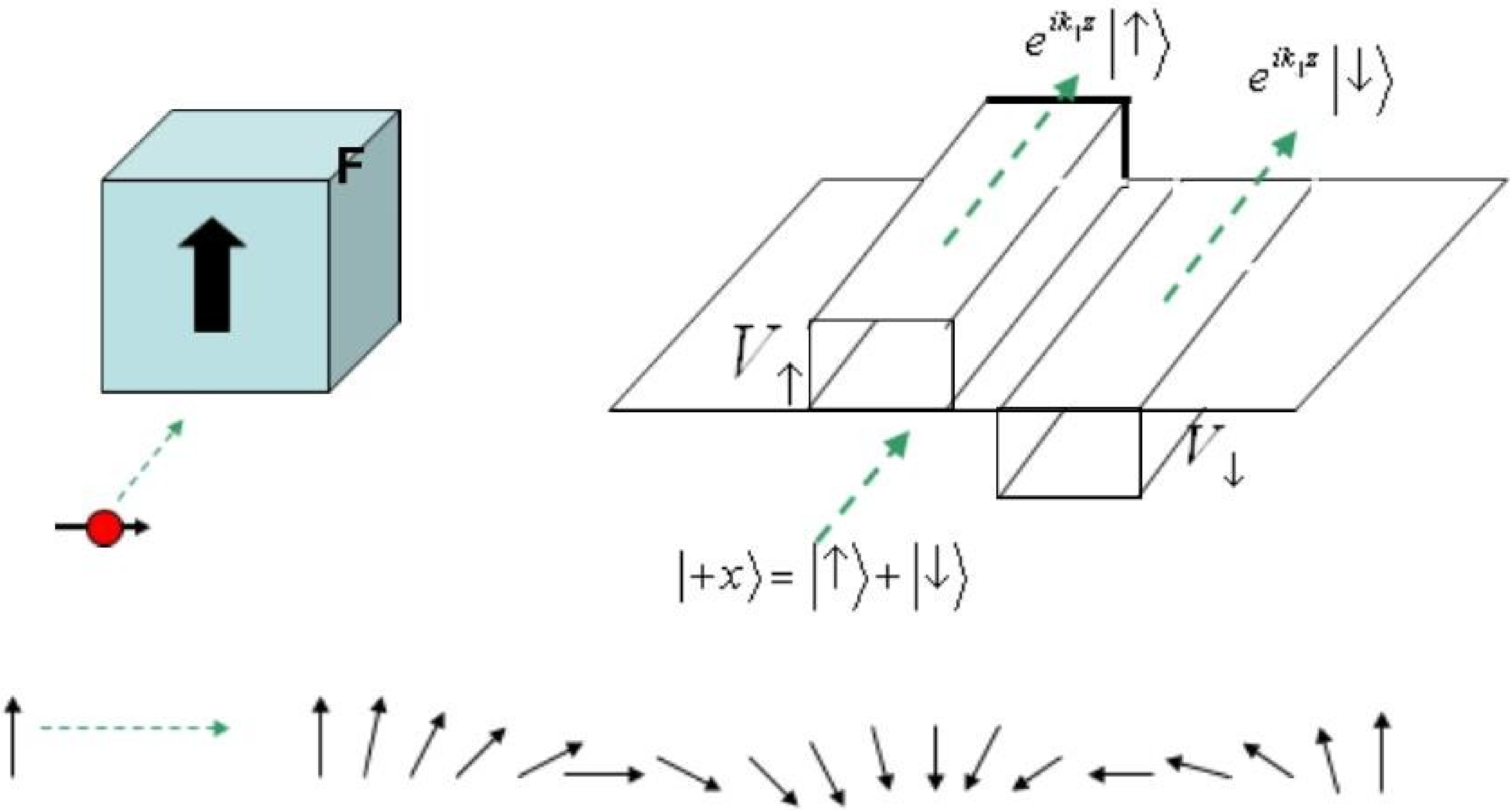


Predicted theoretically by Slonczewksi and Berger in 1996





Spin precession in single channel scattering.



$$\bar{S}_\perp(z) \propto \mathrm{Sin}\left[\left(k_\uparrow - k_\downarrow\right)z\right]\hat{x} + \mathrm{Cos}\left[\left(k_\uparrow - k_\downarrow\right)z\right]\hat{y}$$

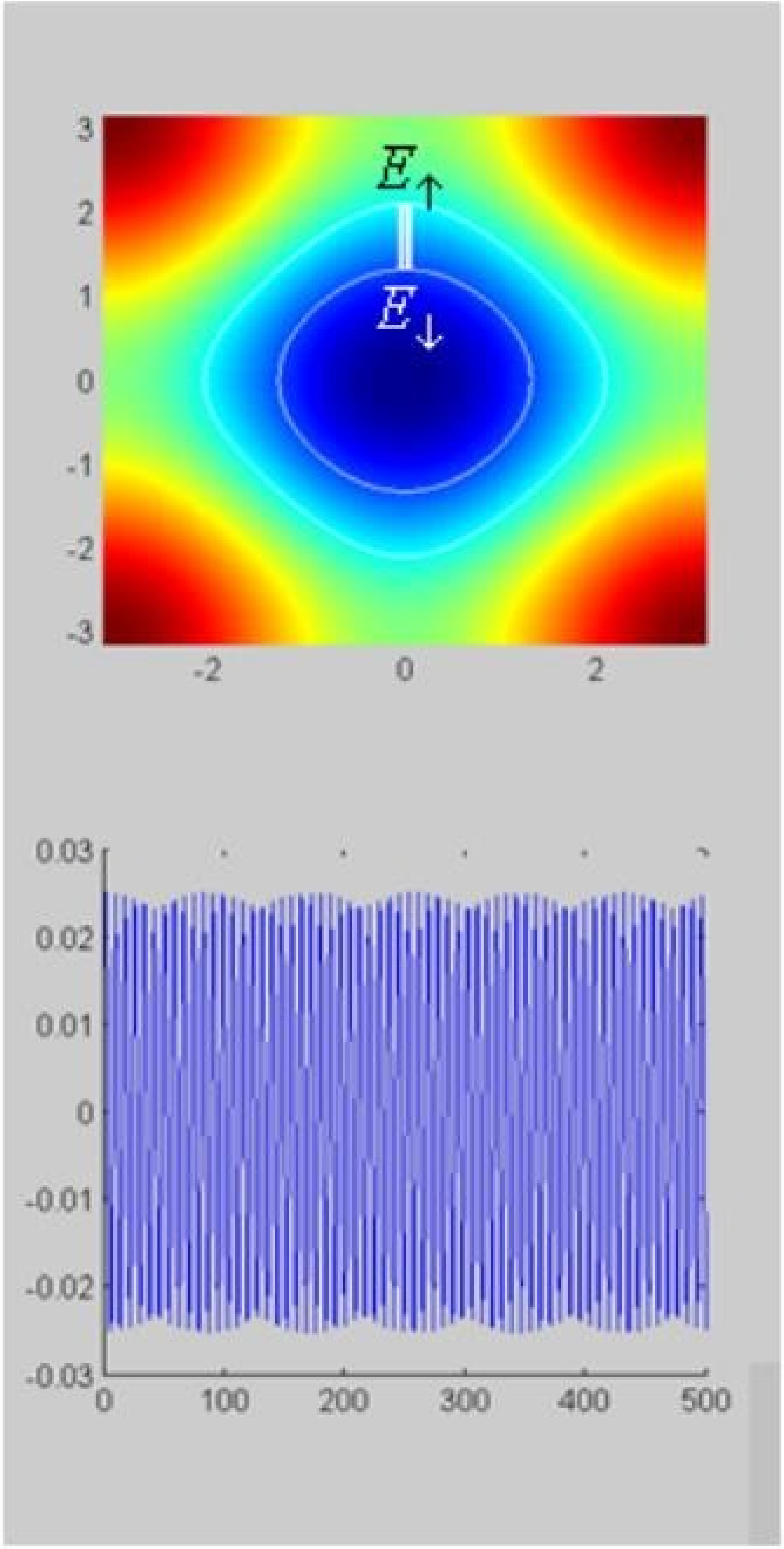
Spin precession in multiple channel scattering

Contributions from different channels (with differing kup-kdown) tend to cancel each other

$$l_{sp} \propto \frac{1}{k_\uparrow - k_\downarrow}$$

Length scale over which transverse spin decays.

Transverse component of carrier spin is destroyed.



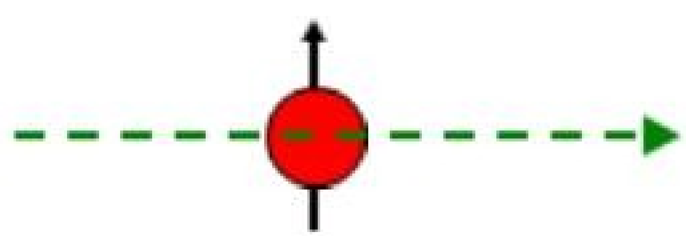
Role of spin transfer in magnetization dynamics

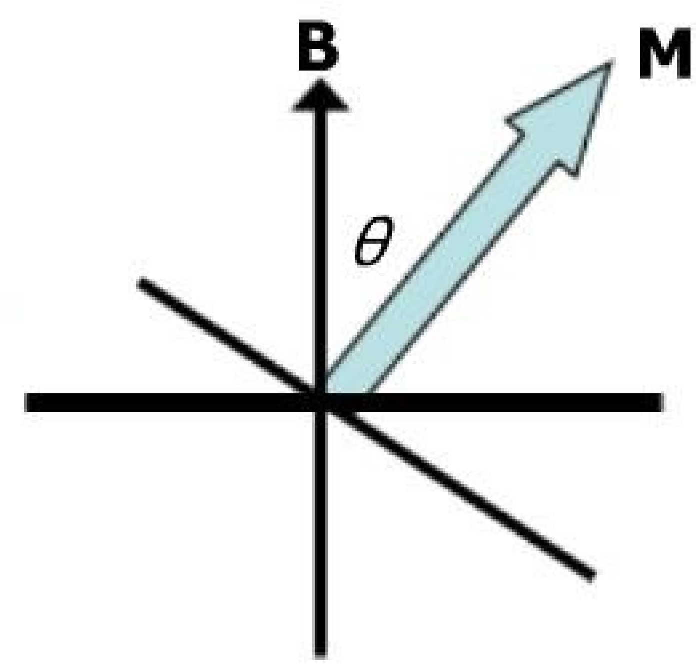
$$\boxed{\frac{1}{\gamma}\frac{d\hat{\Omega}}{dt} = -\hat{\Omega}\times\bar{B}_{eff} + \alpha\left(\hat{\Omega}\times\bar{B}_{eff}\times\hat{\Omega}\right) + \frac{g\bar{\mathbf{I}}_{s,\perp}}{M_s V}}$$

Spin transfer

$$\frac{I_{crit}}{A} = \frac{\alpha B_{eff} M_s t}{g}$$

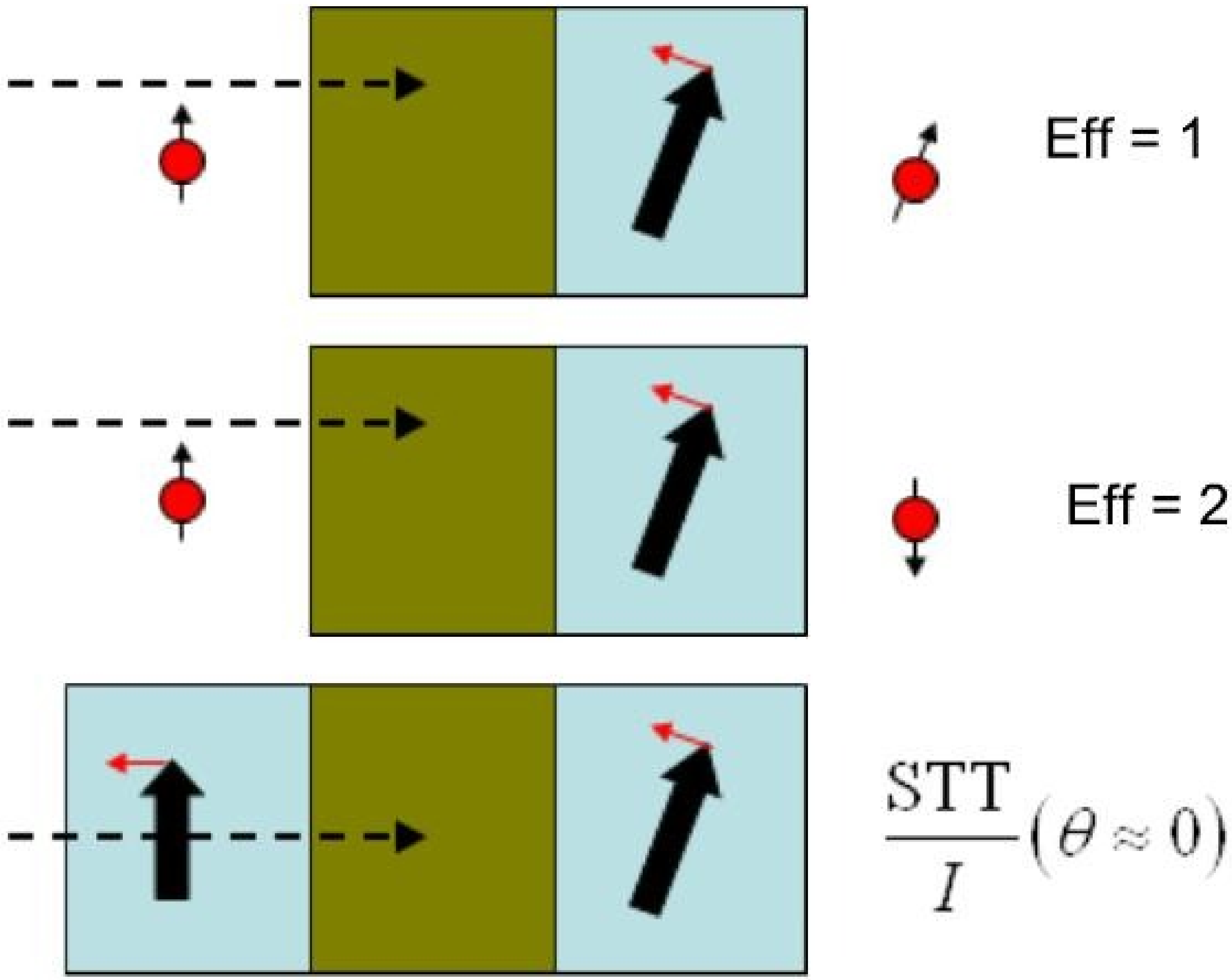
g characterizes the efficiency of transverse spin current to in exerting torques





Spin transfer efficiency

If you want to use spin transfer – you'd like to know (and maximize) the torque per electron you get:



$$P = \frac{I_{\uparrow} - I_{\downarrow}}{I_{\uparrow} + I_{\downarrow}}$$

$$\frac{\mathrm{STT}}{I}(\theta \approx 0) = \frac{P}{2}\theta$$

Calculation of spin transfer torques from first principles

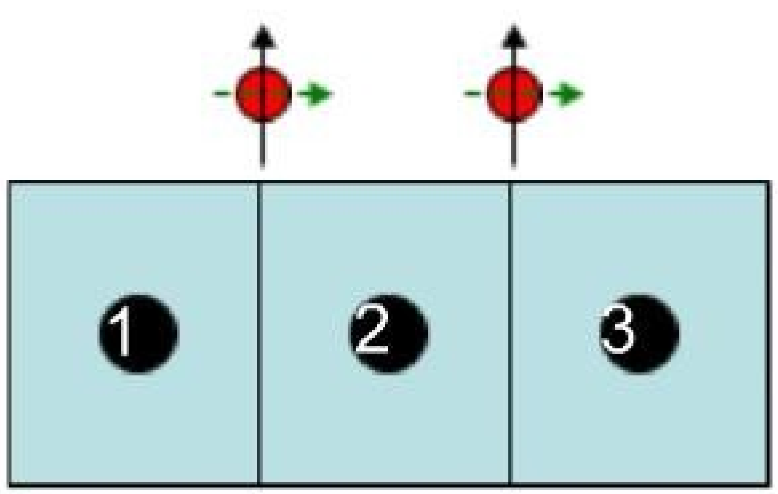
Reminder: how do we calculate STT? Evaluate net spin current flux…

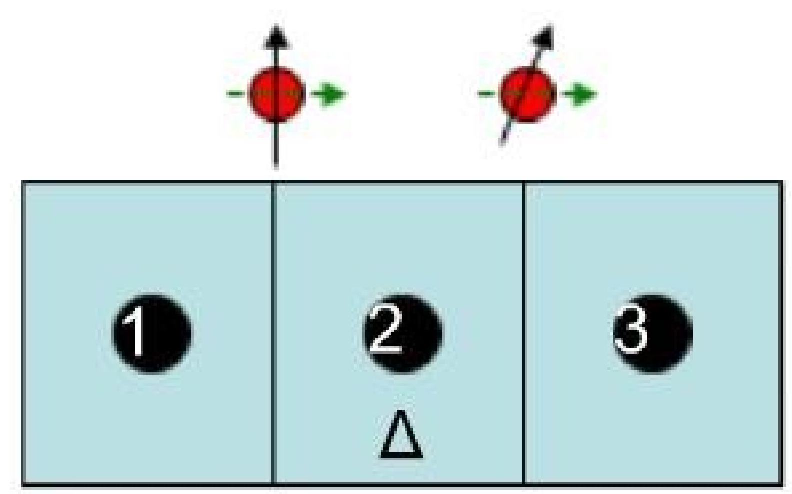
In steady state.

$$\frac{d\bar{s}_i}{dt} = \frac{1}{i\hbar}\left[\bar{\sigma}_i, H\right] = \frac{1}{i\hbar}\sum_{i<j}\mathrm{Tr}\left[H^T_{i,j}\bar{\tau}G^<_{i,j} - \mathrm{h.c.}\right] + 2\left(\bar{\Delta}_i \times \bar{s}_i\right) = 0$$

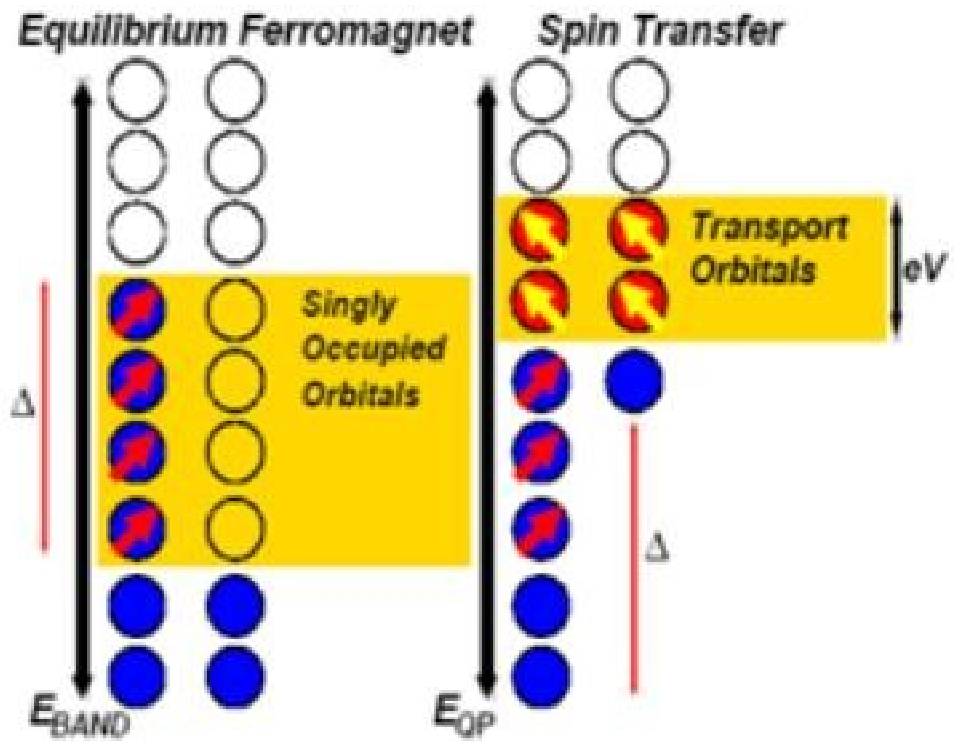
Describes spin current flux

Describes precession of quasi-particle spin around local moment





This motivates a new picture of spin transfer



Non-equilibrium electrons alter exchange-correlation field seen by all other electrons.

$$\boxed{\vec{\Delta}^{\mathrm{tr}} = \Delta_0(n,m)\,\frac{\vec{m}^{\mathrm{tr}}}{m}}$$

The ensuing precession ☐ STT dynamics

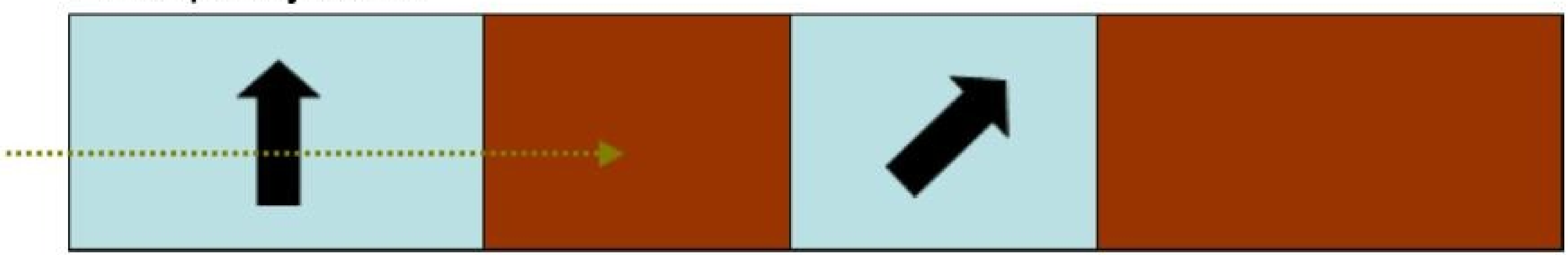
Does not rely on conservation of angular momentum!

New reminder: how do we calculated spin transfer? Calculate non-equilibrium spin densities

Calculation for Co-Cu system:

Consider a bias such that electrons flow from Co lead – use non-SC spin density to get spin torques

Example system:



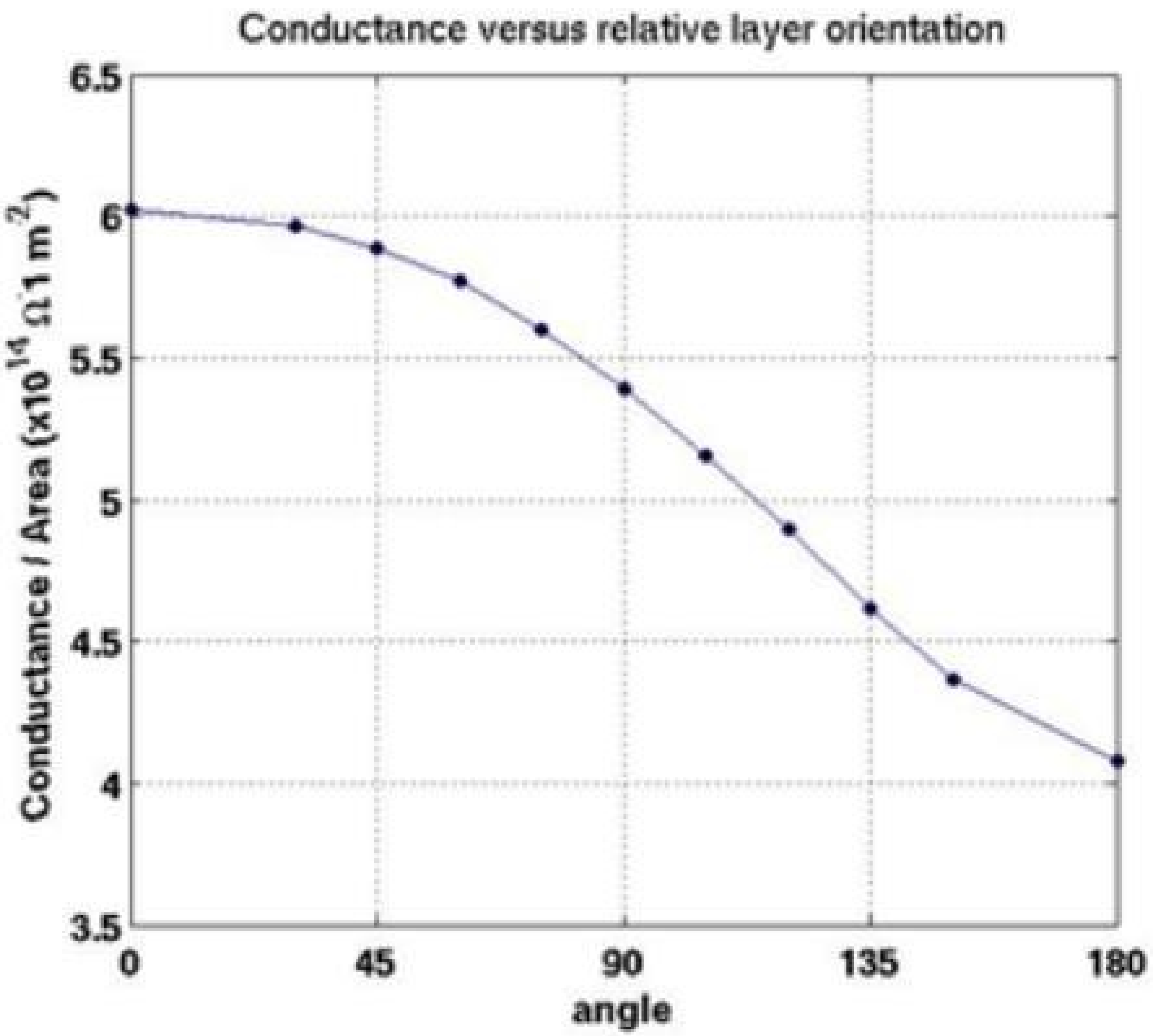
Semi-infinite Co | Cu (9 ML) | Co (15 ML) | Semi-infinite Cu

Basis set = single zeta, (s,p,d) orbital, with pseudopotential.

System length = 6.3 nm. Could do > 20 nm systems □ experimental realm

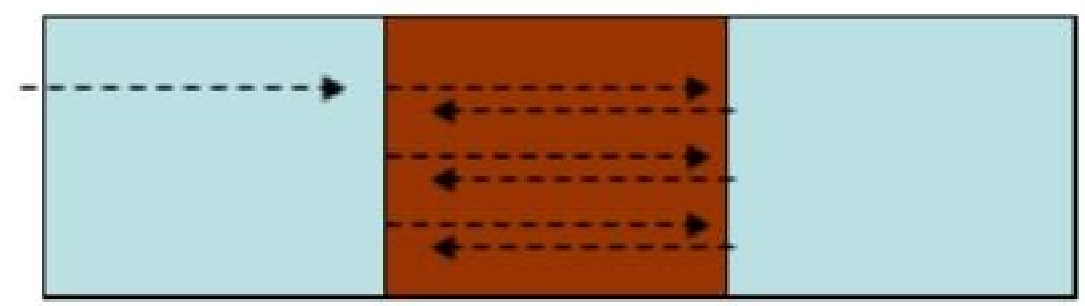
Lattice structure = fcc with constant 3.54 A

Results: GMR



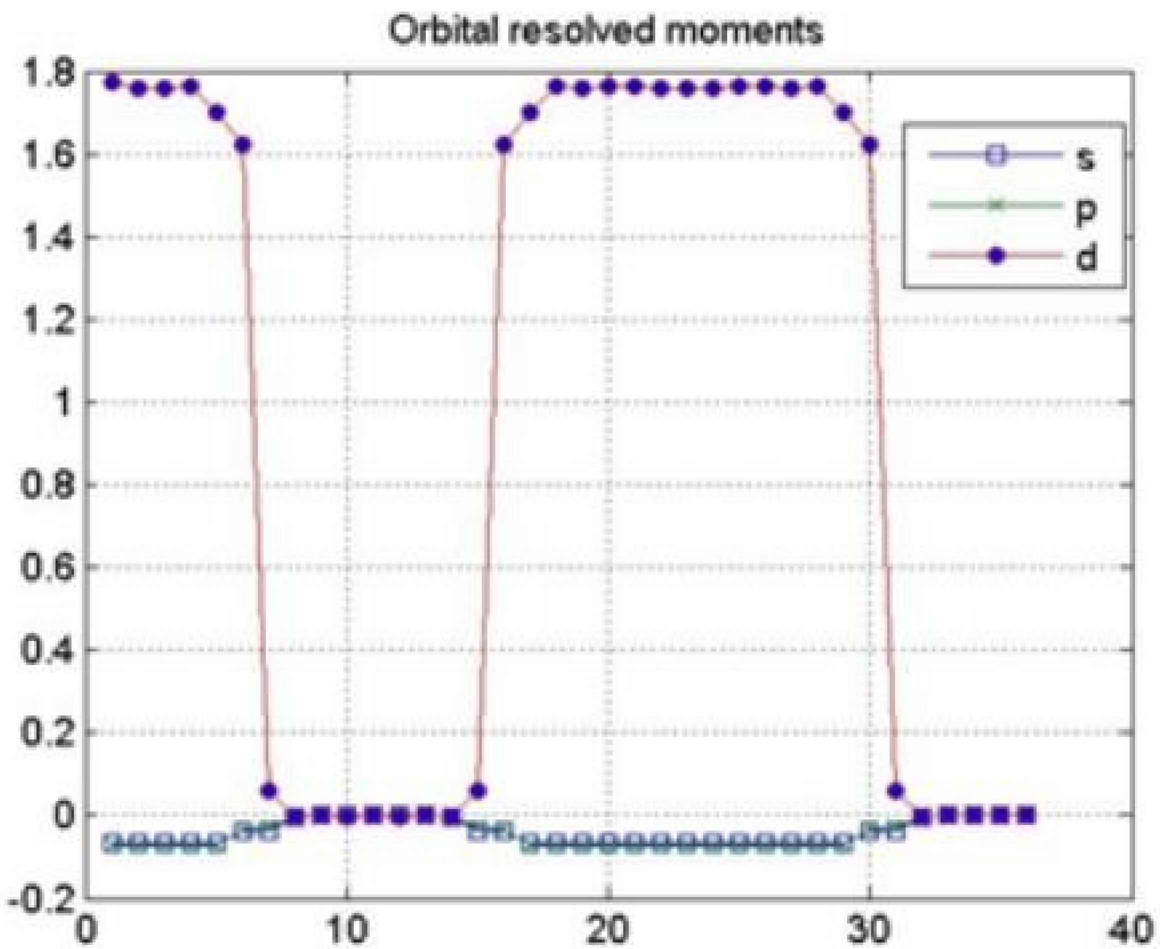
GMR ratio of 48%.

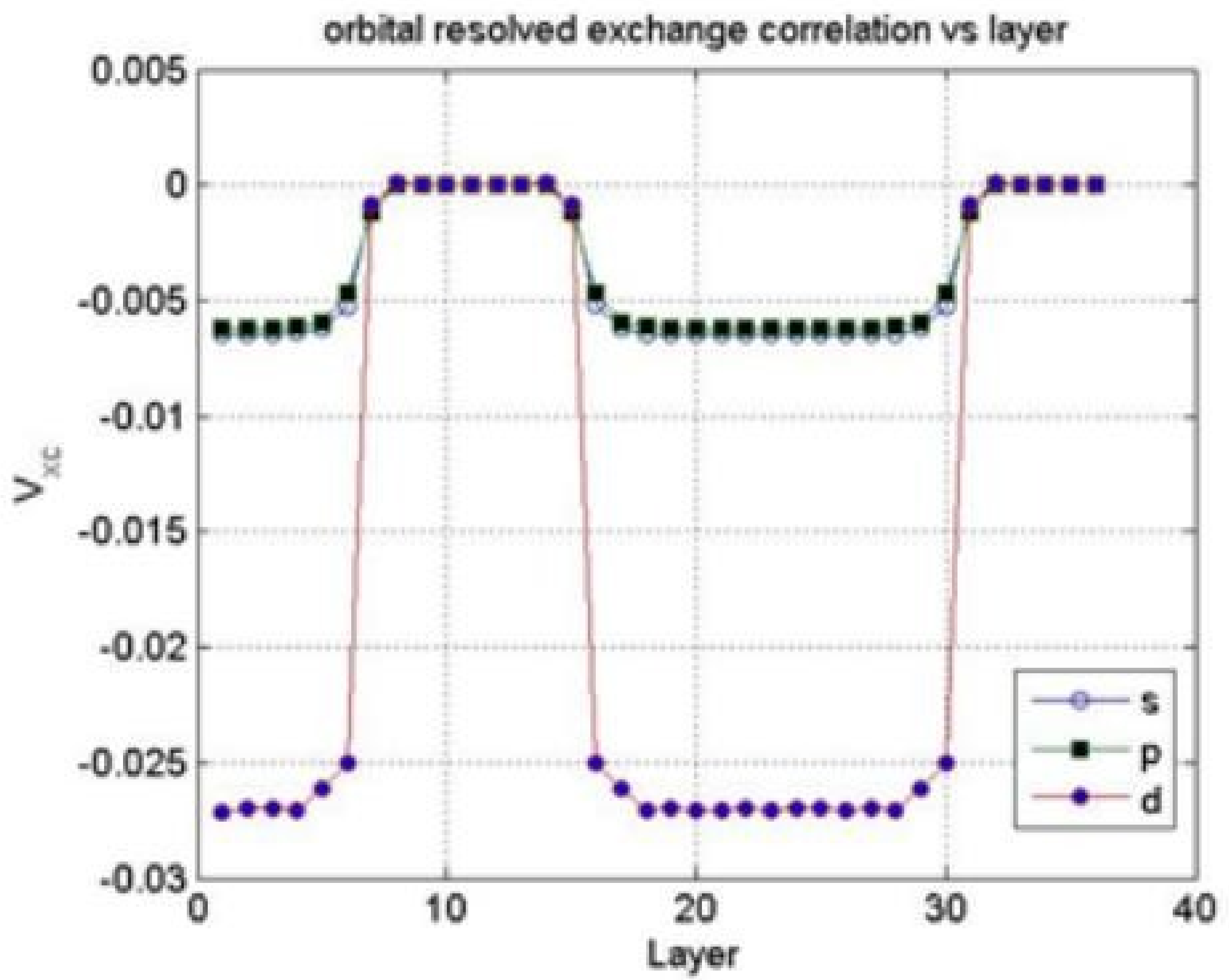
Deviation from cos(θ) implies multiple scattering



Keep in mind calculation is ballistic!

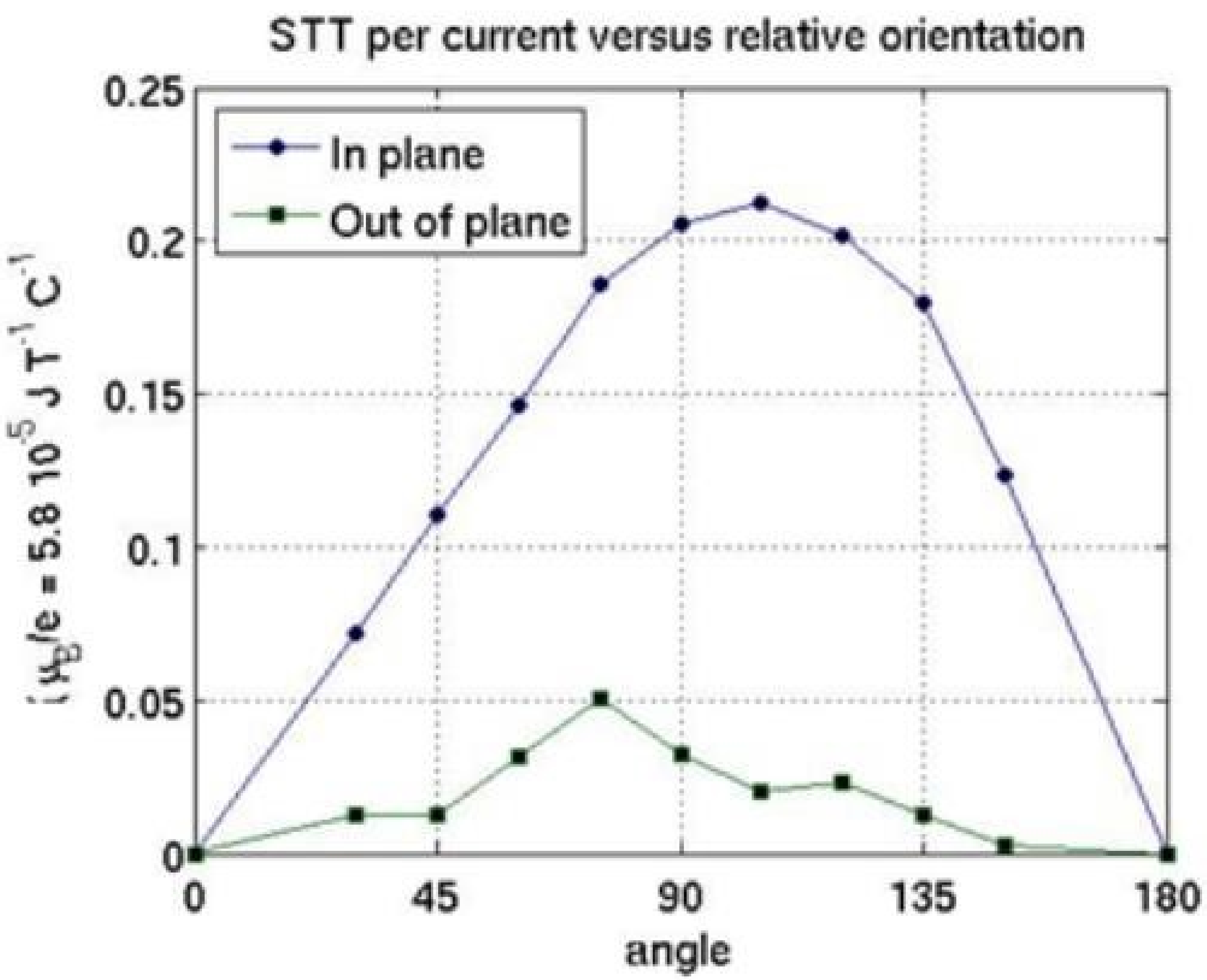
0 bias results – layer moments:





Slight decrease in moment at interface – moments dominated by d electons

Spin Torque per Current



Efficiency at θ=0 : 14%

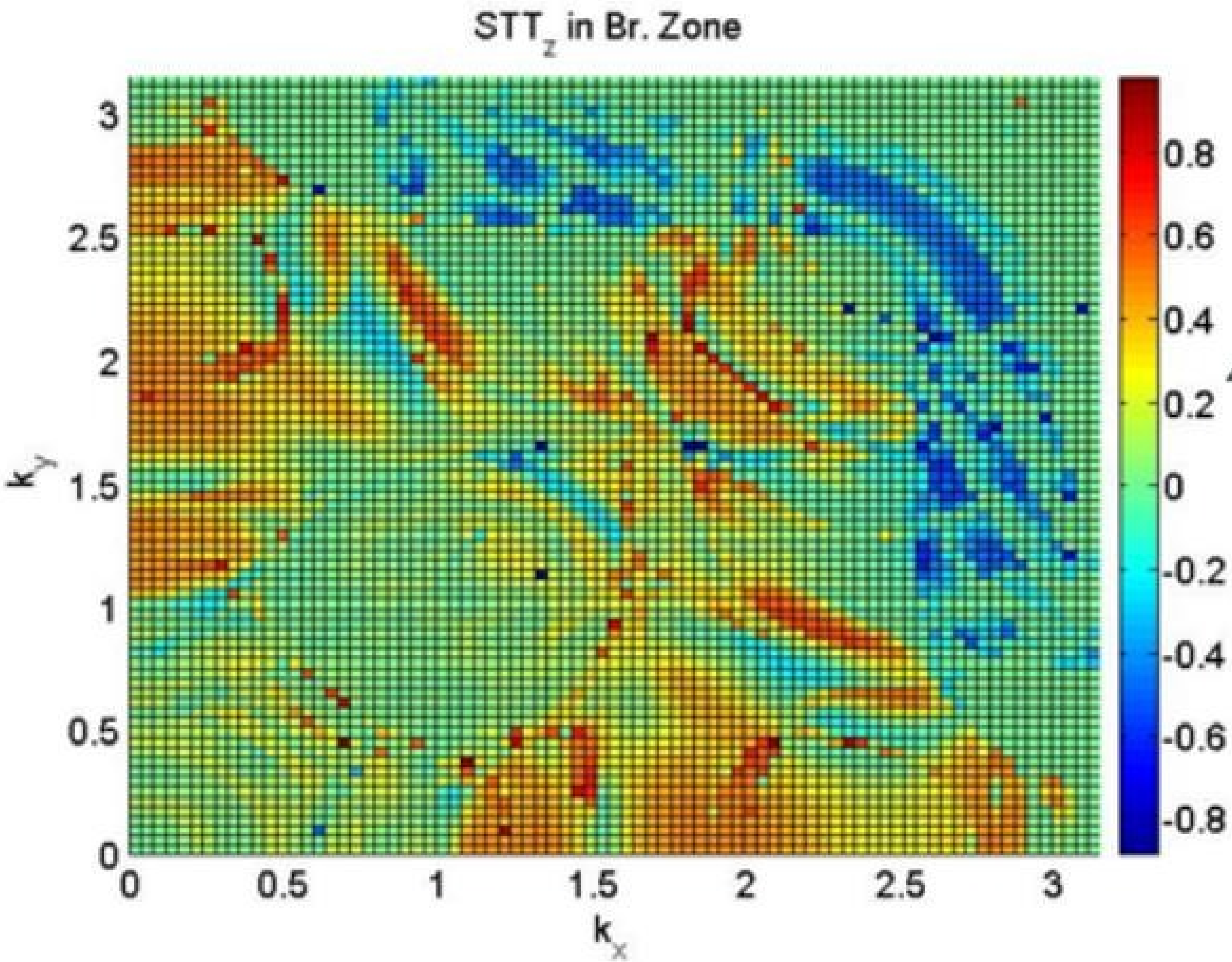
Compare to ideal result of P/2=18%

Out of plane torque up 10% of in-plane torque, in agreement With some calc, disagreement With others…

One experimental value: 34%

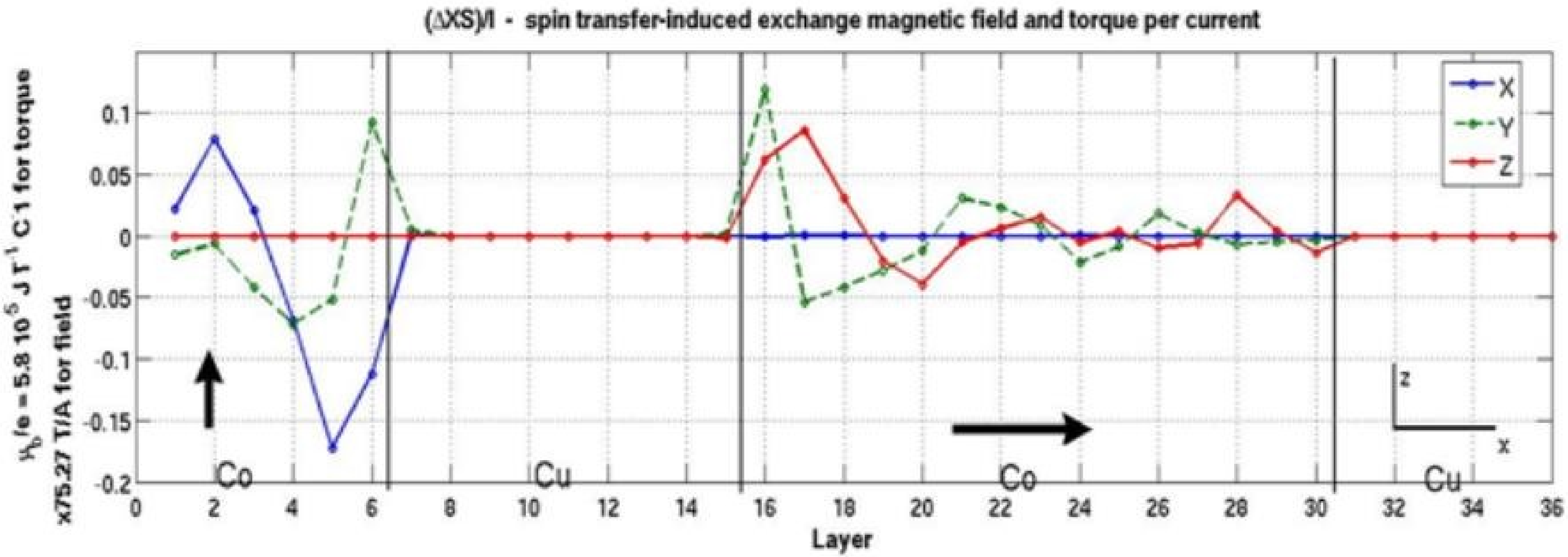
Can microscopic origin of loss of efficiency be found??

Spin torque resolved in k-space



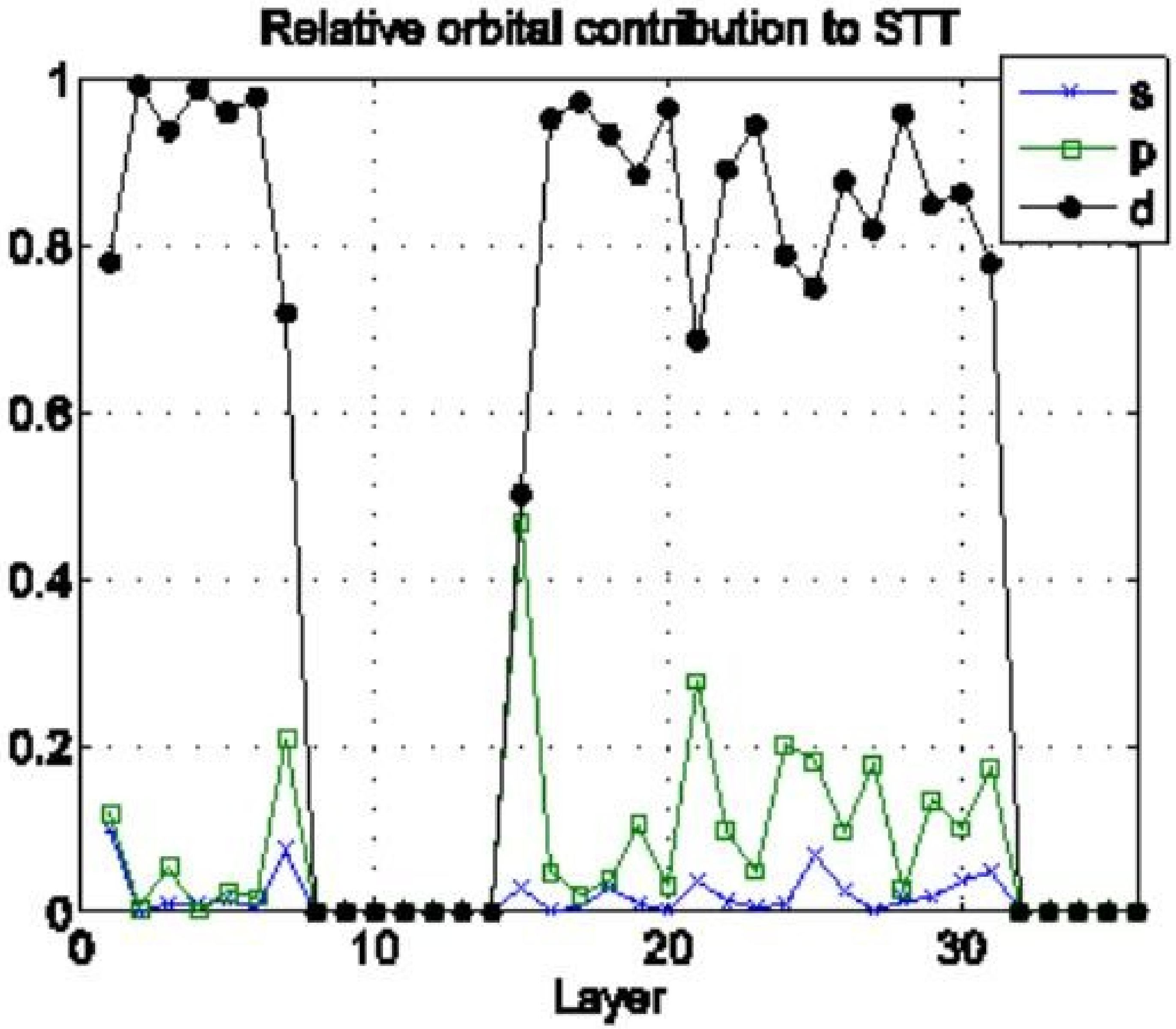
Understand in terms of kup-kdown…
Multi-valued minority channel makes it more difficult…

Layer resolved torques

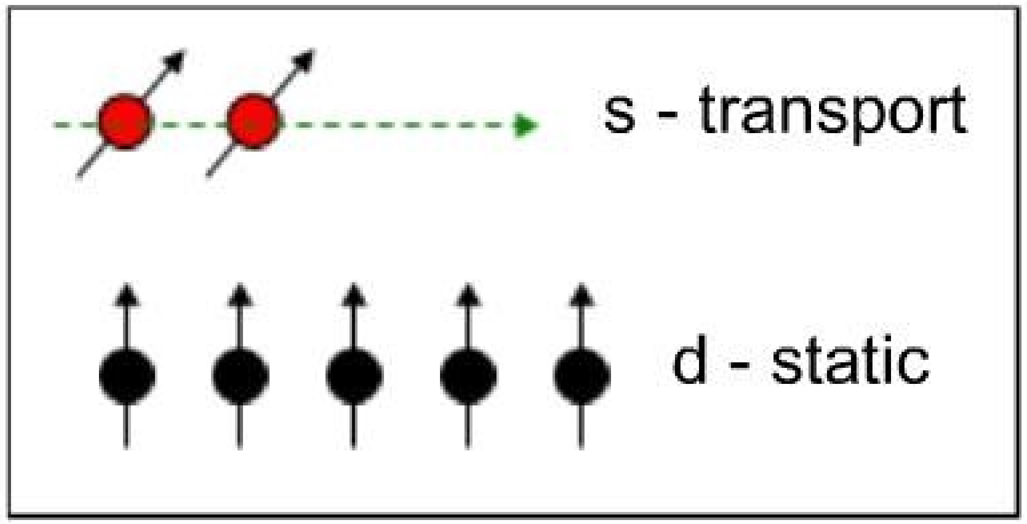


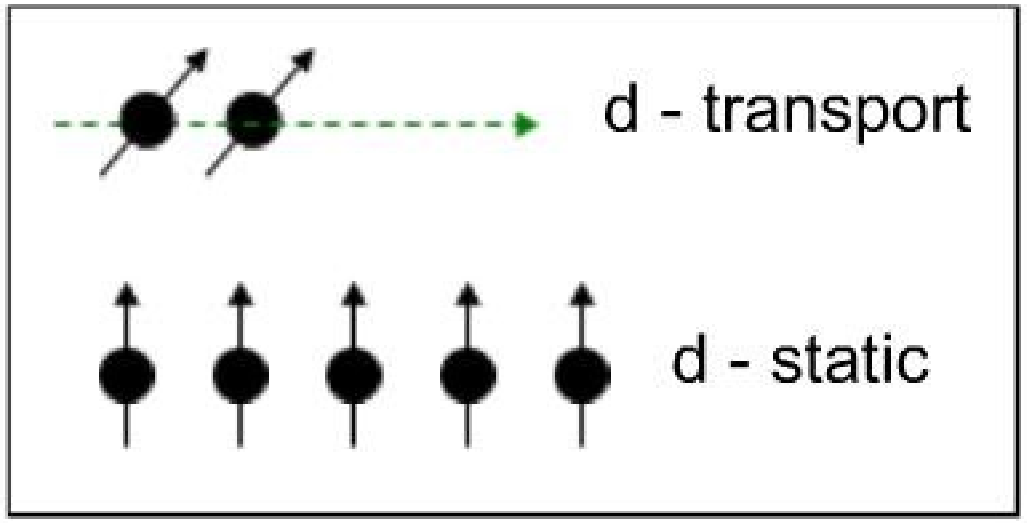
Shows decay (although not complete) of transverse components

Orbital resolved STT



In contrast to s-d model picture

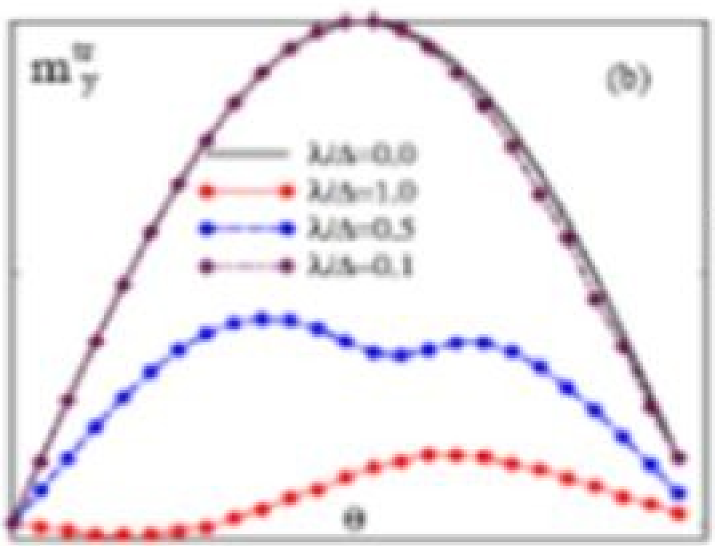




Extensions: spin-orbit coupling

$$V_{so} = \sum_{l,M} V_l^{SO} \bar{L} \cdot \bar{S} \left| l,M \right\rangle \left\langle l,M \right|$$

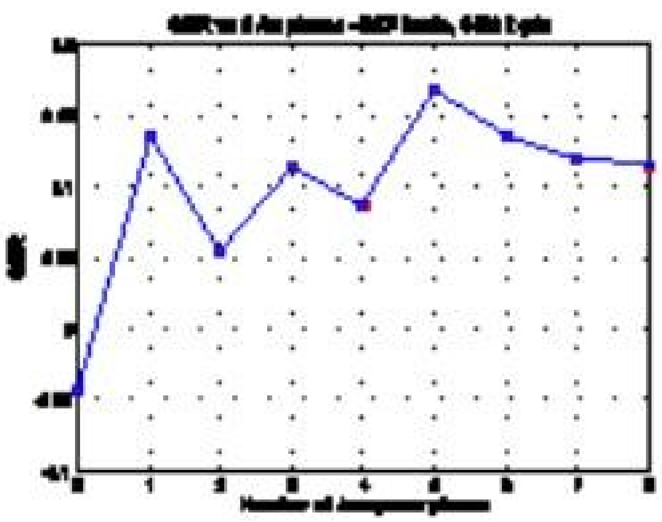
In the case where spin is not conserved (not a good quantum #), our approach to spin transfer is required.



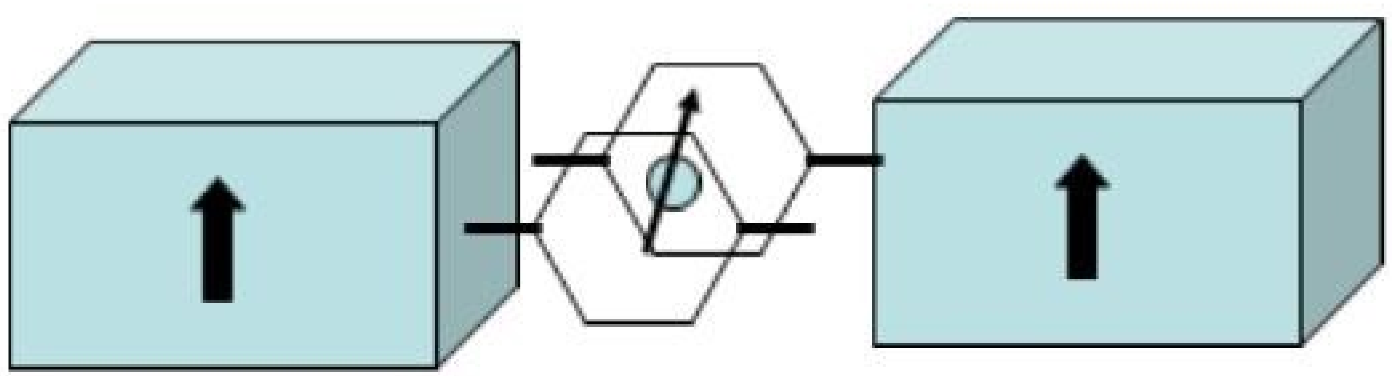
Calculation for toy-model. For our scheme inclusion of S-O coupling is straightforward…

Other calculations in progress:

- Do Anti-Ferromagnets show spin transfer/GMR effects? Yes: Cr-Au-Cr



- Current can change the direction of the magnetization. What else can it change (the magnitude, stiffness, anisotropy?)
- What's the effect of reducing dimensionality? What are spin torques like in 0-d (molecular), or 1-d systems?

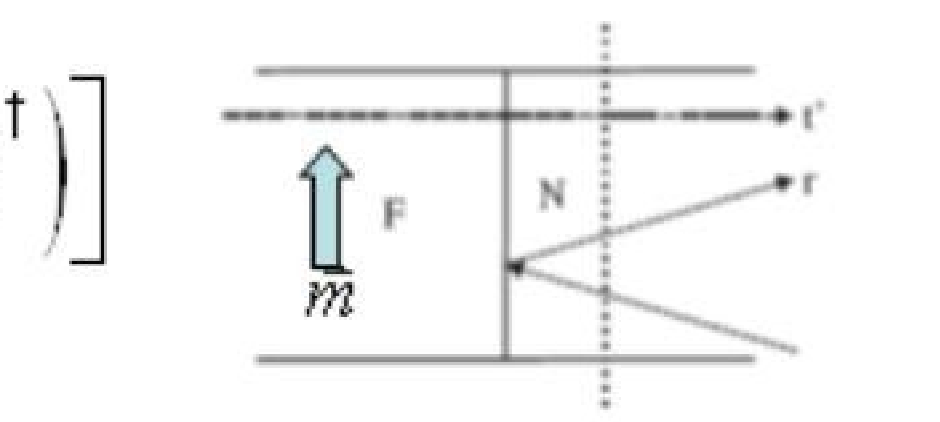


How do we design in spintronics?

- Once we can calculate things realistically, then can engineer things to be the way we want, a la MgO barriers, etc…
- How can we lower the critical current for spin transfer induced switching (for MRAM)??
- Let's start with toy models…

Magneto-electronics background

$$\hat{I} = \frac{e}{h}\sum_{nm}\left[\hat{t}^{nm}\hat{f}^{F}\left(\hat{t}^{mn}\right)^{\dagger} - \left(\delta_{nm}\hat{f}^{N} - \hat{r}^{nm}\hat{f}^{N}\left(\hat{r}^{mn}\right)^{\dagger}\right)\right]$$



$$\hat{I} = \begin{pmatrix} I_{\uparrow\uparrow} & I_{\uparrow\downarrow} \\ I_{\downarrow\uparrow} & I_{\downarrow\downarrow} \end{pmatrix} = \frac{1}{2}\left(I_C + \boldsymbol{\sigma}\cdot\mathbf{I}_S\right)$$

$$\hat{f} = \begin{pmatrix} f_{\uparrow\uparrow} & f_{\uparrow\downarrow} \\ f_{\downarrow\uparrow} & f_{\downarrow\downarrow} \end{pmatrix} = f_C + \left(\boldsymbol{\sigma}\cdot\mathbf{s}\right) f_S$$

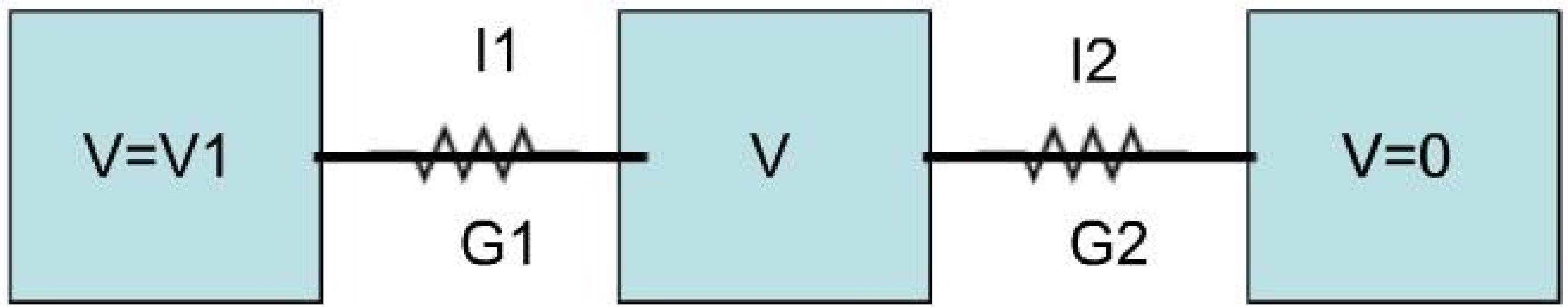
All objects are in spin space

Ohm's Law in spin space:

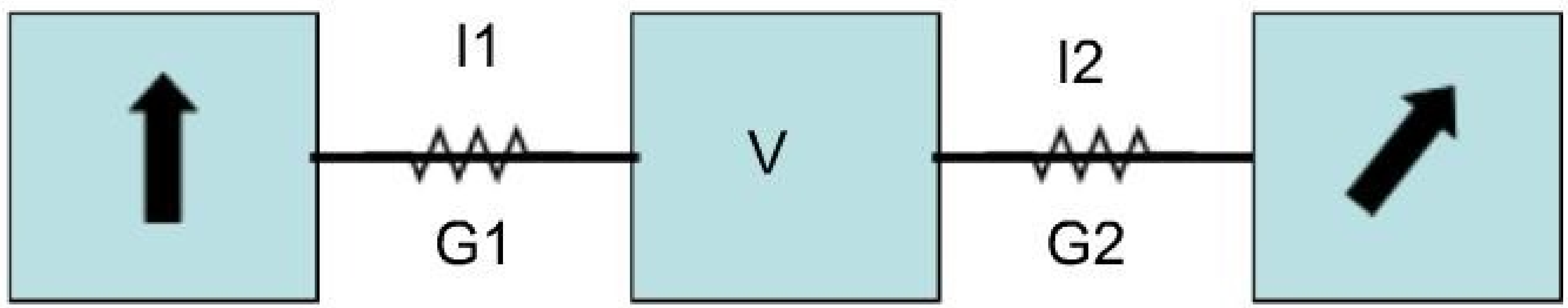
$$I_C = \left(G^{\uparrow} + G^{\downarrow}\right)\left(f_C^F - f_C^N\right) + \left(G^{\uparrow} - G^{\downarrow}\right)\left(f_S^F - \bar{m}\cdot\bar{s} f_S^N\right)$$

$$\bar{I}_S = \left[\left(G^{\uparrow} - G^{\downarrow}\right)\left(f_C^F - f_C^N\right) + \left(G^{\uparrow} + G^{\downarrow}\right) f_S^N + \left(2\,\mathrm{Re}\,G^{\uparrow\downarrow} - G^{\uparrow} - G^{\downarrow}\right)\bar{m}\cdot\bar{s} f_S^N\right]\bar{m}$$
$$- 2\,\mathrm{Re}\,G^{\uparrow\downarrow} f_S^N \bar{s} + 2\,\mathrm{Im}\,G^{\uparrow\downarrow} f_S^N \bar{m}\times\bar{s}$$

Magneto-electronics nuts and bolts



I1=G1*(V1-V)
I2=G2*(V-0)
I1+I2=0



G1 (V) is has now a charge + spin vector component – specified by 4 numbers:

$G^{\uparrow\uparrow}$ Specifies conductance of diagonal majority channel

$G^{\downarrow\downarrow}$ Specifies conductance of diagonal minority channel

$G^{\uparrow\downarrow}$ Imaginary #: Specifies propensity to absorb spins transverse to local moment

Kirchoff's Laws in spin space

Conservation laws in spin space
(assuming no spin relaxation)

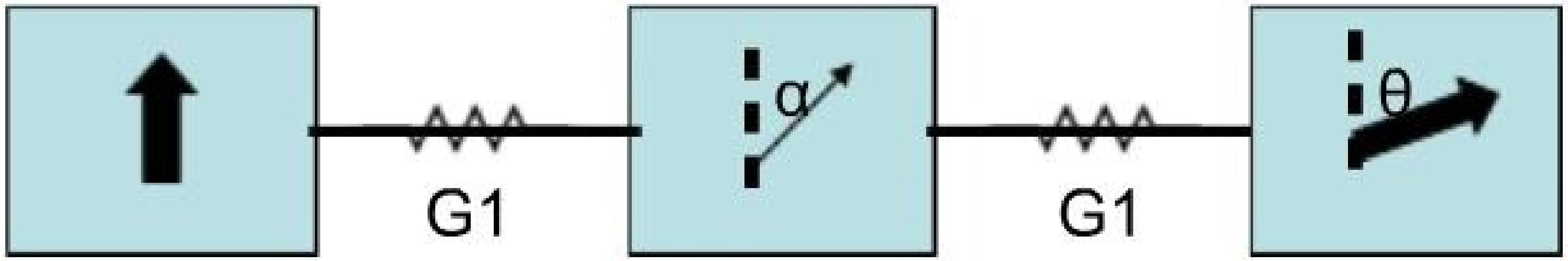
$$\sum_{\alpha} I_{\alpha} = 0$$

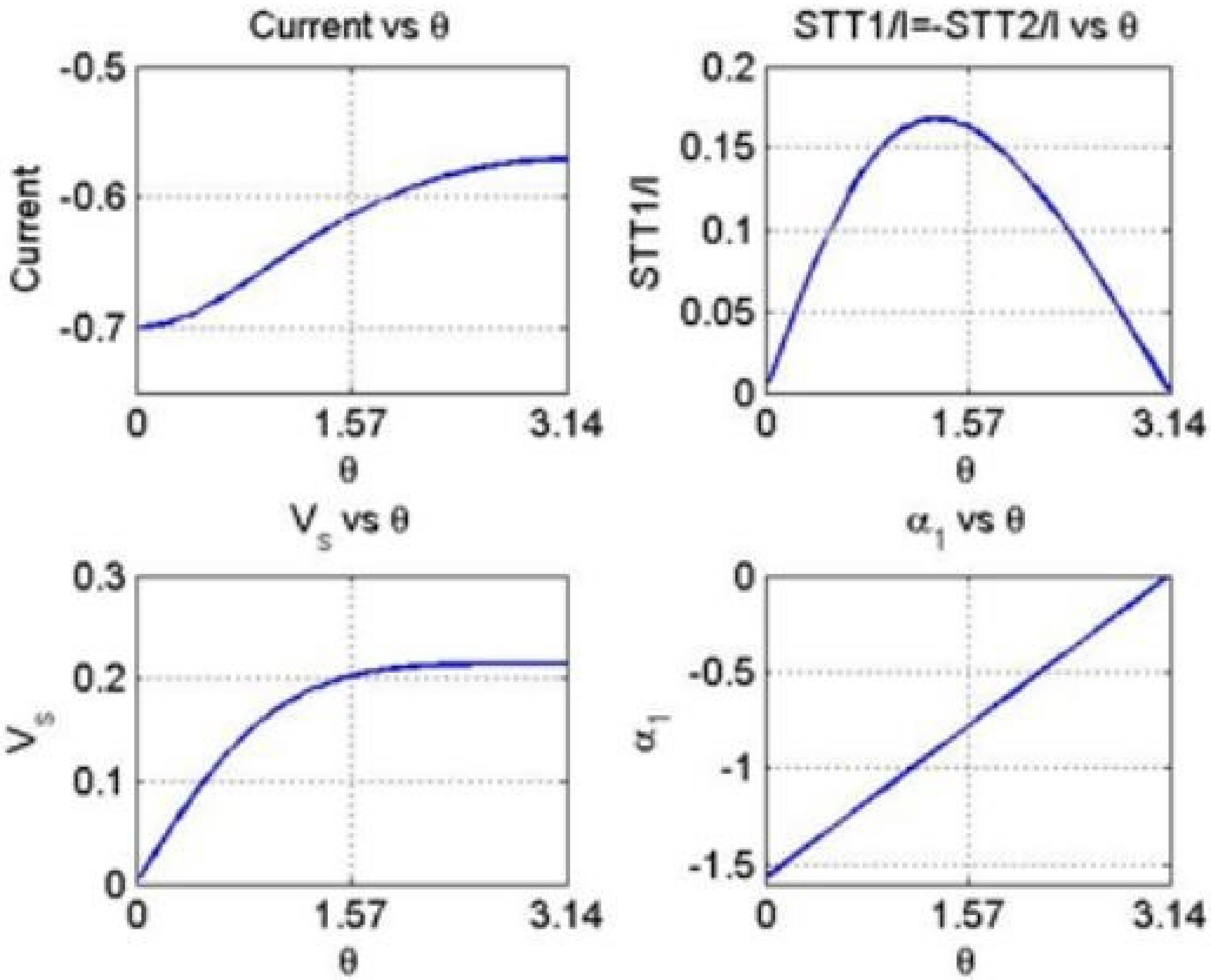
$$\sum_{\alpha} \bar{\mathbf{I}}_S = 0 \qquad \text{(for N node)}$$

$$\sum_{\alpha} \bar{\mathbf{I}}_S \cdot \bar{\mathbf{m}} = 0 \qquad \text{(for F node)}$$

Implies spin accumulation in FM is parallel to magnetization. Assumes length scales are greater than spin dephasing length

2 layer calc example…





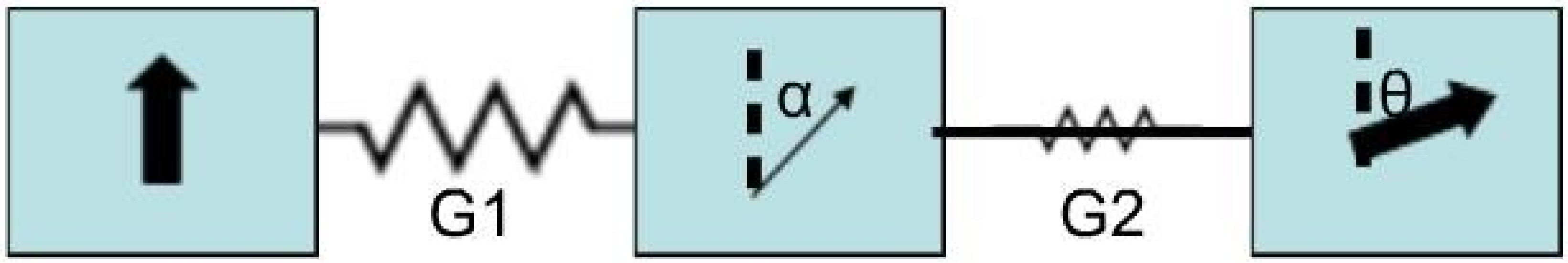
Note alpha is m1-m2
STT efficiency = P/2
Put params in

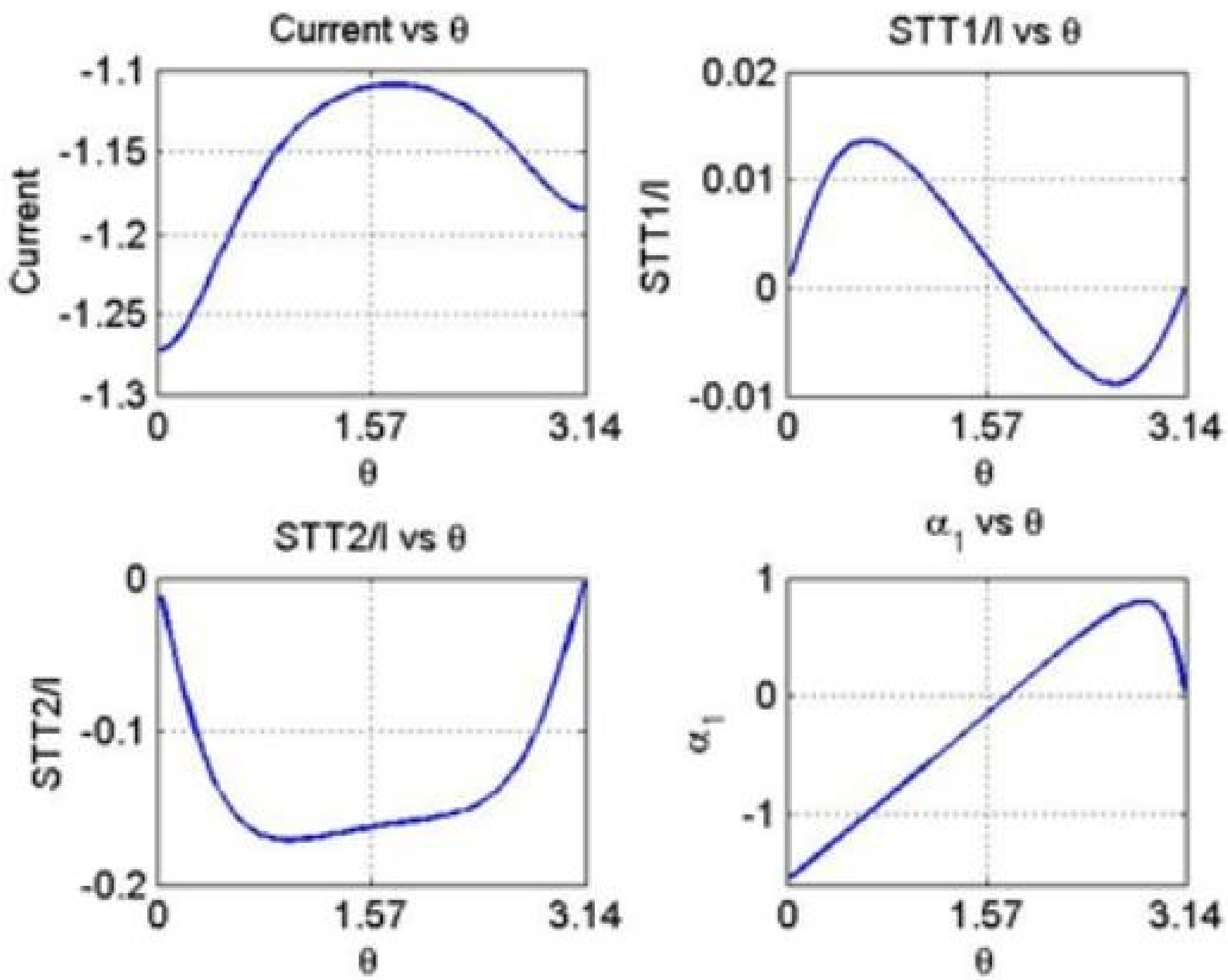
$$G_1 = G^{\uparrow} + G^{\downarrow} = 1.4$$

$$p_1 = \frac{G^{\uparrow} - G^{\downarrow}}{G^{\uparrow} + G^{\downarrow}} = .4$$

$$\eta = \frac{2\mathrm{Re}G^{\uparrow\downarrow}}{G^{\uparrow} + G^{\downarrow}} = .5$$

Small eta





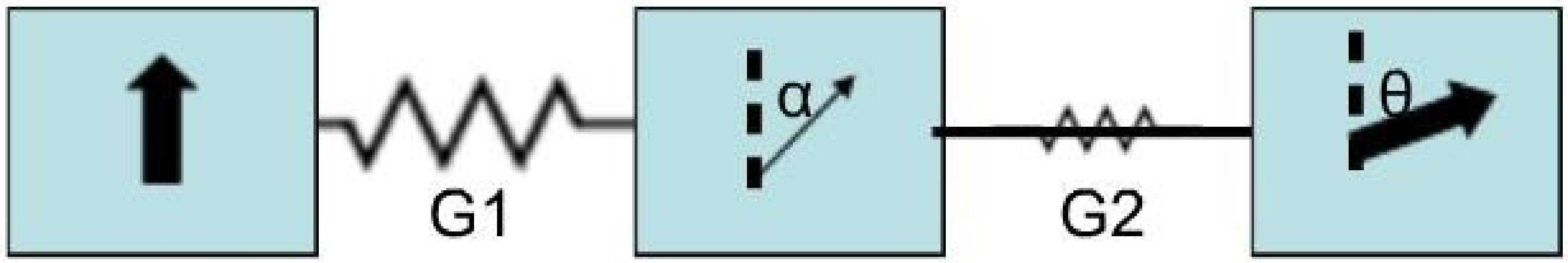
$$G_2 = 14 = 10 \times G_1$$

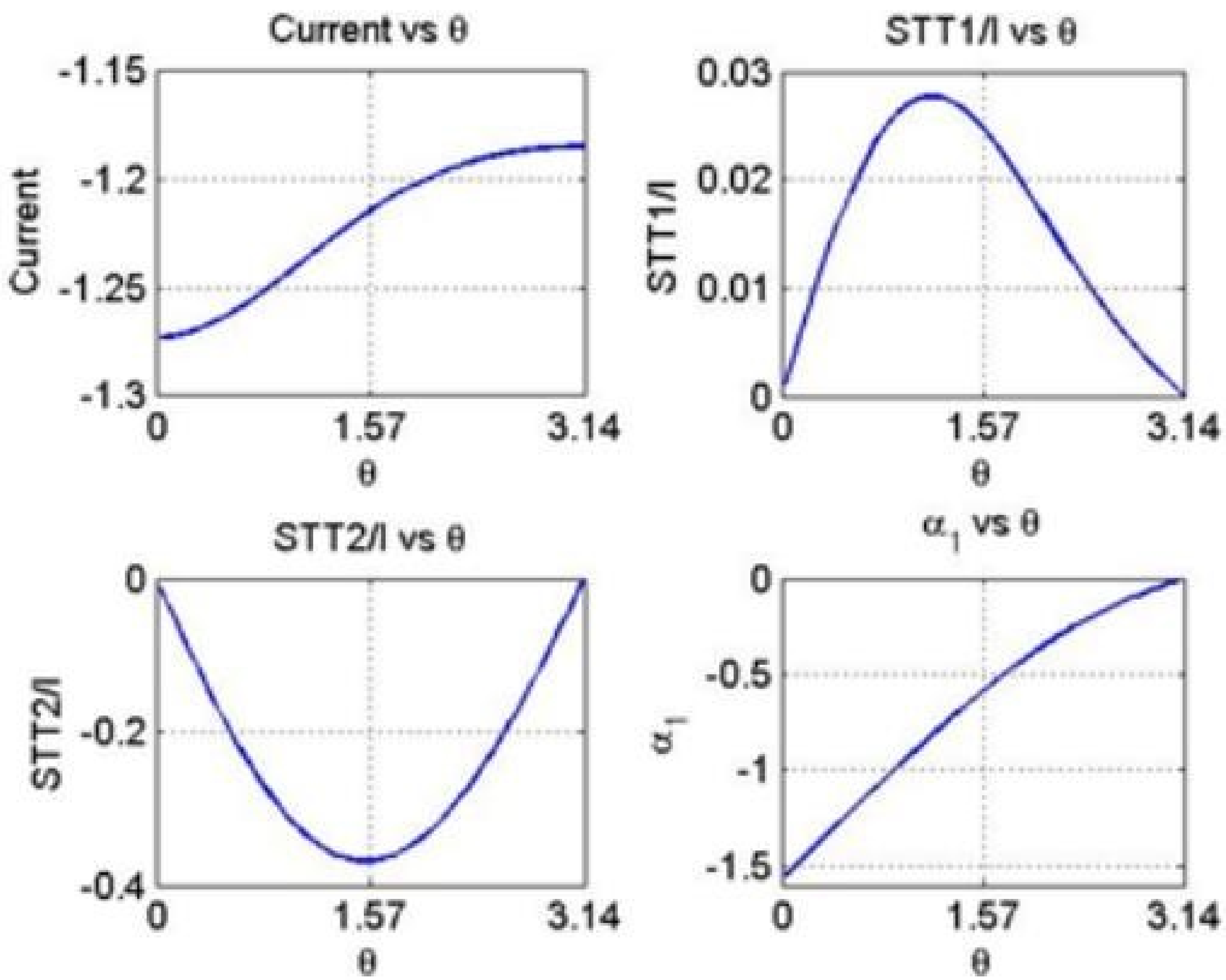
$$p_2 = p_1 = .4$$

$$\eta_2 = \eta_1 = \frac{2\,\mathrm{Re}\,G^{\uparrow\downarrow}}{G^{\uparrow} + G^{\downarrow}} = .05$$

Gain = 1.02

Big eta





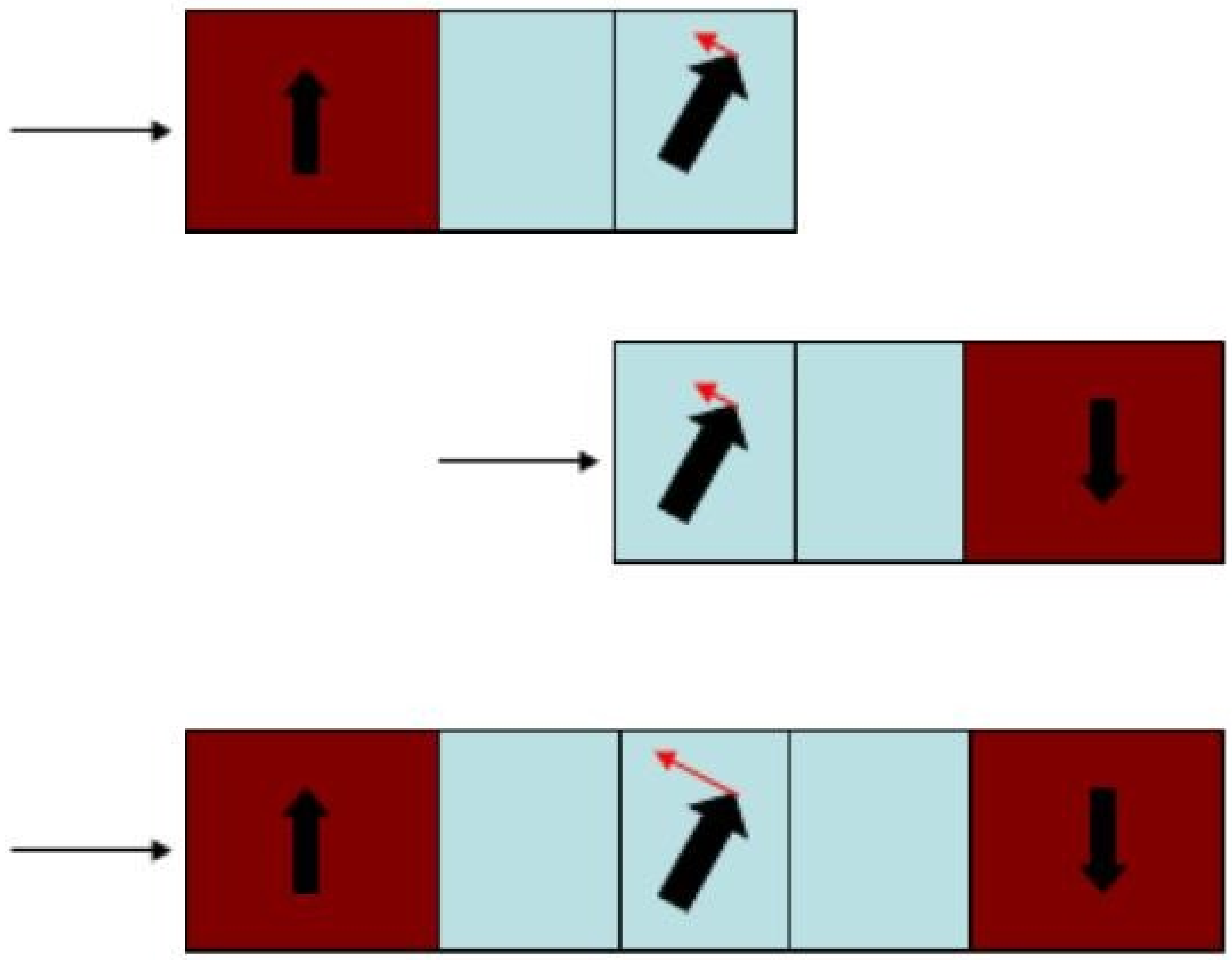
$$G_2 = 14 = 10 \times G_1$$

$$p_2 = p_1 = .4$$

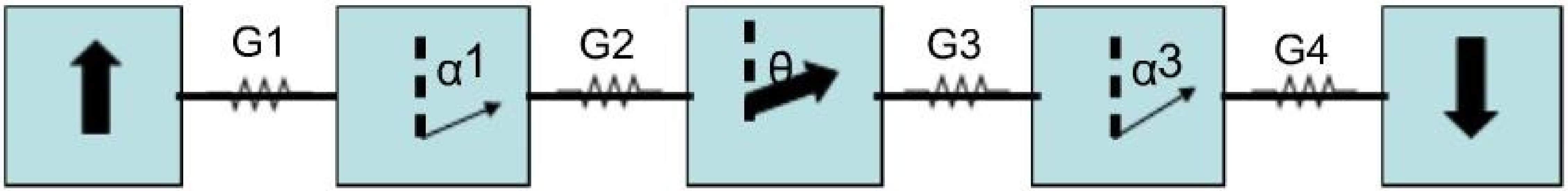
$$\eta_2 = \eta_1 = \frac{2\mathrm{Re}G^{\uparrow\downarrow}}{G^{\uparrow} + G^{\downarrow}} = .5$$

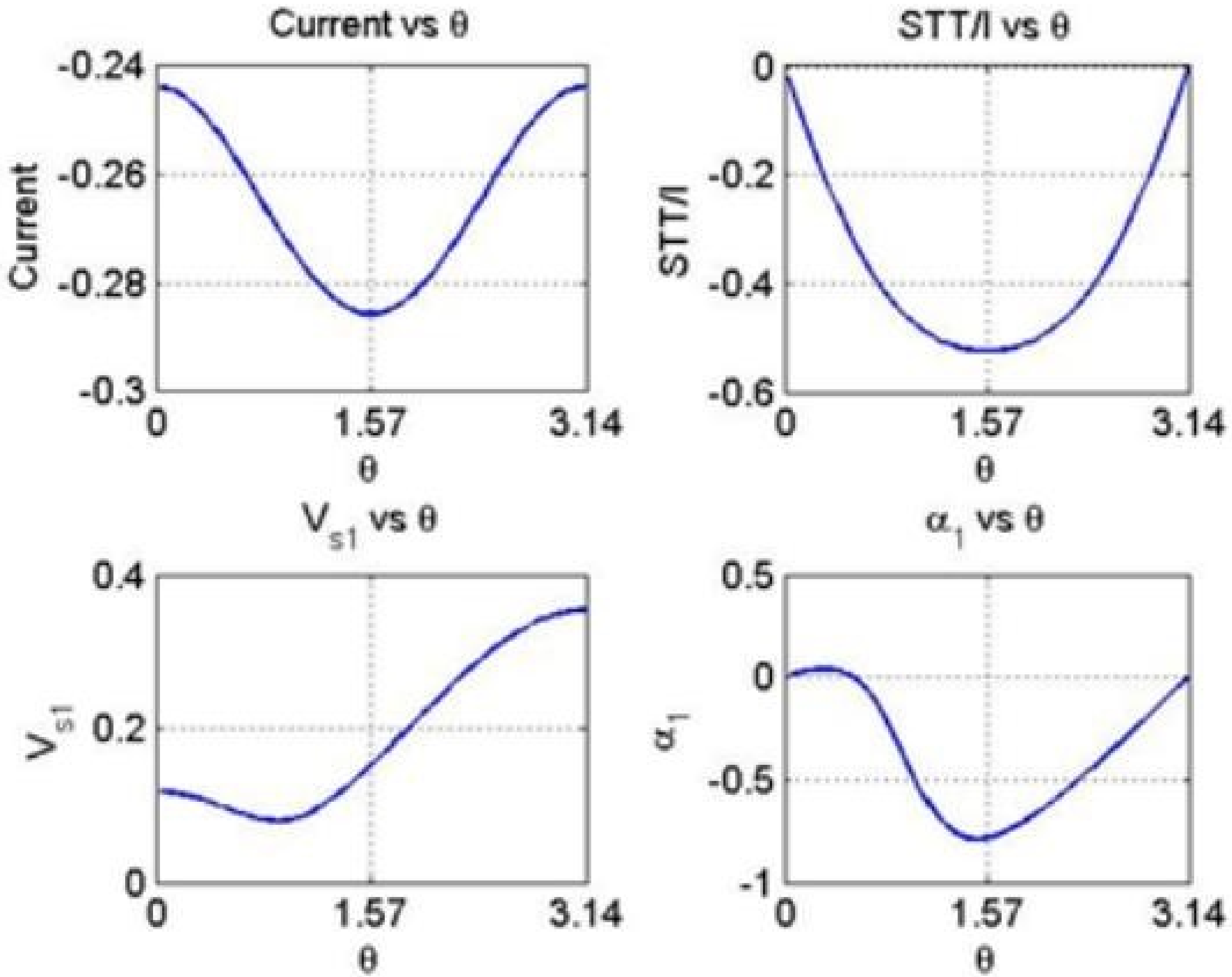
Gain = 2.2

Dual Spin Filter Proposal for increased effeciency



DSF – results 1





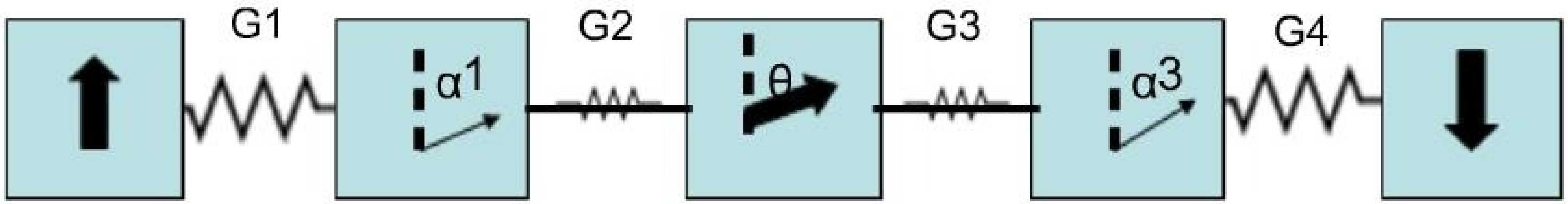
$$G_{1,2,3,4} = 1.4$$

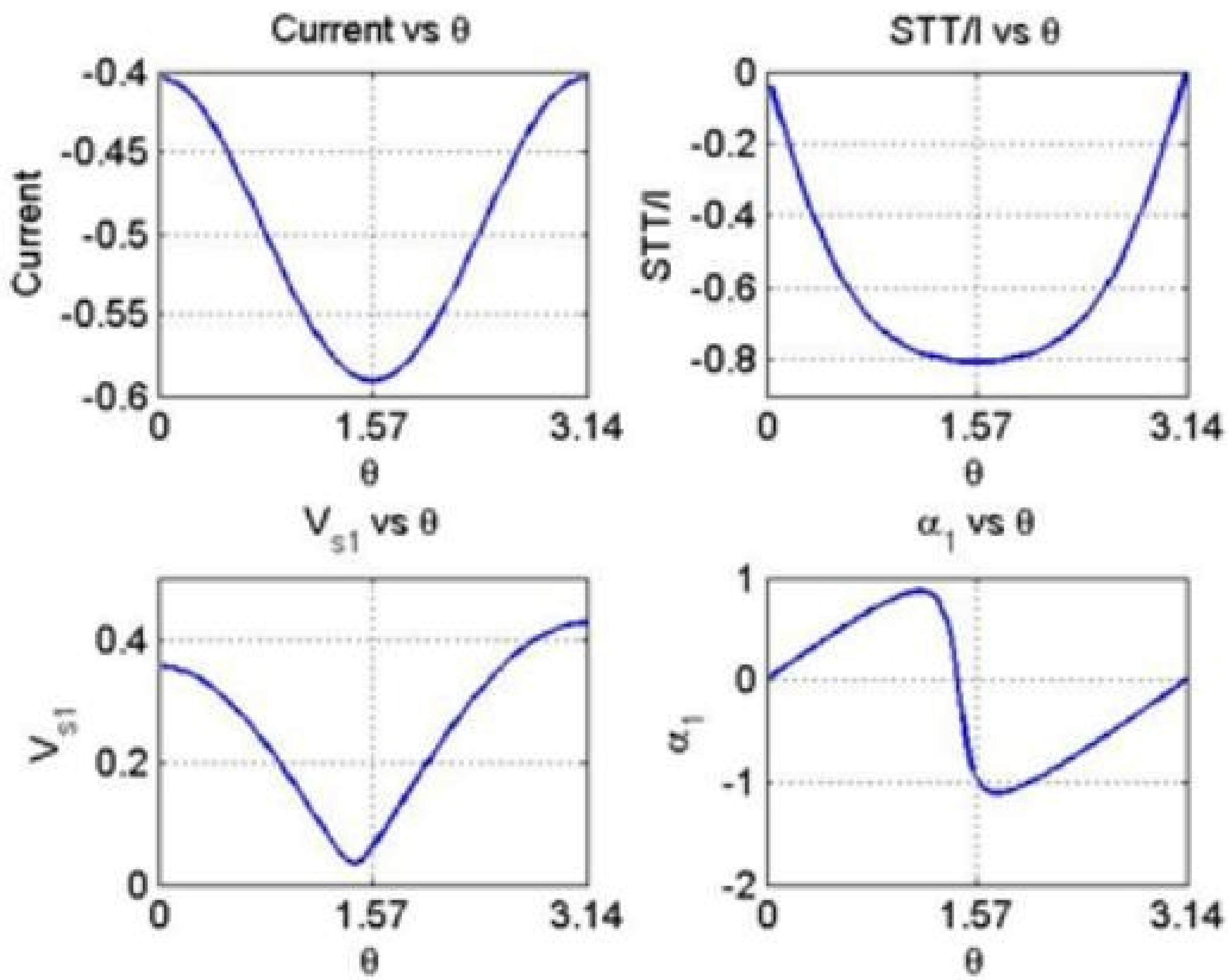
$$p_{1,2,3,4} = .4$$

$$\eta_{1,2,3,4} = .5$$

Gain = 3.13

DSF 2





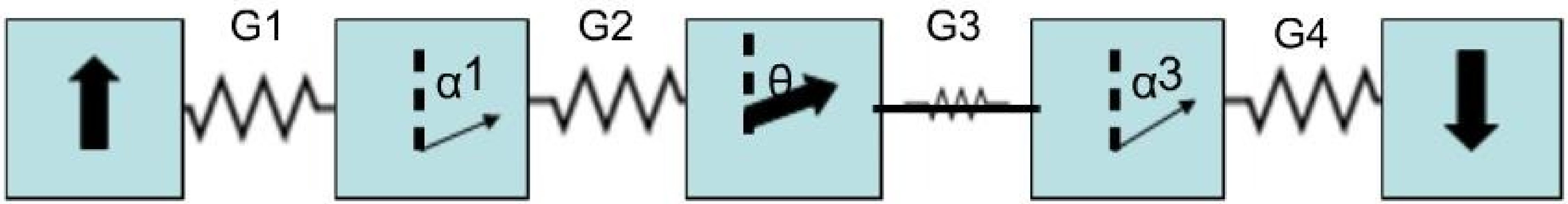
$$G_{2,3} = 14 = 10 \times G_{1,4}$$

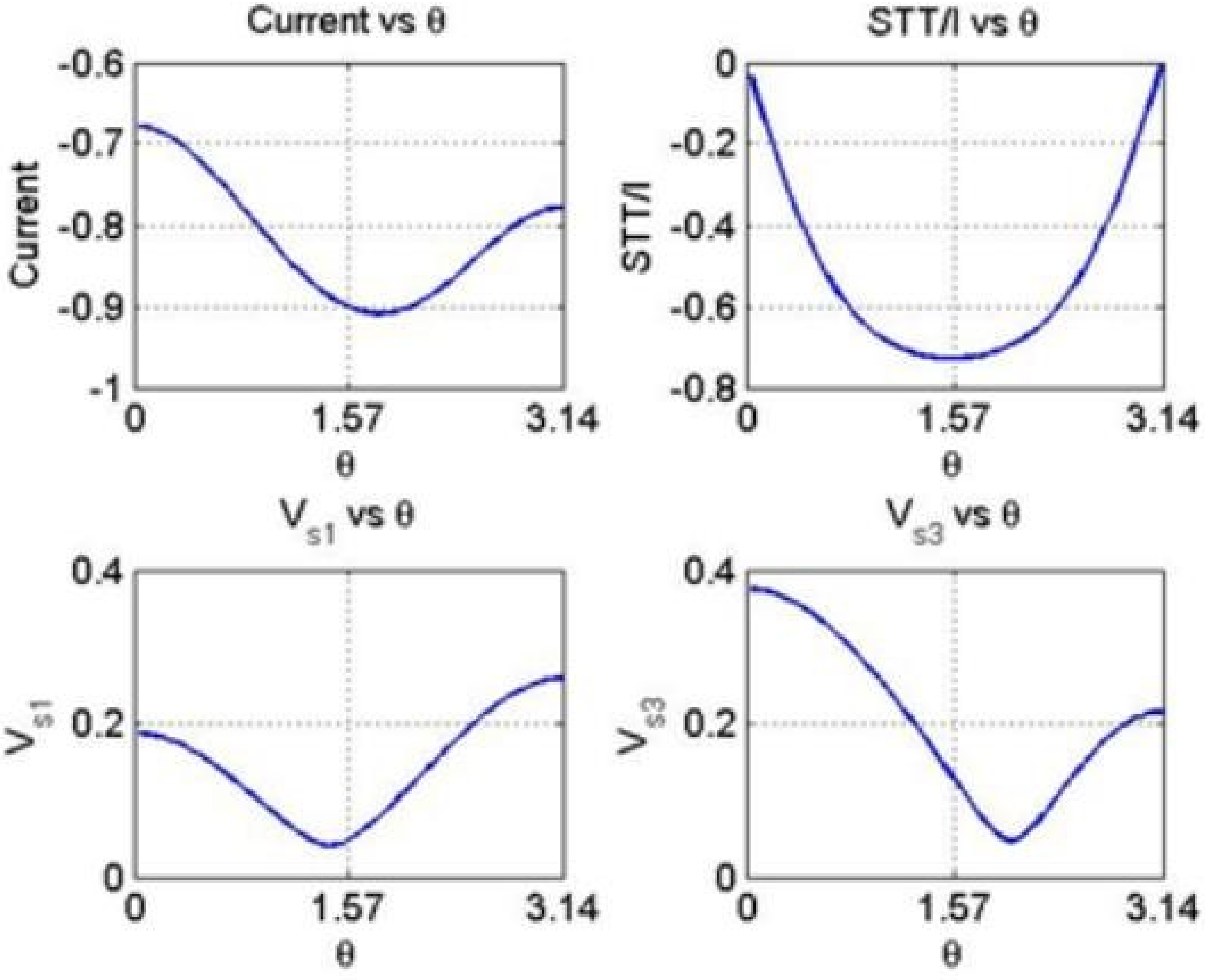
$$p_{1,2,3,4} = .4$$

$$\eta_{1,2,3,4} = .5$$

Gain = 4.87

DSF 3





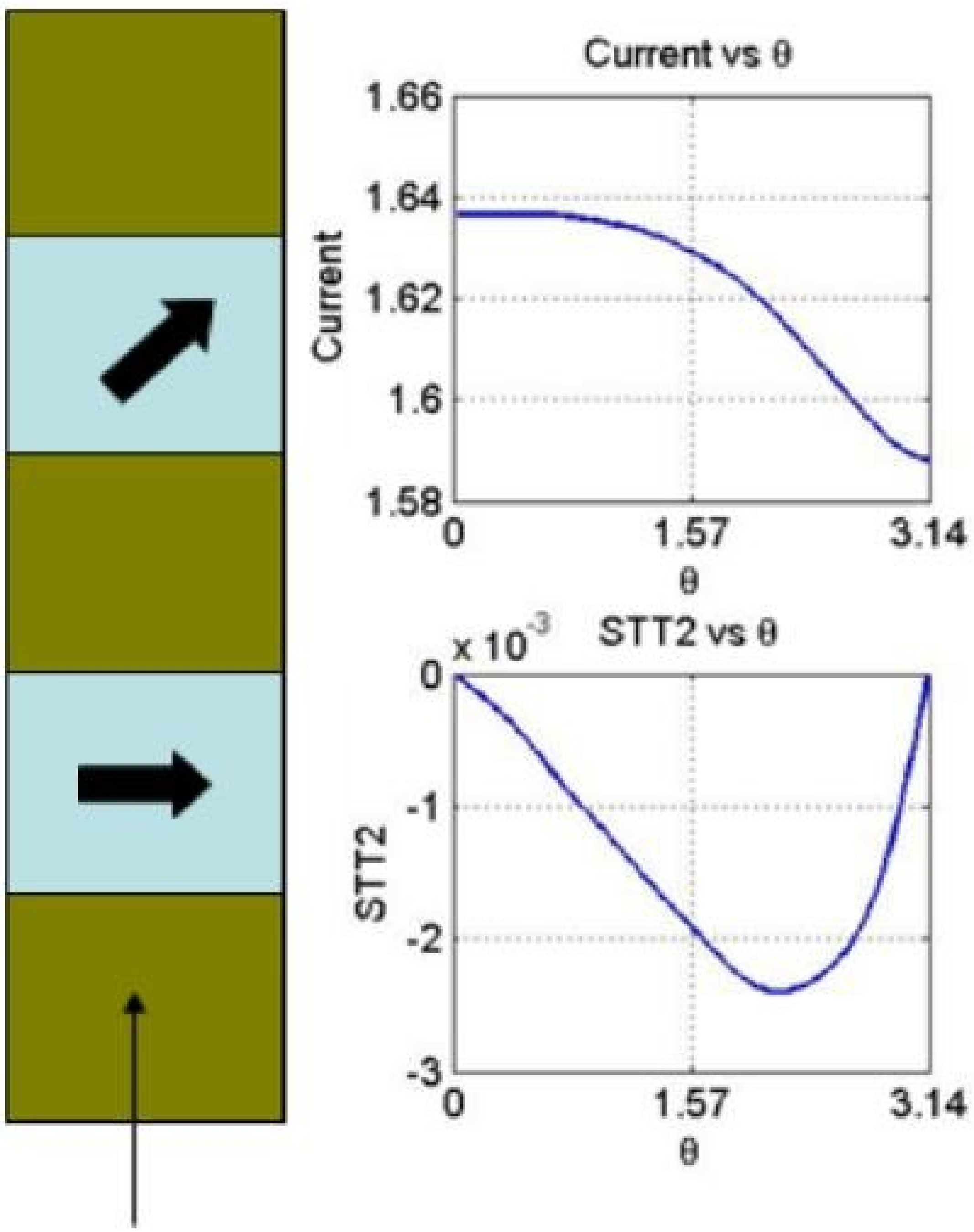
$$G_{2,3} = 14 = 10 \times G_4 = 2 \times G_1$$

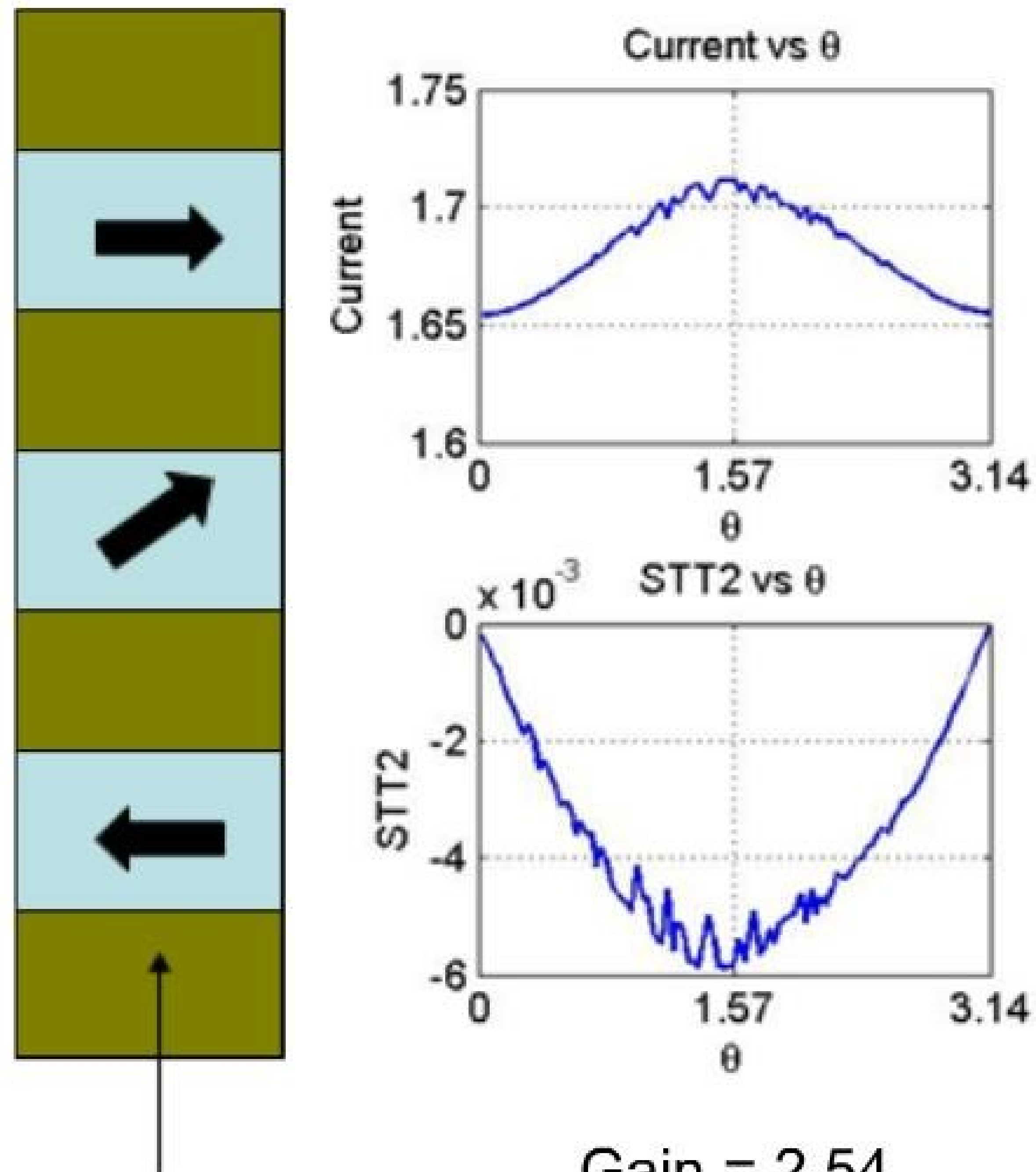
$$p_{1,2,3,4} = .4$$

$$\eta_{1,2,3,4} = .5$$

Gain = 4.34

2-d toy model (ballistic)





Gain = 2.54

Efficiency enhancement ideas:

- From circuit theory and toy ballistic models, the DSF idea should work. How well it works is not clear.
- An uneven distribution of interface resistances may improve efficiency.
- The parameters G in circuit theory can be found from 1stprinciples, and with our code □ guide to material choices.

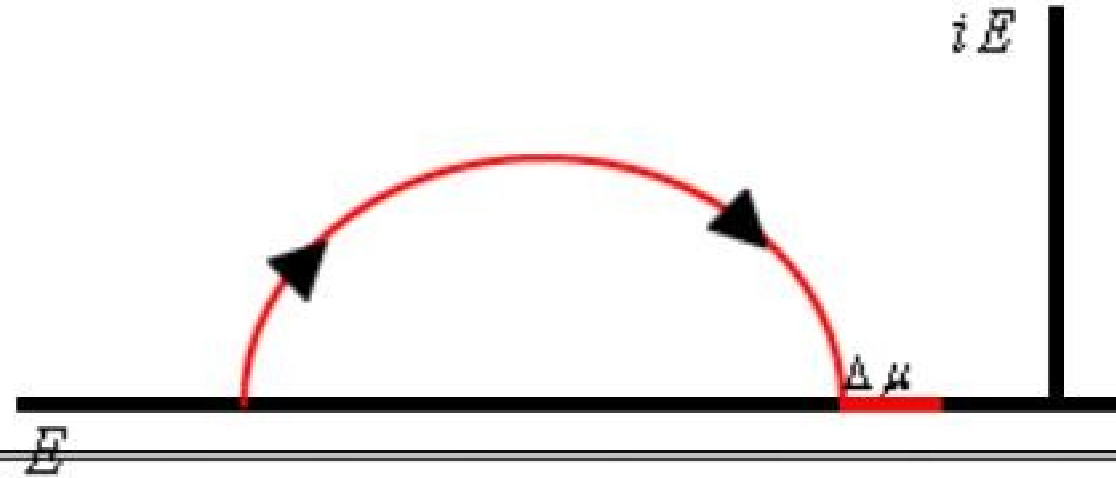
Breakdown of circuit theory

- Theory assumes V=IR – not true for MgO.
- Theory assumes short spin coherence length. For small moment materials, may not be true.
- Spin transfer currently understood mostly on a circuit theory, toy model level – our tool can extend that understanding the same way GMR understanding has been extended.

Systems to calculate with full machinery:

- Fe-MgO single barrier spin transfer □ (recent experiments show efficiency is constant over bias, even though TMR is not).
- DSF with MgO.
- Calculate spin torque parameters of circuit theory, and compare to ballistic result.

Computational stuff



$$\boxed{G^{<} = \int dE\left[f(E-\mu_1)A_1(\hat{\rho}) + f(E-\mu_2)A_2(\hat{\rho})\right]}\ .$$

Software technology used:

Parallel, Portable — MPI-2

Simple, Flexible, Powerful — MATLAB 7

Object-oriented, Fast — JAVA

Calculation done in parallel: