spintec
SPIN IN ELECTRONICS

Theory of spin transport phenomena in magnetic tunnel junctions

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Spintronics

Conventional spintronics

Spin-orbit phenomena -> Spin orbitronics

- GMR & TMR
- Interlayer Exchange (IEC)
- Spin Filtering (SF)
- Spin Transfer Torques (STT)
- Magneto crystalline anisotropy
- Spin Hall Effect (SHE)
- Rashba Effect
- Dzyaloshinskii-Moriya (DMI)
- Spin-orbit Torques (SOT)

…

Spin valves

Single & double barrier MTJs

AFM metals

AFM insulators

Frustrated magnets

Interfaces

Rutiles

Heusler alloys

perovskites

Ferrites ($CoFe_2O_4$)

Garnets ($Y_3Fe_5O_{12}$)

Domain walls

Graphene

Alloys (BiCu, IrCu…)

Layered structures (Pt/Co/AlOx, Ta/CoFe/MgO

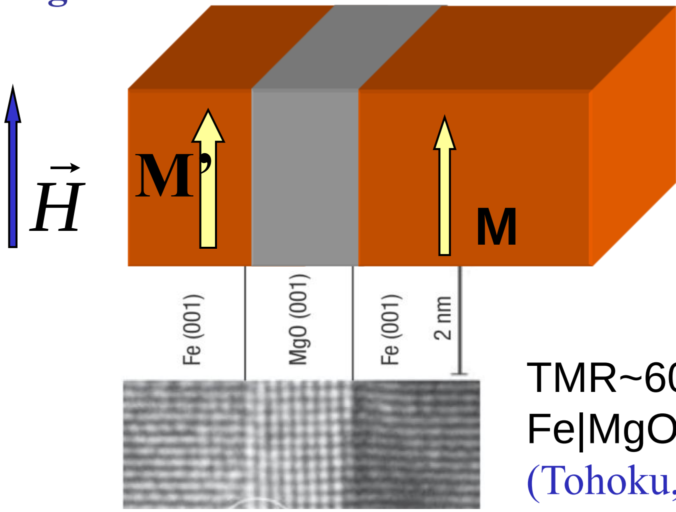
…

This lecture:

- Tunnel magnetoresistance (TMR)
- Spin transfer torques (STT)
  - Quantum origin of spin transfer torque
  - Description of spin currents and spin transfer torques
    - Free electron model
    - Tight-binding model
  - Voltage dependence of STT
    - symmetric MTJs
    - asymmetric MTJs
- Interlayer exchange coupling
- …

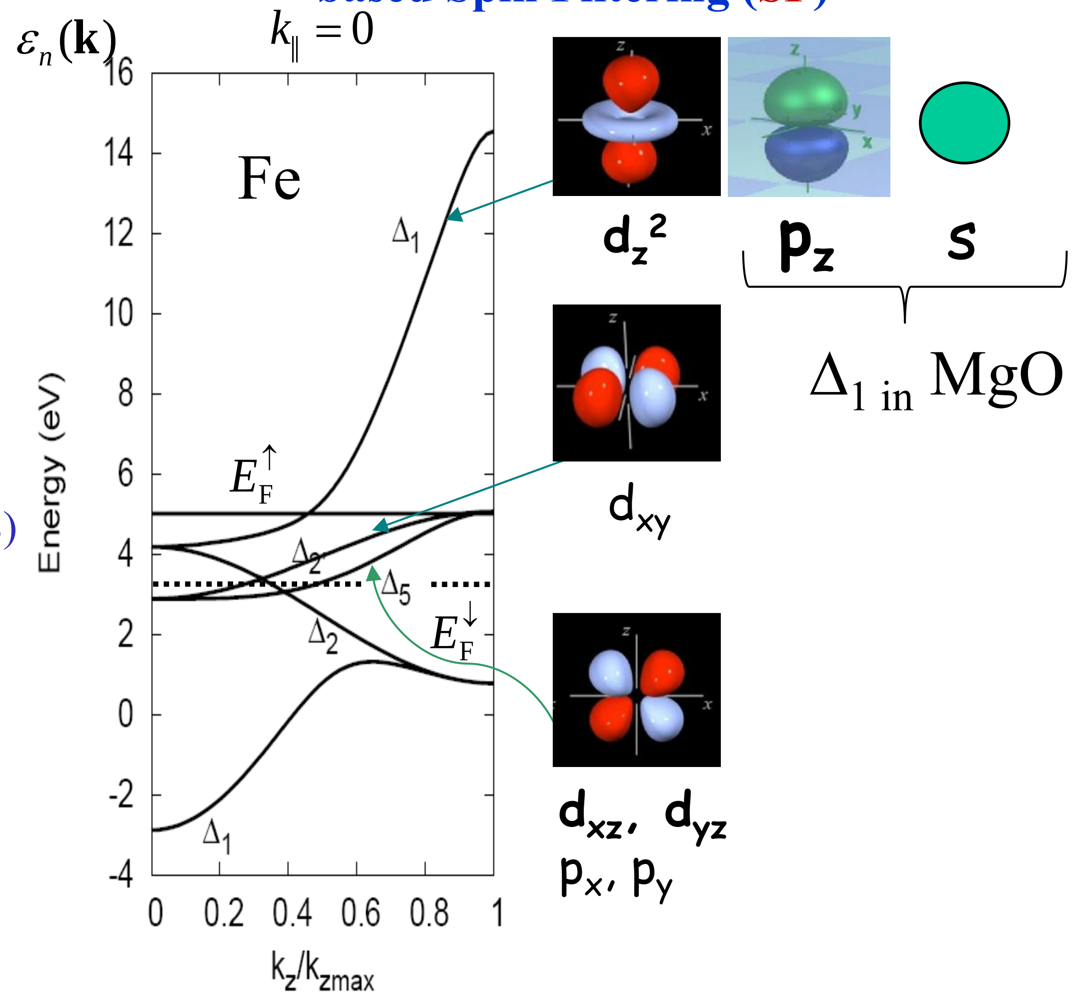
Spintronics

Tunnel (TMR) magnetoresistance:
magnetization acts on current



TMR~600%
Fe|MgO|Fe
(Tohoku,2008)

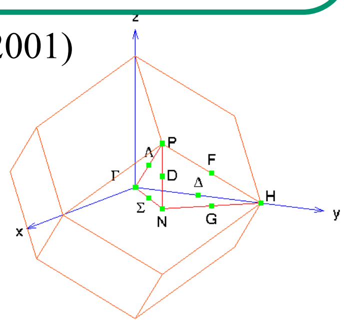
Bloch state symmetry based Spin Filtering (SF)

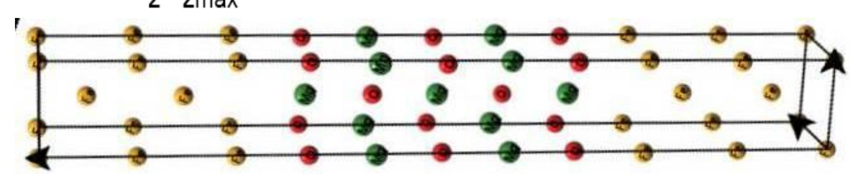


Huge TMR in crystalline MTJ if:
- Good epitaxial fit between FM and I(SC)
- Evanescent states in I(SC) with the same Bloch state symmetry
- High symmetry Bloch state (Δ_1) for one of two e^- spin states in FM electrodes ("**half-metallic**"-like)

W. H. Butler et al, PRB (2001)

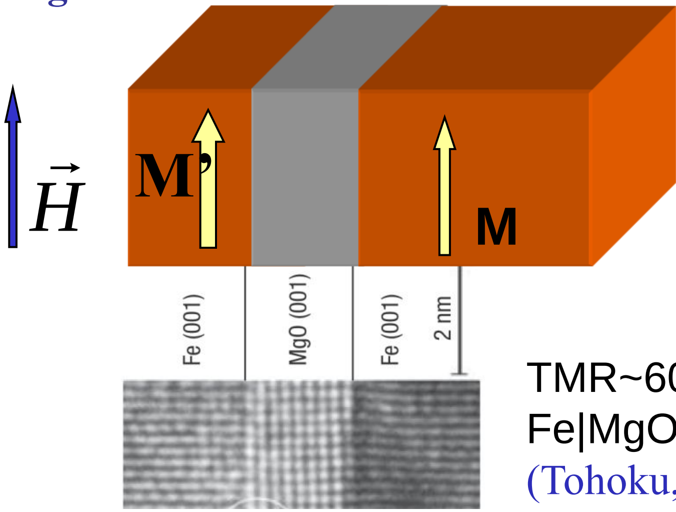
The 1st Brillouin zone with high symmetry k-points





Spintronics

Tunnel (TMR) magnetoresistance:
magnetization acts on current



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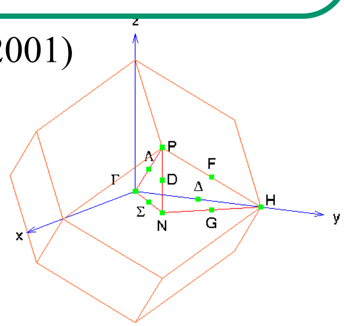
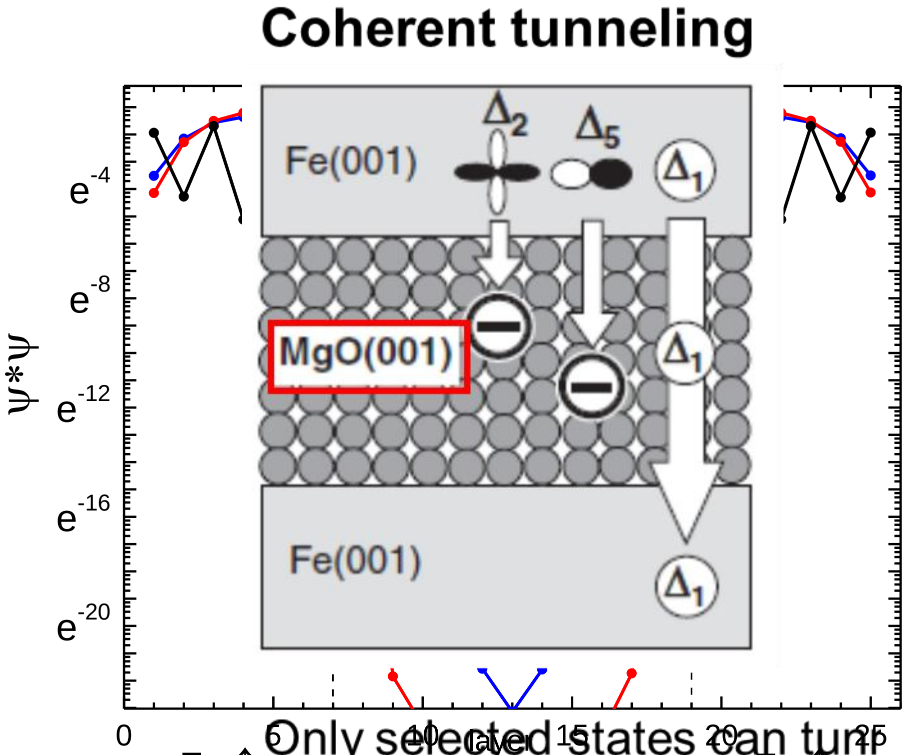
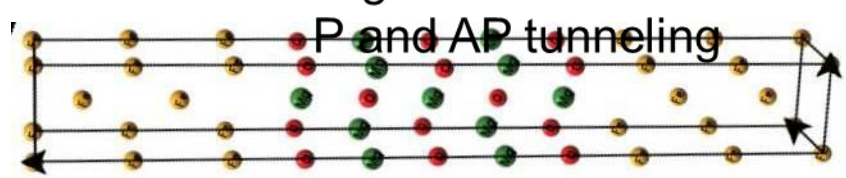


Bloch state symmetry based Spin Filtering (SF)

W. H. Butler et al, PRB (2001)
IEEE Trans. Mag., **41** (2005) 2645
Sci. Technol. Adv. Mater. 9 (2008) 014106

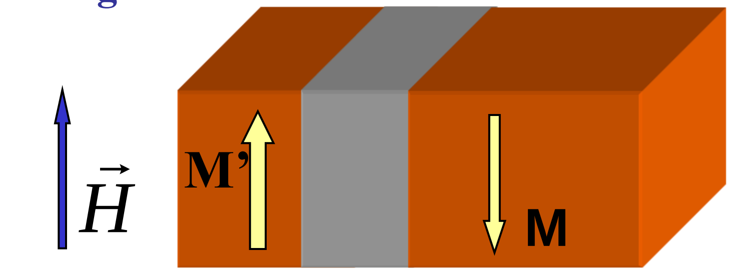


Only selected states can turn
→ Stronger contraste between P and AP tunneling

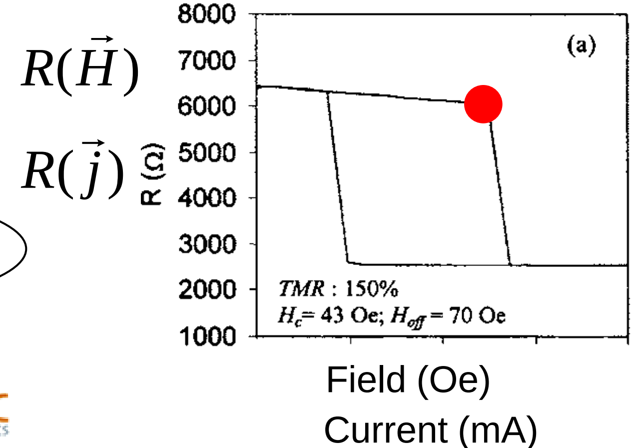


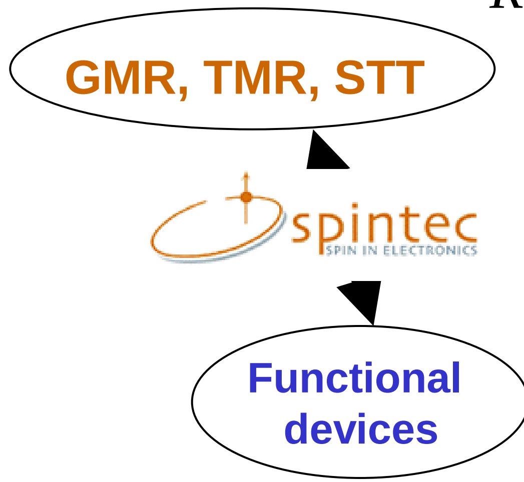
Spintronics

Tunnel (TMR) magnetoresistance:
magnetization acts on current

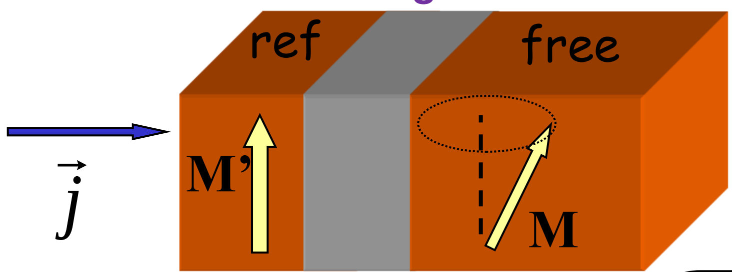


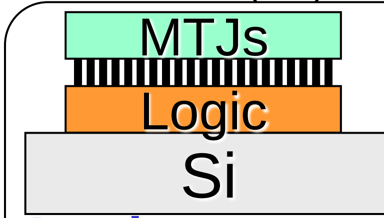
$$\mathrm{TMR} = \frac{R_{AP} - R_P}{R_P}$$



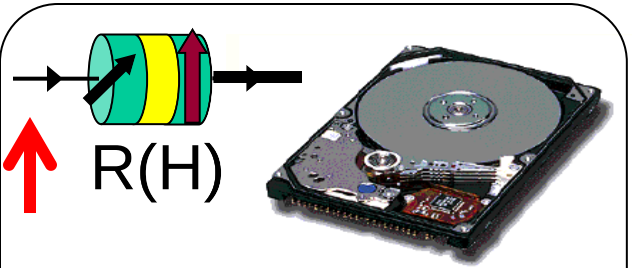


Spin Transfer Torque (STT):
current acts on magnetization

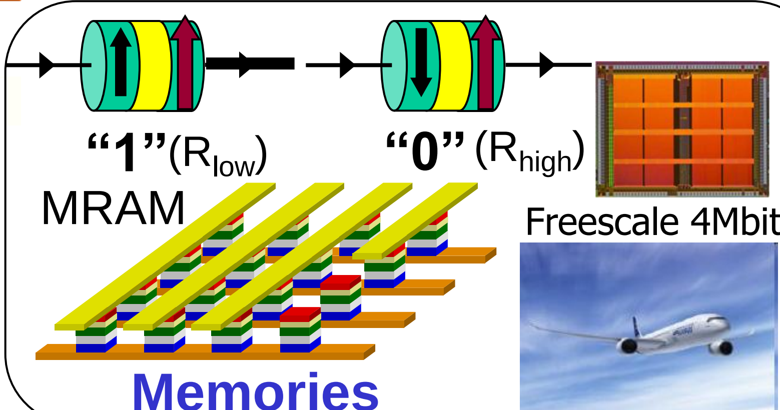




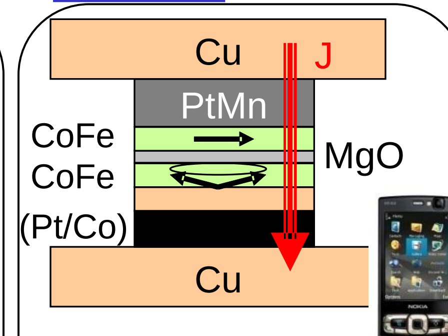
Logics



Sensors



Memories



RF components

Spintronics

Quantum transport theory and electronic structure of materials for spintronics

Giant magnetoresistance (GMR)
metallic nanostructures

Tunnel magnetoresistance (TMR)
amorphous and crystalline, single and double barrier tunnel junctions

Spin transfer torque (STT), exchange coupling (IEC), anisotropy
amorphous and crystalline tunnel junctions

Spin filtering
crystalline magnetic tunnel junctions

Materials for spintronics
chalcogenides, rutiles, spinels, Heusler alloys, Graphene, frustrated magnets

Spin Hall Effect (SHE)
alloys

Boltzmann approach (drift-diffusion)

Kubo formalism
Free electron model

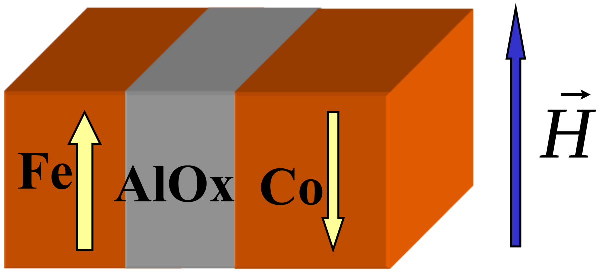
Keldysh formalism
Tight-binding model

Ab-initio (DFT)

Calculation techniques

Condensed Matter Theory + Computational Materials Science

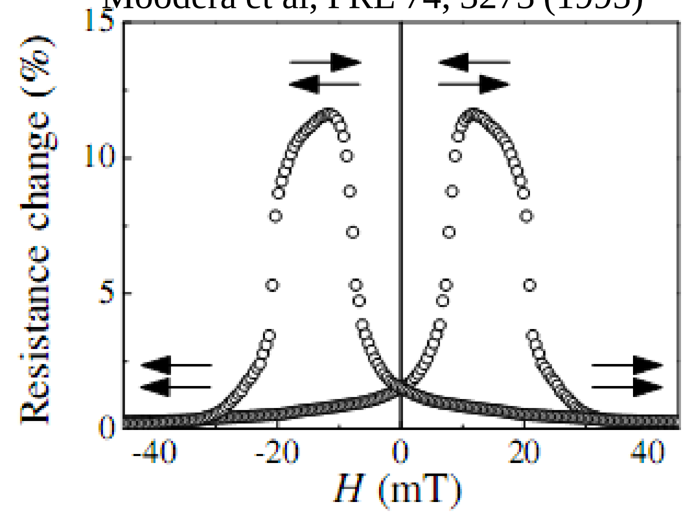
Julliere 1975 -> Moodera 1995



Different coercive fields For Co, Fe

Miyazaki

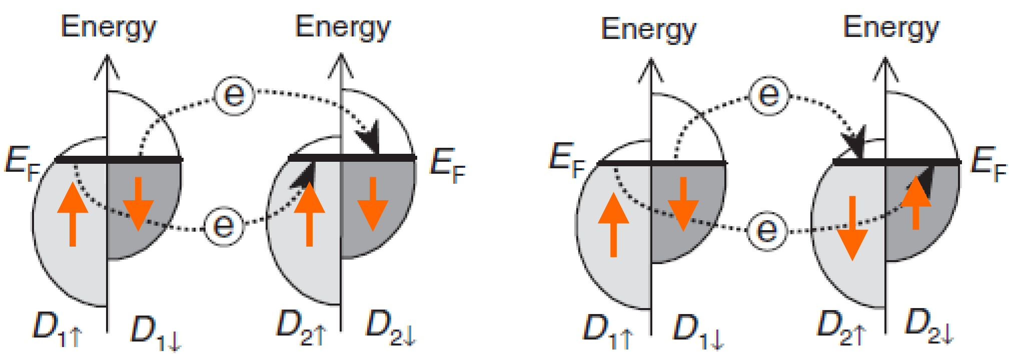
Moodera et al, PRL 74, 3273 (1995)



300K ΔR/R~ 15% → P+0.26

Parallel configuration

Antiparallel configuration



$$J^{parallel} \propto D_L^{\uparrow} D_R^{\uparrow} + D_L^{\downarrow} D_R^{\downarrow}$$

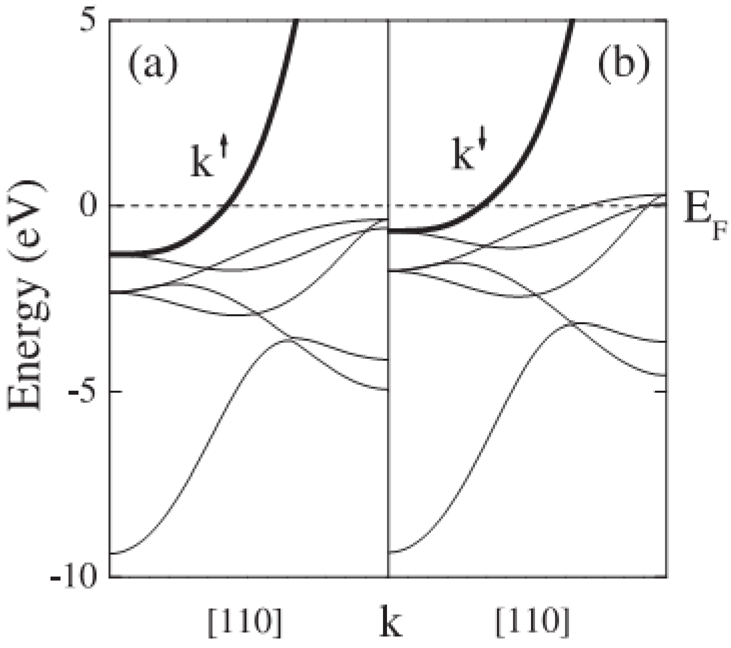
$$J^{antiparallel} \propto D_L^{\uparrow} D_R^{\downarrow} + D_L^{\downarrow} D_R^{\uparrow}$$

$$P_{L(R)} = \frac{D^{\uparrow}_{L(R)}(E_F) - D^{\downarrow}_{L(R)}(E_F)}{D^{\uparrow}_{L(R)}(E_F) + D^{\downarrow}_{L(R)}(E_F)}$$

$$TMR = \frac{\Delta R}{R_P} = \frac{2\,P_L\,P_R}{1 - P_L\,P_R}$$

P>0 (~50%) in Fe, Co → ΔR/R~40 - 70% with alumina barriers at low T

Stearns' polarization



$$P_{L(R)} = \frac{D^{\uparrow}_{L(R)}(E_F) - D^{\downarrow}_{L(R)}(E_F)}{D^{\uparrow}_{L(R)}(E_F) + D^{\downarrow}_{L(R)}(E_F)}$$

Julliere's model is insufficient!

$$P_{L(R)} = \frac{k^{\uparrow}_{L(R)} - k^{\downarrow}_{L(R)}}{k^{\uparrow}_{L(R)} + k^{\downarrow}_{L(R)})}$$

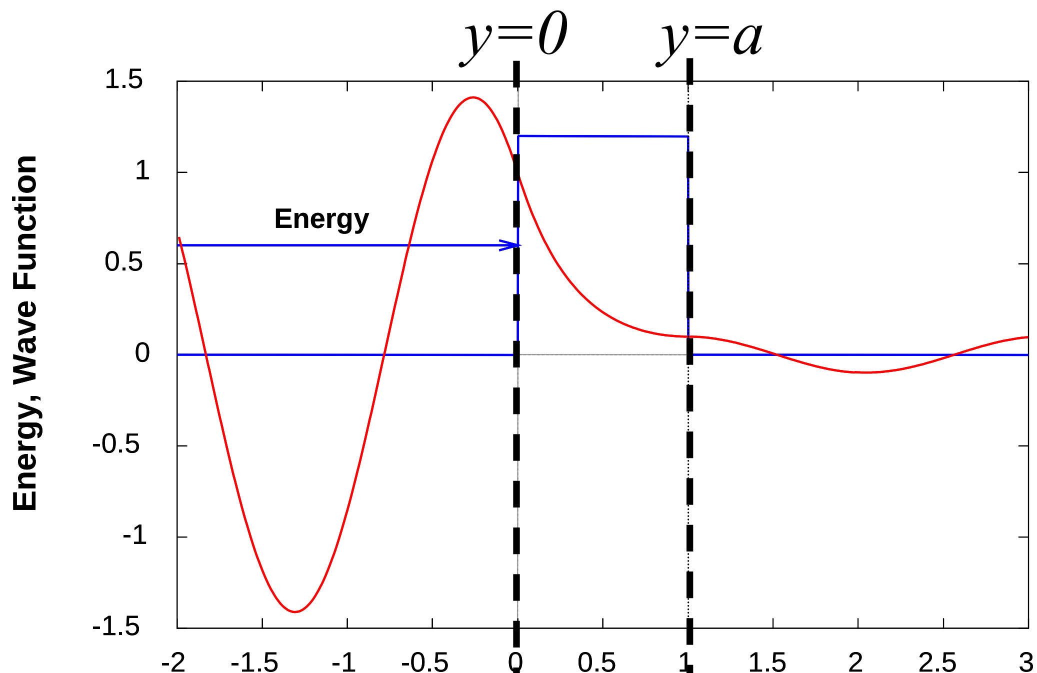
Not overall density of states important but specific bands at the Fermi level and their properties

→ Stearns first explanation in this way

M. B. Stearns, JMMM 5, 1062 (1977)

Free electron model for tunneling (no spin)

Matching Boundary Conditions (4 linear equations with 4 unknowns) allows the solution for the transmission probability.



E_F at equal potential

$$|\psi\rangle \propto \quad e^{ik_L y} + re^{-ik_L y} \qquad \mathbf{y} \qquad te^{ik_R y}$$

t transmission amplitude

$$Ae^{-\kappa_0 y} + Be^{\kappa_0 y}$$

Boundary conditions :
continuity of $|\Psi>$ and its derivative

Free electron model for tunneling (no spin)

Transmission probability : T=|t|²

$$T = \frac{8\kappa_0^2 k_1 k_2}{(k_L^2+\kappa_0^2)(k_R^2+\kappa_0^2)\cosh(2\kappa_0 a) + 4\kappa_0^2 k_L k_R - (k_L^2-\kappa_0^2)(k_R^2-\kappa_0^2)}$$

When system is thick enough that $e^{2\kappa_0 a} >> 1$:

$$T = \frac{16\kappa_0^2 k_L k_R e^{-2\kappa_0 a}}{(k_L^2+\kappa_0^2)(k_R^2+\kappa_0^2)}$$

- Depends on barrier thickness + height
- $k=k_F$
- Given by transmission probabilities L, R

Note that this can be written as :

$$T = \frac{4\kappa_0 k_L}{(k_L^2+\kappa_0^2)} \frac{4\kappa_0 k_R}{(k_R^2+\kappa_0^2)} e^{-2\kappa_0 a} = T_L T_R e^{-2\kappa_0 a} \quad = T(k_{//})$$

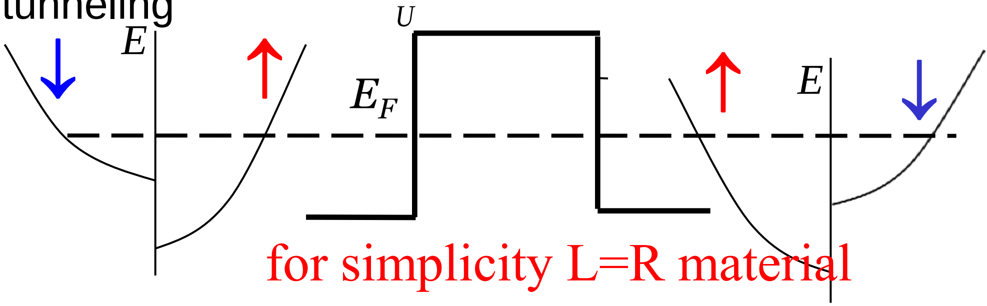
$$G = \frac{I}{V} = \frac{e^2}{h} \sum_{\mathbf{k}_\parallel} \left[T(\mathbf{k}_\parallel) \right]_{E_F}$$

Landauer Formula for Conductance

Slonczewski model for tunneling (with spin)

Slonczewski (1989) Delocalized electrons contribute most to the current *(sp* states*)*
Localized states don't (*d* states) → free electron tunneling

$$T^{\sigma\sigma'} = \frac{16\kappa_0^2 k_\sigma k_{\sigma'} e^{-2\kappa_0 a}}{(k_\sigma^2+\kappa_0^2)(k_{\sigma'}^2+\kappa_0^2)}$$



Spin ↑ and spin ↓ channels conduct in parallel (two current model):

$$G_{Parallel} = G^{\uparrow\uparrow} + G^{\downarrow\downarrow} \quad \text{and} \quad G_{Antiparallel} = G^{\uparrow\downarrow} + G^{\downarrow\uparrow}$$

$$G_{Parallel} - G_{antiparallel} \propto 16\kappa_0^2 e^{-2\kappa_0 a}\left[\frac{(k_\uparrow - k_\downarrow)(\kappa_0^2 - k_\uparrow k_\downarrow)}{(\kappa_0^2 + k_\uparrow^2)(\kappa_0^2 + k_\downarrow^2)}\right]^2$$

Tunnel magnetoresistance

$$\frac{\Delta G}{G_{Parallel}} \propto \frac{G_{Parallel} - G_{antiparallel}}{G_{parallel}} = \frac{2P^2}{1+P^2}$$

Slonczewski Polarisation

$$P = \left(\frac{k_{F\uparrow} - k_{F\downarrow}}{k_{F\uparrow} + k_{F\downarrow}}\right)\left(\frac{\kappa_0^2 - k_{F\uparrow}k_{F\downarrow}}{\kappa_0^2 + k_{F\uparrow}k_{F\downarrow}}\right)$$

- Depends on properties of FM and barrier!
- Bandstructure details are important!

Slonczewski model for tunneling (with spin)

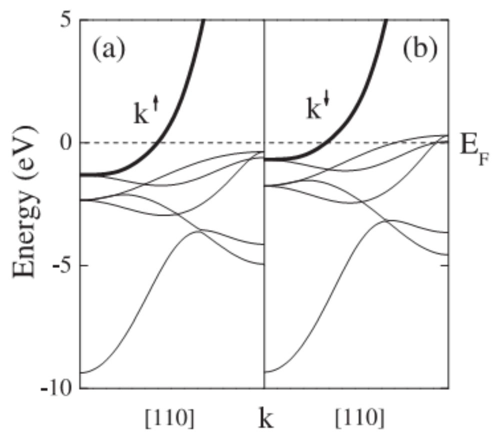
$$P = \left(\frac{k_{F\uparrow} - k_{F\downarrow}}{k_{F\uparrow} + k_{F\downarrow}}\right)\left(\frac{\kappa_0^2 - k_{F\uparrow}k_{F\downarrow}}{\kappa_0^2 + k_{F\uparrow}k_{F\downarrow}}\right) \qquad \kappa_0 = \pm\sqrt{\frac{2m(U-E)}{\hbar^2} + k_{\parallel}^2}$$

In Julliere's model, only the polarization within the magnetic electrodes influences the TMR. In Slonczewski's model, the barrier height also plays a role.

Case of high barrier: $\kappa >> k_{F\uparrow}, k_{F\downarrow}$

$$P \approx \frac{k_{F\uparrow} - k_{F\downarrow}}{k_{F\uparrow} + k_{F\downarrow}} > 0$$

Electrons with highest velocity give strongest contribution to tunneling



Free electrons: $DOS(E) = \frac{mk}{\hbar^2\pi^2} \propto k$

$$P \approx \frac{D_\uparrow - D_\downarrow}{D_\uparrow + D_\downarrow}$$

Back to Julliere formula
With P defined via DOS

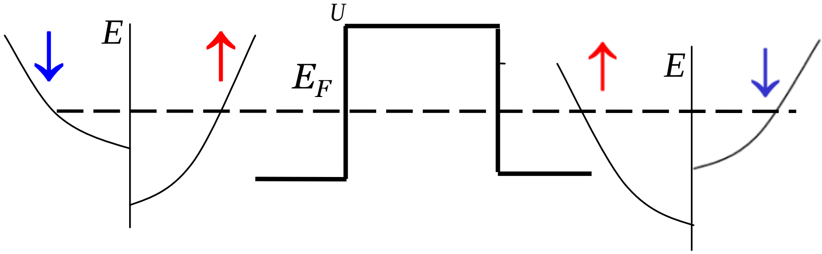
$$\frac{\Delta R}{R_{Antiparallel}} = \frac{\Delta G}{G_{Parallel}} = \frac{2P^2}{1+P^2}$$

Generalized model for tunneling (with spin)

Generalization: Write TMR in terms of the transmission probability

$$T^{\sigma\sigma'} = \frac{16\kappa_0^2 k_\sigma k_{\sigma'} e^{-2\kappa_0 a}}{(k_\sigma^2+\kappa_0^2)(k_{\sigma'}^2+\kappa_0^2)} = T_L^\sigma T_R^{\sigma'} e^{-2\kappa_0 a}$$

$$T_L^\sigma = \frac{4\kappa_0 k_{L\sigma}}{(k_{L\sigma}^2+\kappa_0^2)}; \quad T_R^\sigma = \frac{4\kappa_0 k_{R\sigma'}}{(k_{R\sigma}^2+\kappa_0^2)}$$



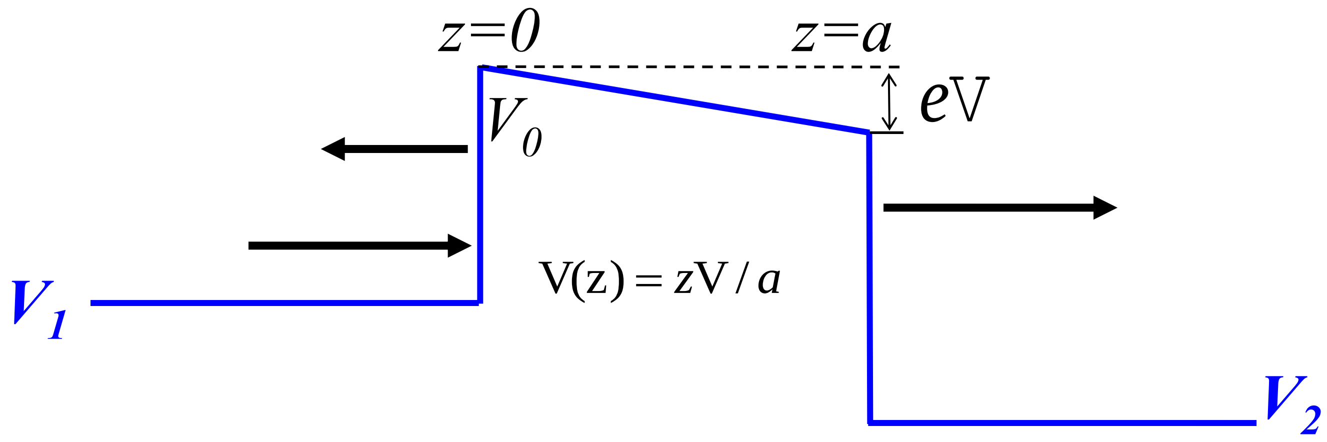
$$\mathrm{TMR} = \frac{T^P - T^{AP}}{T^{AP}} = \frac{\left(T^{\uparrow\uparrow}+T^{\downarrow\downarrow}\right)-\left(T^{\uparrow\downarrow}+T^{\downarrow\uparrow}\right)}{\left(T^{\uparrow\downarrow}+T^{\downarrow\uparrow}\right)} = \frac{\left(T_L^\uparrow T_R^\uparrow + T_L^\downarrow T_R^\downarrow\right)-\left(T_L^\uparrow T_R^\downarrow + T_L^\downarrow T_R^\uparrow\right)}{\left(T_L^\uparrow T_R^\downarrow + T_L^\downarrow T_R^\uparrow\right)}$$

$$\mathrm{TMR} = \frac{2P_L P_R}{1-P_L P_R} \quad \text{where} \quad P_L = \frac{T_L^\uparrow - T_L^\downarrow}{T_L^\uparrow + T_L^\downarrow} \quad P_R = \frac{T_R^\uparrow - T_R^\downarrow}{T_R^\uparrow + T_R^\downarrow}$$

Jullière model

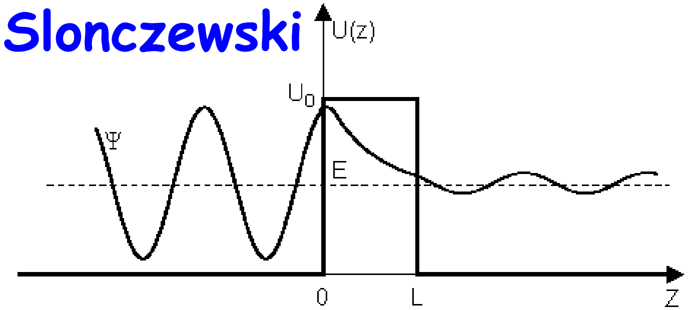
Provides defintion that can be generalized to complex bandstructures

Voltage dependence of tunnel current



Voltage dependence of tunnel current

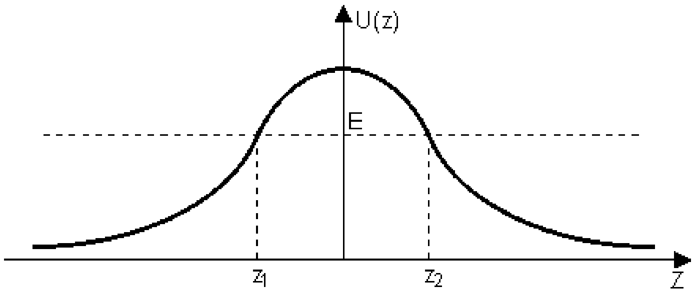
Slonczewski



When system is thick enough that $e^{2\kappa_0 L} >> 1$:

$$T = \frac{16\kappa_0^2 k_1 k_2 e^{-2\kappa_0 L}}{(k_1^2+\kappa_0^2)(k_2^2+\kappa_0^2)} = D_0 \exp\left[-\frac{2L}{\hbar}\sqrt{U_0 - E}\right]$$

But what if the barrier is not rectangular???



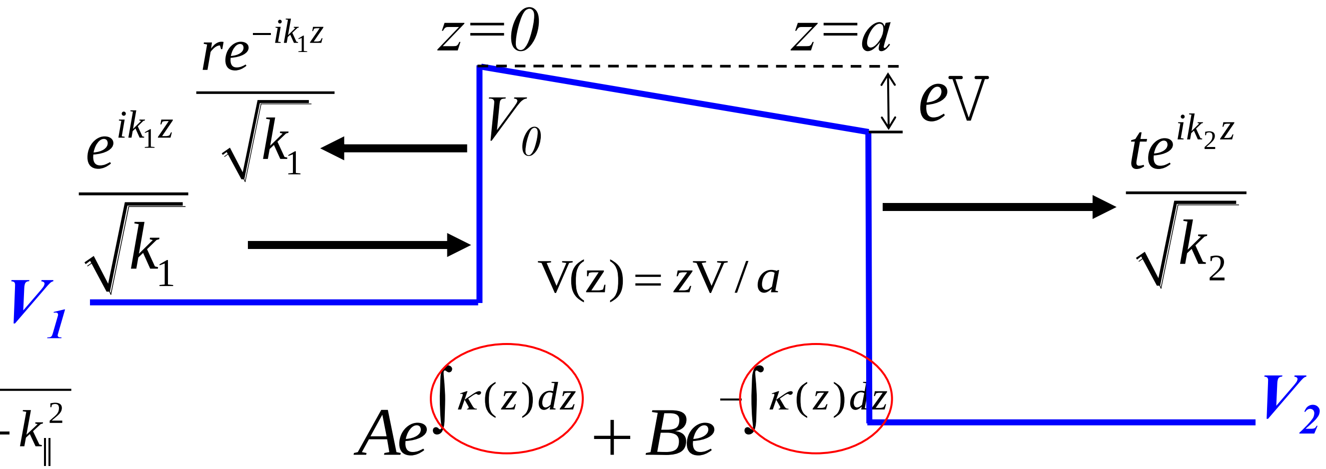
We use WKB approximation :

$$T = D_0 \exp\left[-\frac{2}{\hbar}\int_{z_1}^{z_2} dz\sqrt{U(z)-E}\right]$$

- de Broglie wavelength $\lambda = \hbar / p_z$ is much smaller than (z_2-z_1)
- U(z) should vary slowly over (z_2-z_1)

→ Simmons model based on WKB is usually used to estimate potential barrier height and width

Voltage dependence tunnel current



$$k_1 = \sqrt{k_{1E}^2 - k_\parallel^2}$$

$$k_{1E} = \sqrt{\frac{2m}{\hbar^2}(E - V_1)}$$

$$\kappa(z) = \sqrt{\kappa_0^2 + k_\parallel^2 - \frac{2m}{\hbar^2} e\mathrm{V}(z)}$$

$$\kappa_0 = \sqrt{\frac{2m}{\hbar^2}(V_0 - E)}$$

$$k_2 = \sqrt{k_{2E}^2 - k_\parallel^2 + \frac{2m}{\hbar^2} e\mathrm{V}}$$

$$k_{2E} = \sqrt{\frac{2m}{\hbar^2}(E - V_2)}$$

voltage dependence appears

Current density: $$j = \frac{e}{2\pi h}\int dE\left[f(E) - f(E + e\mathrm{V})\right]\int T(E, \mathrm{V}, k_\parallel) k_\parallel dk_\parallel$$ → **I(V)**

$$T(E, \mathrm{V}, k_\parallel) = \frac{8k_1 k_2 \kappa(0)\kappa(a)}{\left[\kappa^2(0) + k_1^2\right]\left[\kappa^2(a) + k_2^2\right]\cosh\left(2\int_0^a \kappa(z)dz\right) + 4k_1 k_2 \kappa(0)\kappa(a) - \left[\kappa^2(0) - k_1^2\right]\left[\kappa^2(a) - k_2^2\right]}$$

Voltage dependence of TMR and tunnel current

Current density: $$j = \frac{e}{2\pi h}\int dE\,[\underbrace{f(E) - f(E+eV)}]\int T(E, V, k_\parallel)k_\parallel dk_\parallel$$ → **I(V)**

Fermi Dirac, gives window ~V

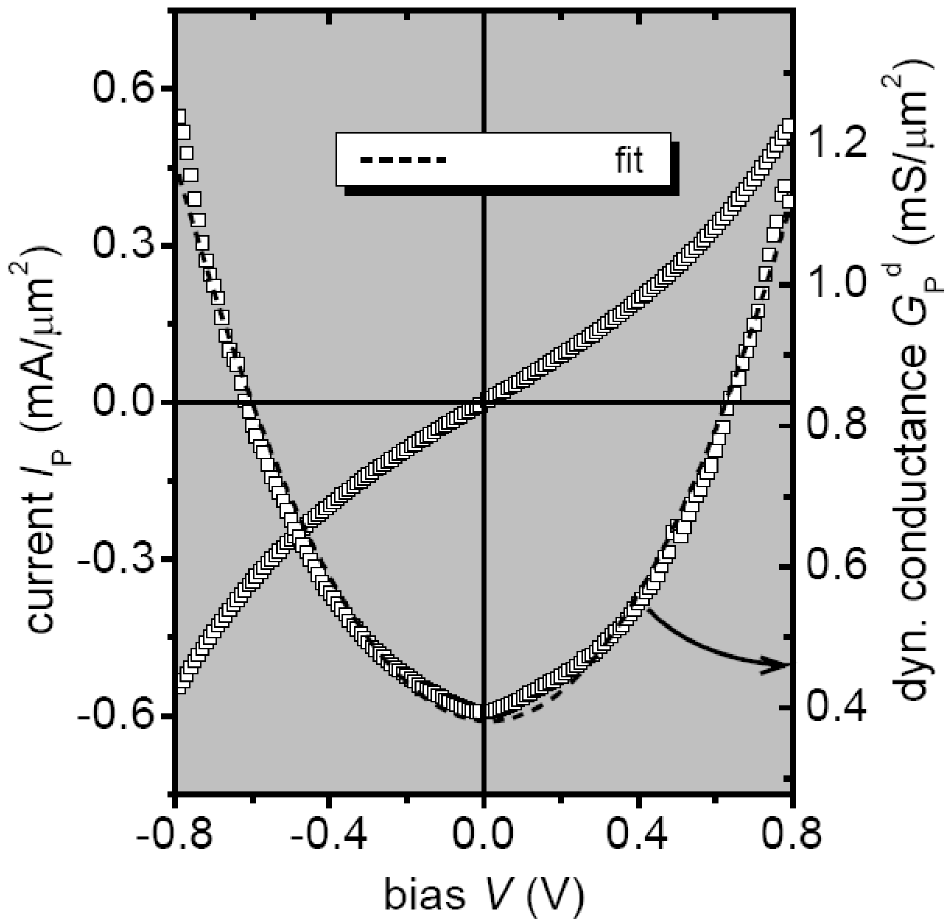
I/V=G = conductance =Integral of T

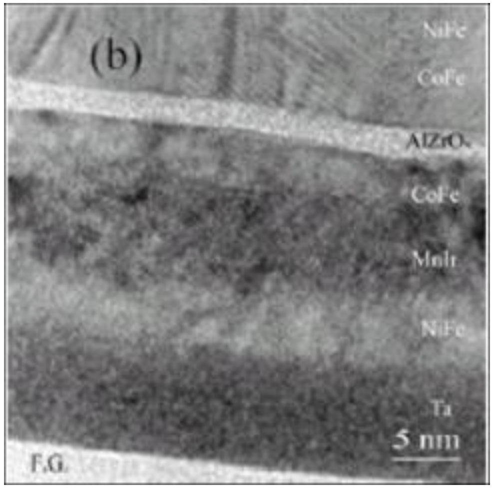
Note

1) increase of G with V since more states available for tunneling
2) For symmetric barriers $G \sim V^2$
3) For asymmetric barrier only $G \sim V + const * V^2$

Voltage dependence of TMR and tunnel current

Exemple of experimental I(V) characteristics in Co|AlOx|Co tunnel junction





Barrier height: φ=1.04 eV

Barrier asymmetry: $\Delta\varphi$=0.20 eV

Barrier thickness: d=1.6 nm

Effective mass: m_{eff}/m_e= α=0.4

Dynamic conductance=dI/dV

T. Dimopoulos et al

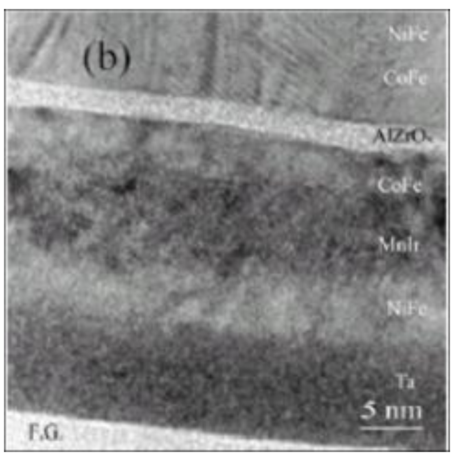
See lectures of C. Tiusan and S. Valenzuela for epitaxial Fe|MgO MTJs

Pros/Cons of Julliere/Slonczewski Models

• AlOx tunnel barriers are amorphous.
• In amorphous materials, all electronic effects related to crystal symmetry are smeared out.
• Evanescent waves in alumina have “free like” character.
• Free electron models work OK in this case.
• However, they fail with crystalline barriers. Additional band structures effect in the electrodes and barrier must be taken into account (Bloch state symmetry based spin filtering).

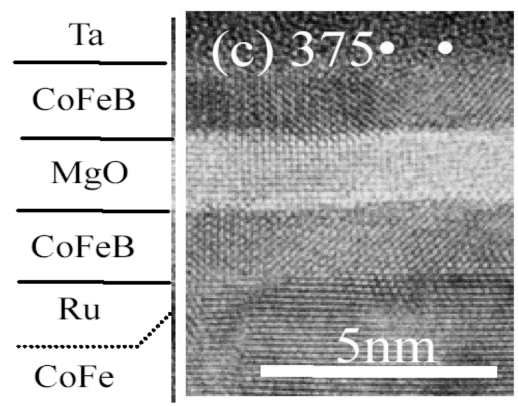
1995-2005 AlOx barriers

>2005 MgO barriers



Best MR~80%

Best MR~600%



See lectures of C. Tiusan, S. Valenzuela for cristalline Fe|MgO MTJs

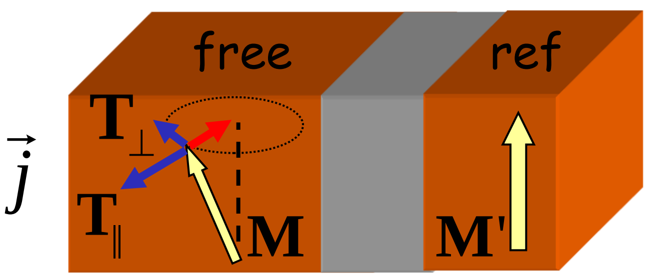
This lecture:

- Tunnel magnetoresistance (TMR)
- Spin transfer torques (STT)
  - Landau Lifshitz equation (LLG)
  - Quantum origin of spin transfer torque
  - Description of spin currents and spin transfer torques
    - Free electron model
    - Tight-binding model
  - Voltage dependence of STT
    - symmetric MTJs
    - asymmetric MTJs
- Interlayer exchange coupling
- ...

$P \rightarrow AP$ $\qquad\qquad$ $AP \rightarrow P$

- **exchange of angular momentum between conduction and localized electrons**
- **conservation of total angular momentum**

Spin Transfer Torque (STT): current acts on magnetization



Prediction:
J. Slonczewski (1996)
L. Berger (1996)

First observations:
M. Tsoi et al, PRL 80, 4281 (1998)
J. Katine et al, PRL 84, 3149 (2000)
Y. Huai et al, APL 84, 3118 (2004)
G. Fuchs, et al., APL 85, 1205 (2004)

$T_\perp \sim 0$ for metallic spin valves
S. Zhang, P. M. Levy and A. Fert (2002)
M. D. Stiles and A. Zangwill (2002)

$T_\perp(V) \neq 0$ for MTJs
A. Kalitsov et al, JAP 99, 08G501 (2006)

Landau-Lifshitz-Gilbert-Slonczewski (LLGS) equation:

$$\frac{d\mathbf{M}}{dt} = -\gamma_0 \mathbf{M} \times \mathbf{H} + \frac{\alpha}{M_s} \mathbf{M} \times \frac{d\mathbf{M}}{dt} - \frac{|g_e|\mu_B}{\hbar}\left(T_\parallel \mathbf{M} \times \mathbf{M} \times \mathbf{M}' + T_\perp \mathbf{M}' \times \mathbf{M}\right)$$

precession $\quad$ damping $\quad$ parallel $\quad$ field-like

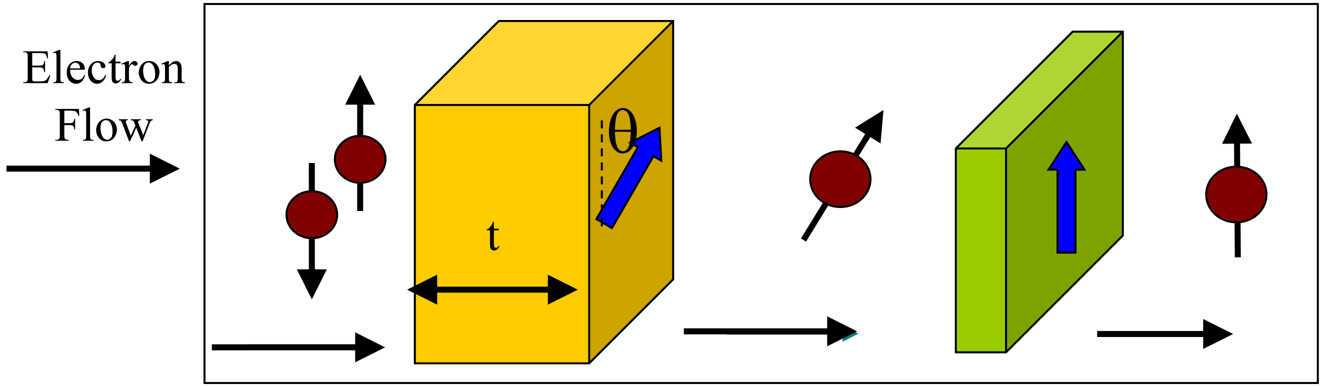
Quantum origin?

J. Slonczewski (1989), R.P. Erickson (1993)

Interlayer Exchange Coupling (IEC) ← $T_\perp^0 + T_\perp^1(V)$

Spin Momentum Transfer - Concept

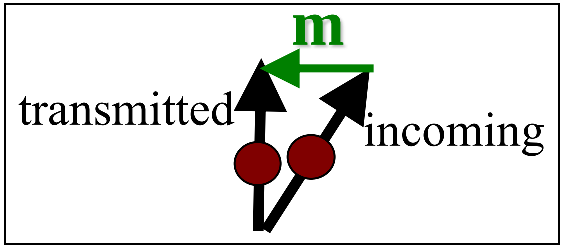
Unpolarized Electrons | **Polarized Electrons** | **Transmitted Electrons**



Local exchange interaction between conduction electron spins and local magnetization **M**

Polarizer P | **Free Layer M**

Conduction Electrons

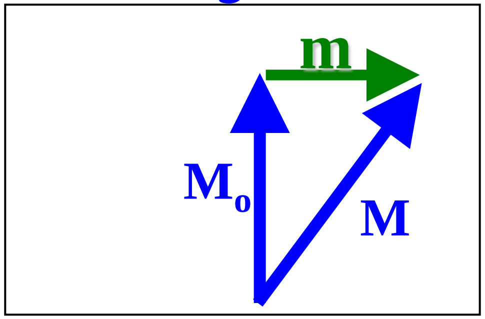


Transfer of spin angular momentum m

=

Spin Torque

Local Magnetization



Flow of angular momentum has a source or sink

Spin Transfer Torque

Continuity equation

Particle transport → Spin transport

current density
particle density
} conserved

spin current density
spin density
} not conserved

↓

Torque

M.D.Stiles and A.Zangwill, PRB 66 (2002) 014407

Particle transport

Spin transport

Particle density:

$$n(\mathbf{r}) = \sum_{i\sigma} \psi^*_{i\sigma}(\mathbf{r})\, \psi_{i\sigma}(\mathbf{r})$$

Current

$$\mathbf{j}(\mathbf{r}) = \mathrm{Re} \sum_{i\sigma} \psi^*_{i\sigma}(\mathbf{r})\, \hat{\mathbf{v}}\, \psi_{i\sigma}(\mathbf{r})$$

where $\hat{\mathbf{v}} = -(i\hbar/m)\nabla$

Continuity equation:

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

Spin density:

$$\mathbf{s}(\mathbf{r}) = \sum_{i\sigma\sigma'} \psi^*_{i\sigma}(\mathbf{r})\, \mathbf{s}_{\sigma,\sigma'}\, \psi_{i\sigma'}(\mathbf{r})$$

Spin current

$$\mathbf{Q}(\mathbf{r}) = \sum_{i\sigma\sigma'} \mathrm{Re}[\psi^*_{i\sigma}(\mathbf{r})\, \mathbf{s}_{\sigma,\sigma'} \otimes \hat{\mathbf{v}}\, \psi_{i\sigma'}(\mathbf{r})]$$

where $\mathbf{s} = (\hbar/2)\boldsymbol{\sigma}$ ← Vector of Pauli matrices

Continuity equation:

$$\nabla \bullet \mathbf{Q} + \frac{\partial \mathbf{s}}{\partial t} \neq 0$$

Spin density:

$$\mathbf{s}(\mathbf{r}) = \sum_{i\sigma\sigma'} \psi^*_{i\sigma}(\mathbf{r})\, \mathbf{s}_{\sigma,\sigma'}\, \psi_{i\sigma'}(\mathbf{r})$$

$$\begin{cases} s_x = \frac{\hbar}{2}\sum_i \left(\psi^*_{i\uparrow}\psi_{i\downarrow} + \psi^*_{i\downarrow}\psi_{i\uparrow}\right) \\ s_y = \frac{\hbar}{2}\sum_i \left(i\psi^*_{i\downarrow}\psi_{i\uparrow} - i\psi^*_{i\uparrow}\psi_{i\downarrow}\right) \\ s_z = \frac{\hbar}{2}\sum_i \left(\psi^*_{i\uparrow}\psi_{i\uparrow} - \psi^*_{i\downarrow}\psi_{i\downarrow}\right) \end{cases}$$

Spin current density:

$$\mathbf{Q}(\mathbf{r}) = \sum_{i\sigma\sigma'} \mathrm{Re}[\psi^*_{i\sigma}(\mathbf{r})\, \mathbf{s}_{\sigma,\sigma'} \otimes \hat{\mathbf{v}}\, \psi_{i\sigma'}(\mathbf{r})]$$

$$\begin{cases} \mathbf{Q}_x = \mathrm{Re}\sum_i \left(\psi^*_{i\uparrow}\hat{\mathbf{v}}\psi_{i\downarrow} + \psi^*_{i\downarrow}\hat{\mathbf{v}}\psi_{i\uparrow}\right) \\ \mathbf{Q}_y = \mathrm{Re}\sum_i \left(i\psi^*_{i\downarrow}\hat{\mathbf{v}}\psi_{i\uparrow} - i\psi^*_{i\uparrow}\hat{\mathbf{v}}\psi_{i\downarrow}\right) \\ \mathbf{Q}_z = \mathrm{Re}\sum_i \left(\psi^*_{i\uparrow}\hat{\mathbf{v}}\psi_{i\uparrow} - \psi^*_{i\downarrow}\hat{\mathbf{v}}\psi_{i\downarrow}\right) \end{cases}$$

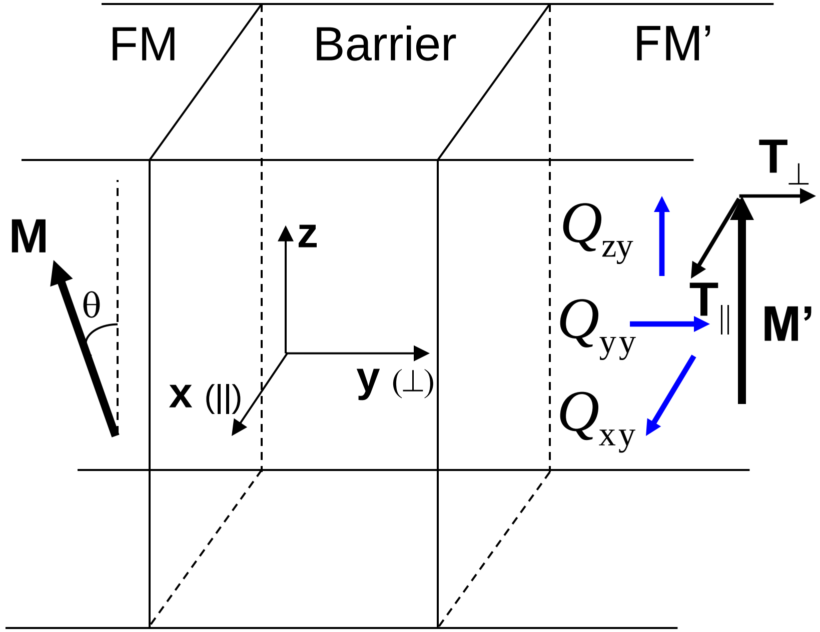
Tensor quantity with elements Q_{ij} with $i=x,y,z$ in spin space and $j=x,y,z$ in real space

$$\nabla \cdot \mathbf{Q} = \partial_k Q_{ik}$$

Current flows in **y** direction

$$\begin{cases} Q_{xy} \neq 0 \\ Q_{yy} \neq 0 \\ Q_{zy} \neq 0 \end{cases}$$

Spin current and spin torque in non-collinear case



Spin current tensor:

$$Q_{ik}$$

i=x, y, z in spin space
k=x, y, z in real space

Spin torque:

$$\mathbf{T} = \nabla \bullet \mathbf{Q} = \partial_k Q_{ik}$$

$$Q_{zy}(\theta) = \frac{\hbar}{2e}\left(J^{\uparrow\uparrow}(\theta) - J^{\downarrow\downarrow}(\theta)\right)$$

$$J(\theta) = \frac{\hbar}{2e}\left(J^{\uparrow\uparrow}(\theta) + J^{\downarrow\downarrow}(\theta)\right)$$

Current flows in **y** direction ⇒

$$Q_{zy} \neq 0$$ conserved

$$Q_{xy} \neq 0, \quad Q_{yy} \neq 0$$ not conserved

⇓

$$T_{x(\|)} \neq 0, \; T_{y(\perp)} \neq 0$$

$T_{x(\|)}$: parallel (Slonczewski)

$T_{y(\perp)}$: perpendicular (field-like)

$$\mathrm{TMR} = \frac{J(0) - J(\pi)}{J(\pi)}$$

- **Current matrix:** $\begin{pmatrix} J^{\uparrow\uparrow} & J^{\uparrow\downarrow} \\ J^{\downarrow\uparrow} & J^{\downarrow\downarrow} \end{pmatrix}$

M. D. Stiles and A.Zangwill, PRB 66 (2002) 014407
A. Manchon et al, JPCM 20 (2008) 145208

Physical origin of Spin transfer torque (sd model)

Consider two populations of electrons:
-1) s conduction electrons (spin-polarized)
-2) d more localized electrons responsible for magnetization

The spin-polarized conduction electrons and localized d electrons interact by exchange interactions

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Hamiltonian of propagating s electrons:

$$H = \frac{p^2}{2m} + U(r) - J_{sd}(\vec{\boldsymbol{\sigma}}.\mathbf{S_d})$$

Kinetic — Potential — Exchange sd

Pauli matrices vector: $\vec{\boldsymbol{\sigma}}$

Unit vector//M: $\mathbf{S_d}$

In non-colinear geometry, exchange of angular momentum takes place between the two populations of electrons but total angular moment is conserved.

$$\boxed{\text{Torque on } \mathbf{S}_d \text{ due to s electrons} = \frac{J_{sd}}{\hbar}\mathbf{S_d} \times \mathbf{s}(r,t)}$$

s=local spin-density of s electrons

A. Manchon et al, JPCM 20 (2008) 145208

Physical origin of Spin transfer (sd model) (cont'd)

Electron wave-function
$$\psi(r,t)\ \begin{cases}\psi^{\uparrow}(r,t)\\ \psi^{\downarrow}(r,t)\end{cases}$$

Local spin density at r and t :
$$\mathbf{s}(r,t)=\psi^{*}(r,t)\frac{\hbar}{2}\vec{\boldsymbol{\sigma}}\psi(r,t)$$

Temporal variation of local spin density:
$$\dot{\mathbf{s}}(r,t)=\frac{\hbar}{2}\left[\dot{\psi}^{*}\vec{\boldsymbol{\sigma}}\psi+\psi^{*}\vec{\boldsymbol{\sigma}}\dot{\psi}\right] \qquad (1)$$

Schrödinger equation :
$$\dot{\psi}(r,t)=-\frac{i}{\hbar}H\psi(r,t) \qquad (2)$$

Substitution (2) in (1) :
$$\dot{\mathbf{s}}(r,t)=\frac{1}{2i}\left[\psi^{*}\vec{\boldsymbol{\sigma}}H\psi+\left(H\psi\right)^{*}\vec{\boldsymbol{\sigma}}\psi\right]$$

$\ldots\Rightarrow$
$$\dot{\mathbf{s}}(r,t)=-\nabla\bullet\mathbf{Q}\left(r,t\right)+\frac{J_{sd}}{\hbar}\mathbf{S_d}\times\mathbf{s}(r,t)$$

$\mathbf{Q}$ is the spin density current
3x3 tensor
Spin space x real space

$$\mathbf{Q}=-\frac{\hbar^{2}}{2m}\mathrm{Im}\left[\psi^{*}(r,t)\vec{\boldsymbol{\sigma}}\otimes\nabla_{\mathbf{r}}\psi\left(r,t\right)\right]$$

A. Manchon et al, JPCM 20 (2008) 145208

Physical origin of Spin transfer (sd model) (cont'd)

In ballistic systems:

$$\mathbf{T} = \nabla \bullet \mathbf{Q}(r,t) = \frac{J_{sd}}{\hbar} \mathbf{S_d} \times \mathbf{s}(r,t)$$

The exchange interaction between spin-polarized s electrons and more localized d electrons is responsible for spin-transfer torque. This interaction yields a precessional motion of spin-density of s electrons around the local magnetization. In ballistic regime, the spin-transfer torque is also equal to the divergence of spin-current.

In diffusive systems:

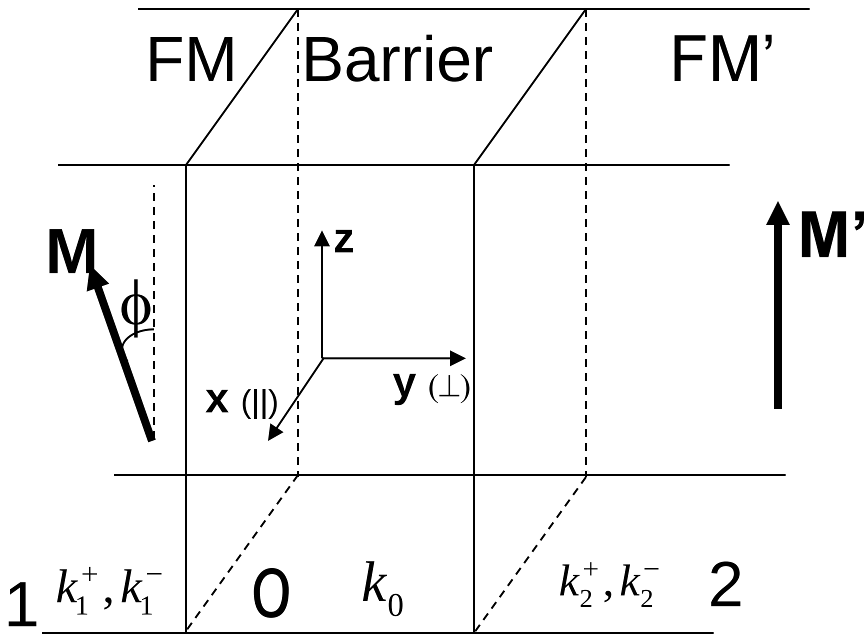
$$\mathbf{T} = \nabla \bullet \mathbf{Q}(r,t) + \frac{\mathbf{s}}{\tau_{SF}} = \frac{J_{sd}}{\hbar} \mathbf{S_d} \times \mathbf{s}(r,t)$$

Takes into account the spin-memory loss by scattering with spin lifetime τ_{SF}

$\mathbf{T}$ can be fully calculated by solving Schrodinger equation in non-colinear geometry

See lectures of G. Bauer, T. Jungwirth, S. Valenzuela for metallic spin valves

Let's derive STT expressions



$\hbar k_1^+ \equiv z-$component of majority spin momentum with $\hat{\mathrm{M}}$ as quantization axis

$\hbar k_1^- \equiv z-$component of minority spin momentum with $\hat{\mathrm{M}}$ as quantization axis

$\hbar k_2^+ \equiv z-$component of majority spin momentum with $\hat{\mathrm{M}}'$ as quantization axis

$\hbar k_2^- \equiv z-$component of minority spin momentum with $\hat{\mathrm{M}}'$ as quantization axis

W.F. in layer 1 (quant. axis || M):

$$\Psi_1 = \begin{pmatrix} e^{ik_1^+ y} + r^{++} e^{-ik_1^+ y} \\ r^{+-} e^{-ik_1^- y} \end{pmatrix}$$

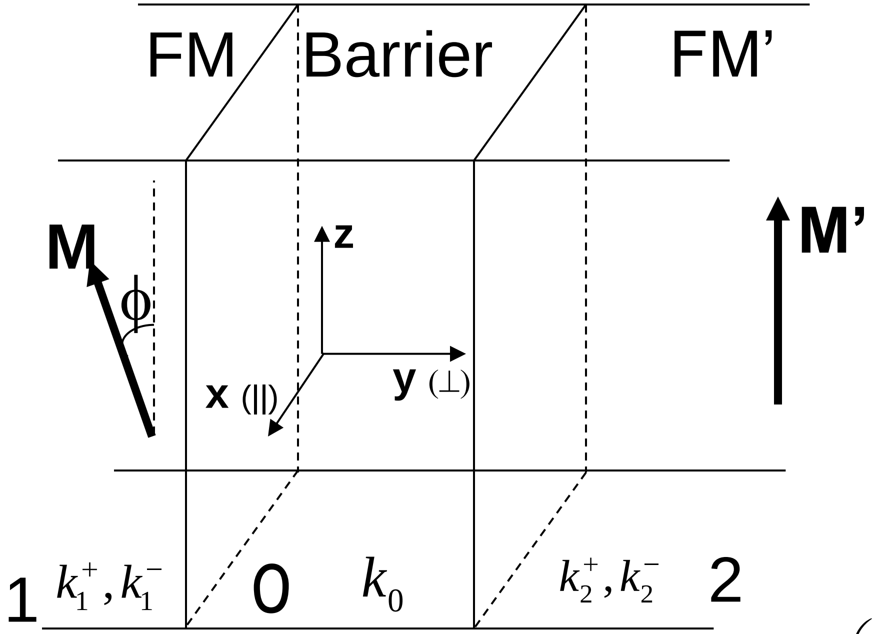
W.F. in layer 2: (quant. axis || M')

$$\Psi_0 = \begin{pmatrix} A^+ e^{k_0 y} + B^+ e^{-k_0 y} \\ A^- e^{k_0 y} + B^- e^{-k_0 y} \end{pmatrix}$$

W.F. in layer 3: (quant. axis || M')

$$\Psi_2 = \begin{pmatrix} t^{++} e^{ik_2^+ y} \\ t^{+-} e^{ik_2^- y} \end{pmatrix}$$

Rotate Ψ_1 in respect to direction of M'



Rotate Ψ_1 about y axis through angle ϕ.

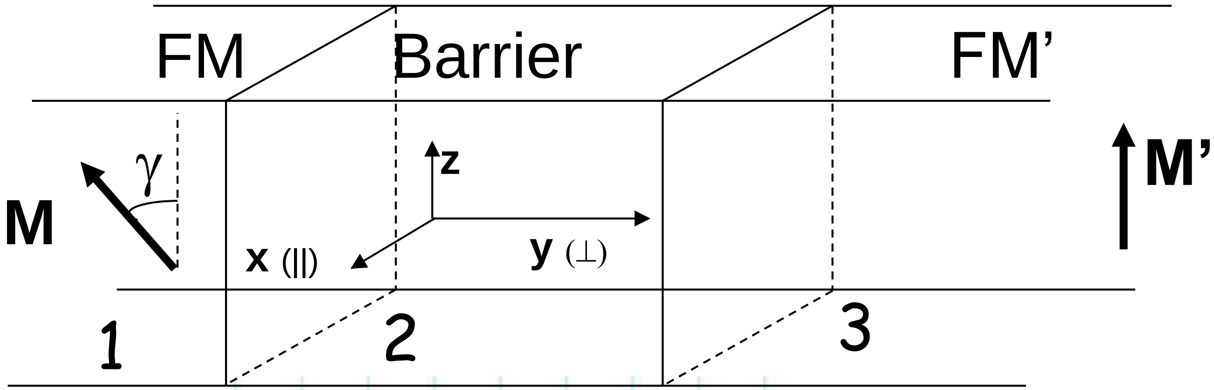
$$\tilde{\Psi}_1 = \begin{pmatrix} \cos(\varphi/2) & -\sin(\varphi/2) \\ \sin(\varphi/2) & \cos(\varphi/2) \end{pmatrix} \begin{pmatrix} e^{ik_1^+ y} + r^{++} e^{-ik_1^+ y} \\ r^{+-} e^{-ik_1^- y} \end{pmatrix}$$

$$= \begin{pmatrix} \cos(\varphi/2)\left(e^{ik_1^+ y} + r^{++} e^{-ik_1^+ y}\right) - \sin(\varphi/2) r^{+-} e^{-ik_1^- y} \\ \sin(\varphi/2)\left(e^{ik_1^+ y} + r^{++} e^{-ik_1^+ y}\right) + \cos(\varphi/2) r^{+-} e^{-ik_1^- y} \end{pmatrix}$$

See G. Bauer's lecture

Wave functions for non-collinear MTJ

4 systems of 8Eqs. and 8Uknowns



$$\Psi_{1R}^{\uparrow\uparrow} = T_{1R}^{\uparrow\uparrow} e^{-ik_1^{\uparrow} z}\cos\frac{\gamma}{2} - T_{1R}^{\downarrow\uparrow} e^{-ik_1^{\downarrow} z}\sin\frac{\gamma}{2}$$

$$\Psi_{1R}^{\downarrow\uparrow} = T_{1R}^{\uparrow\uparrow} e^{-ik_1^{\uparrow} z}\sin\frac{\gamma}{2} + T_{1R}^{\downarrow\uparrow} e^{-ik_1^{\downarrow} z}\cos\frac{\gamma}{2}$$

$$\Psi_{1R}^{\uparrow\downarrow} = T_{1R}^{\uparrow\downarrow} e^{-ik_1^{\uparrow} z}\cos\frac{\gamma}{2} - T_{1R}^{\downarrow\downarrow} e^{-ik_1^{\downarrow} z}\sin\frac{\gamma}{2}$$

$$\Psi_{1R}^{\downarrow\downarrow} = T_{1R}^{\uparrow\downarrow} e^{-ik_1^{\uparrow} z}\sin\frac{\gamma}{2} + T_{1R}^{\downarrow\downarrow} e^{-ik_1^{\downarrow} z}\cos\frac{\gamma}{2}$$

$$\Psi_{1L}^{\uparrow\uparrow} = \left[\frac{e^{ik_1^{\uparrow} z}}{\sqrt{k_1^{\uparrow}}} + R_L^{\uparrow\uparrow} e^{-ik_1^{\uparrow} z}\right]\cos\frac{\gamma}{2} - R_L^{\downarrow\uparrow} e^{-ik_1^{\downarrow} z}\sin\frac{\gamma}{2}$$

$$\Psi_{1L}^{\downarrow\uparrow} = \left[\frac{e^{ik_1^{\uparrow} z}}{\sqrt{k_1^{\uparrow}}} + R_L^{\uparrow\uparrow} e^{-ik_1^{\uparrow} z}\right]\sin\frac{\gamma}{2} + R_L^{\downarrow\uparrow} e^{-ik_1^{\downarrow} z}\cos\frac{\gamma}{2}$$

$$\Psi_{1L}^{\uparrow\downarrow} = -\left[\frac{e^{ik_1^{\downarrow} z}}{\sqrt{k_1^{\downarrow}}} + R_L^{\downarrow\downarrow} e^{-ik_1^{\downarrow} z}\right]\sin\frac{\gamma}{2} + R_L^{\uparrow\downarrow} e^{-ik_1^{\uparrow} z}\cos\frac{\gamma}{2}$$

$$\Psi_{1L}^{\downarrow\downarrow} = \left[\frac{e^{ik_1^{\downarrow} z}}{\sqrt{k_1^{\downarrow}}} + R_L^{\downarrow\downarrow} e^{-ik_1^{\downarrow} z}\right]\cos\frac{\gamma}{2} + R_L^{\uparrow\downarrow} e^{-ik_1^{\uparrow} z}\sin\frac{\gamma}{2}$$

$$\Psi_{2L}^{\uparrow\uparrow} = \frac{A_L^{\uparrow\uparrow}}{\sqrt{q}} e^{\int_0^z q\,dz} + \frac{B_L^{\uparrow\uparrow}}{\sqrt{q}} e^{-\int_0^z q\,dz}$$

$$\Psi_{2L}^{\downarrow\uparrow} = \frac{A_L^{\downarrow\uparrow}}{\sqrt{q}} e^{\int_0^z q\,dz} + \frac{B_L^{\downarrow\uparrow}}{\sqrt{q}} e^{-\int_0^z q\,dz}$$

$$\Psi_{2L}^{\uparrow\downarrow} = \frac{A_L^{\uparrow\downarrow}}{\sqrt{q}} e^{\int_0^z q\,dz} + \frac{B_L^{\uparrow\downarrow}}{\sqrt{q}} e^{-\int_0^z q\,dz}$$

$$\Psi_{2L}^{\downarrow\downarrow} = \frac{A_L^{\downarrow\downarrow}}{\sqrt{q}} e^{\int_0^z q\,dz} + \frac{B_L^{\downarrow\downarrow}}{\sqrt{q}} e^{-\int_0^z q\,dz}$$

$$\Psi_{2R}^{\uparrow\uparrow} = \frac{A_R^{\uparrow\uparrow}}{\sqrt{q}} e^{\int_0^z q\,dz} + \frac{B_R^{\uparrow\uparrow}}{\sqrt{q}} e^{-\int_0^z q\,dz}$$

$$\Psi_{2R}^{\downarrow\uparrow} = \frac{A_R^{\downarrow\uparrow}}{\sqrt{q}} e^{\int_0^z q\,dz} + \frac{B_R^{\downarrow\uparrow}}{\sqrt{q}} e^{-\int_0^z q\,dz}$$

$$\Psi_{2R}^{\uparrow\downarrow} = \frac{A_R^{\uparrow\downarrow}}{\sqrt{q}} e^{\int_0^z q\,dz} + \frac{B_R^{\uparrow\downarrow}}{\sqrt{q}} e^{-\int_0^z q\,dz}$$

$$\Psi_{2R}^{\downarrow\downarrow} = \frac{A_R^{\downarrow\downarrow}}{\sqrt{q}} e^{\int_0^z q\,dz} + \frac{B_R^{\downarrow\downarrow}}{\sqrt{q}} e^{-\int_0^z q\,dz}$$

$$\Psi_{3R}^{\uparrow\uparrow} = \frac{e^{-ik_3^{\uparrow} z}}{\sqrt{k_3^{\uparrow}}} + R_R^{\uparrow\uparrow} e^{ik_3^{\uparrow} z}$$

$$\Psi_{3R}^{\downarrow\uparrow} = R_R^{\downarrow\uparrow} e^{ik_3^{\downarrow} z}$$

$$\Psi_{3R}^{\uparrow\downarrow} = R_R^{\uparrow\downarrow} e^{ik_3^{\uparrow} z}$$

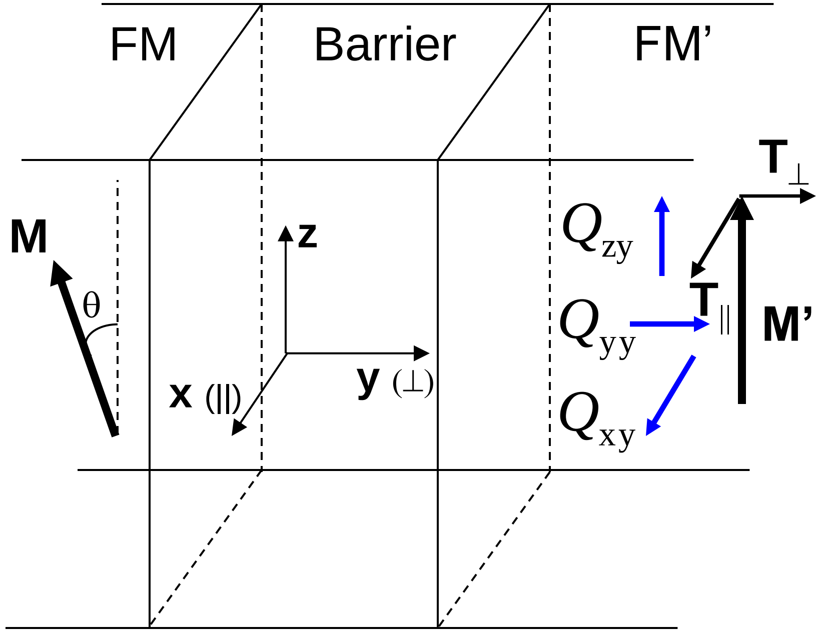
$$\Psi_{3R}^{\downarrow\downarrow} = \frac{e^{-ik_3^{\downarrow} z}}{\sqrt{k_3^{\downarrow}}} + R_R^{\downarrow\downarrow} e^{ik_3^{\downarrow} z}$$

$$\Psi_{3L}^{\uparrow\uparrow} = T_L^{\uparrow\uparrow} e^{ik_3^{\uparrow} z}$$

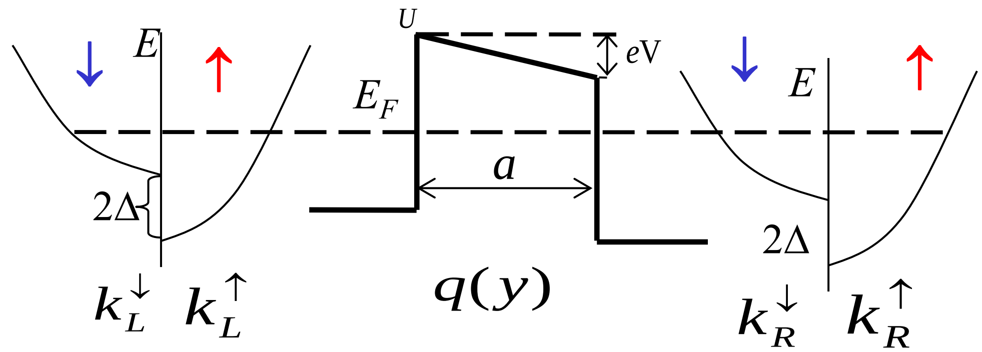
$$\Psi_{3L}^{\downarrow\uparrow} = T_L^{\downarrow\uparrow} e^{ik_3^{\downarrow} z}$$

$$\Psi_{3L}^{\uparrow\downarrow} = T_L^{\uparrow\downarrow} e^{ik_3^{\uparrow} z}$$

$$\Psi_{3L}^{\downarrow\downarrow} = T_L^{\downarrow\downarrow} e^{ik_3^{\downarrow} z}$$



Free electron model



- Wave vectors depends on V and band positions
- Boundary conditions for Green functions and derivatives

In the right FM layer (as an example):

$$T_\parallel(E) \propto \frac{q(0)q(a)(k_L^\uparrow - k_L^\downarrow)(k_R^{\uparrow 2} - k_R^{\downarrow 2})\left[q^2(0) - k_L^\uparrow k_L^\downarrow\right]\sin\gamma}{|Den|^2} e^{-2\int_0^a q(y)dy} \left\{q(a)(k_R^\uparrow - k_R^\downarrow)\cos\left[(k_R^\uparrow - k_R^\downarrow)y'\right] + \left[q^2(a) + k_R^\uparrow k_R^\downarrow\right]\sin\left[(k_R^\uparrow - k_R^\downarrow)y'\right]\right\}\left\{f_L(E) - f_R(E \pm eV)\right\}$$

$$T_\perp(E) = T_\perp^0(E) + T_\perp^1(E), \text{ where}$$

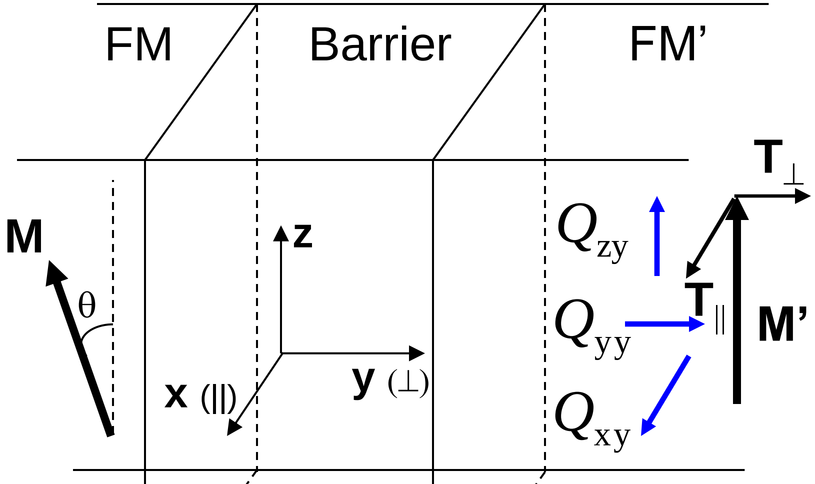
Explicit analytical expressions for STT

$$T_\perp^0(E) \propto \frac{q(0)q(a)(k_L^\uparrow - k_L^\downarrow)(k_R^{\uparrow 2} - k_R^{\downarrow 2})\sin\gamma}{|Den|^2} e^{-2\int_0^a q(y)dy}\, 2 f_R(E \pm eV) \times$$

$$\times \left\{\left[q(0)q(a)(k_L^\uparrow + k_L^\downarrow)(k_R^\uparrow + k_R^\downarrow) - \left(q^2(0) - k_L^\uparrow k_L^\downarrow\right)\left(q^2(a) - k_R^\uparrow k_R^\downarrow\right)\right]\cos\left[(k_R^\uparrow + k_R^\downarrow)y'\right] + \left[q(0)(k_L^\uparrow + k_L^\downarrow)\left(q^2(a) - k_R^\uparrow k_R^\downarrow\right) + q(a)(k_R^\uparrow + k_R^\downarrow)\left(q^2(0) - k_L^\uparrow k_L^\downarrow\right)\right]\sin\left[(k_R^\uparrow + k_R^\downarrow)y'\right]\right\}$$

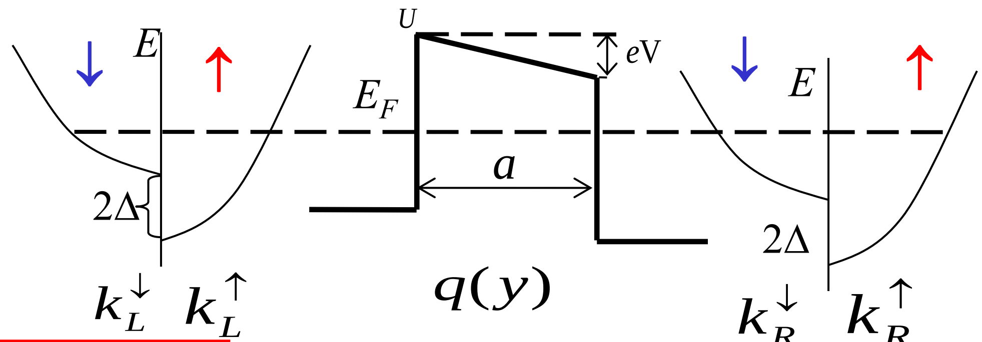
$$T_\perp^1(E) \propto \frac{q(0)q(a)(k_L^\uparrow - k_L^\downarrow)(k_R^{\uparrow 2} - k_R^{\downarrow 2})\left[q^2(0) - k_L^\uparrow k_L^\downarrow\right]\sin\gamma}{|Den|^2} e^{-2\int_0^a q(y)dy} \left\{q(a)(k_R^\uparrow - k_R^\downarrow)\sin\left[(k_R^\uparrow - k_R^\downarrow)y'\right] - \left[q^2(a) + k_R^\uparrow k_R^\downarrow\right]\cos\left[(k_R^\uparrow - k_R^\downarrow)y'\right]\right\}\left\{f_L(E) - f_R(E \pm eV)\right\}$$

M. Chshiev, A. Manchon, A. Kalitsov et al, Phys. Rev. B (2015)



$$E_n = \exp\left(\int_0^d q(y)dy\right)$$

Free electron model



$$P_i = \frac{k_i^\uparrow - k_i^\downarrow}{k_i^\uparrow + k_i^\downarrow} \qquad \alpha_i = \frac{q_i^2 - k_i^\uparrow k_i^\downarrow}{q_i^2 + k_i^\uparrow k_i^\downarrow} \qquad \eta_i = \frac{q_i(k_i^\uparrow + k_i^\downarrow)}{q_i^2 + k_i^\uparrow k_i^\downarrow}$$

Local torques (derivatives of Q):

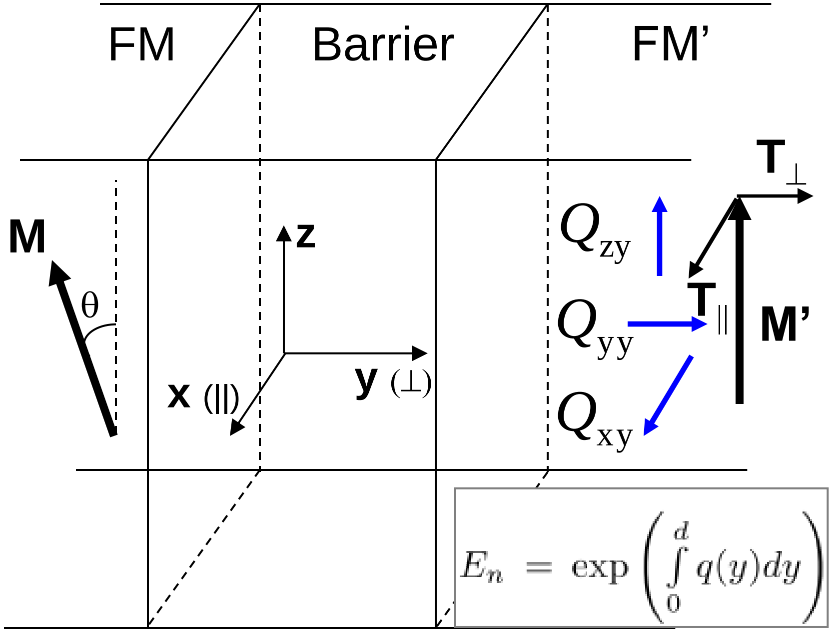
→ Oscillations of different periods

→ Shorter period for RKKY coupling

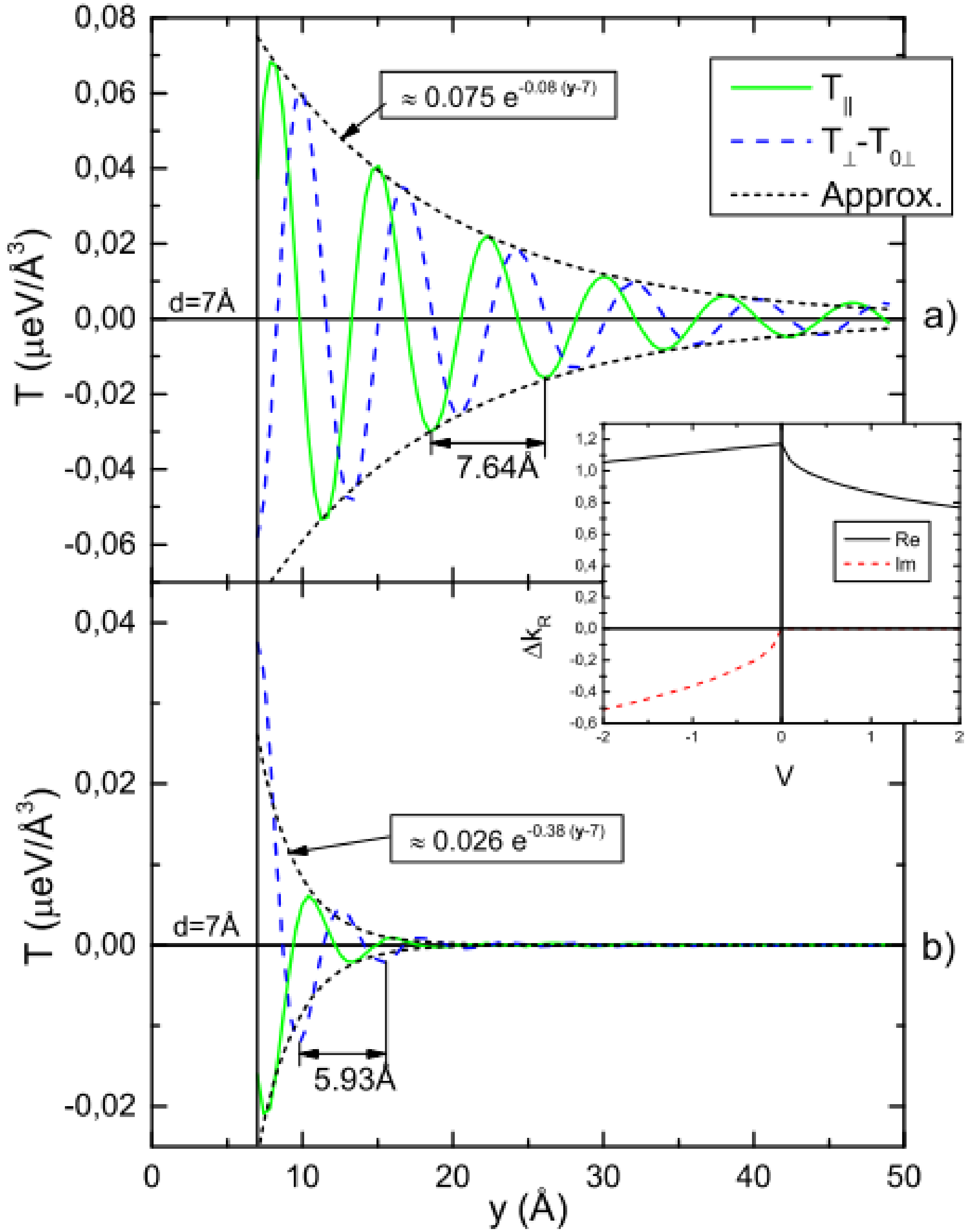
→ Longer period for voltage induced

$$Q_x^R = \frac{4\sin\gamma}{|Den|^2} P_L \; \left[P_R \eta_R \alpha_L [E_n^2 - E_n^{-2}] \sin\{\Delta k_R y\} + (2\alpha_R - \alpha_L[E_n^2 + E_n^{-2}]) \cos\{\Delta k_R y\}\right] [f_L - f_R]$$

$$\begin{aligned} Q_y^R = \frac{4\sin\gamma}{|Den|^2} P_L \; \Big\{ \Big[\Big[& (2\alpha_R - \alpha_L[E_n^2 + E_n^{-2}]) \sin\{\Delta k_R y\} - \\ & P_R \eta_R \alpha_L [E_n^2 - E_n^{-2}] \cos\{\Delta k_R y\} \Big] [f_L - f_R] \\ & + P_R f_R \Big[((\eta_L \eta_R - \alpha_R \alpha_L)\, [E_n^2 + E_n^{-2}] \\ & + 2(1 - \eta_L \eta_R P_L P_R \cos\gamma)) \sin\{\Sigma k_R y\} \\ & - (\eta_L \alpha_R + \eta_R \alpha_L)\, [E_n^2 - E_n^{-2}] \cos\{\Sigma k_R y\} \Big] \Big\} \end{aligned}$$



$$E_n = \exp\left(\int_0^d q(y)dy\right)$$



Local torques (T = ∇Q):

→ Oscillations of different periods

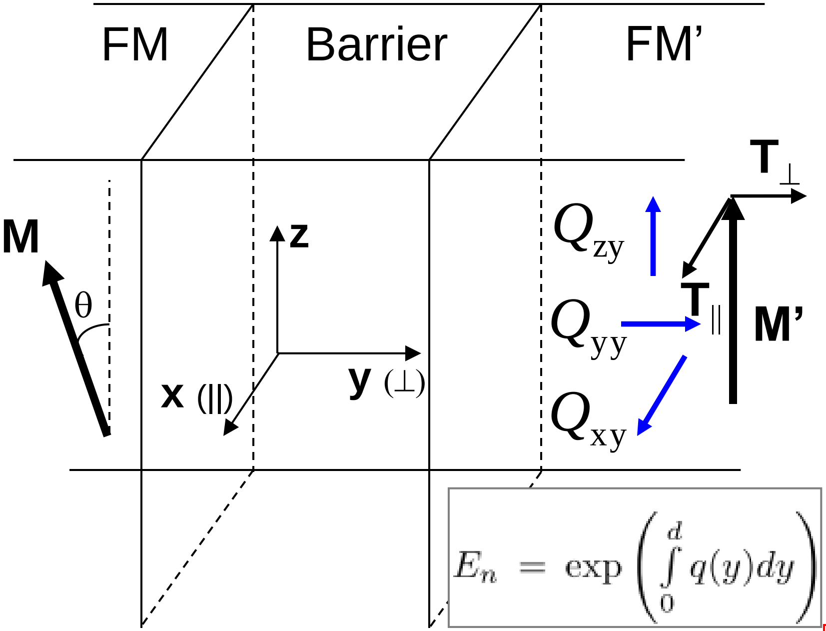
→ Shorter period for RKKY coupling

→ Longer period for voltage induced

Transverse characteristic length scales:

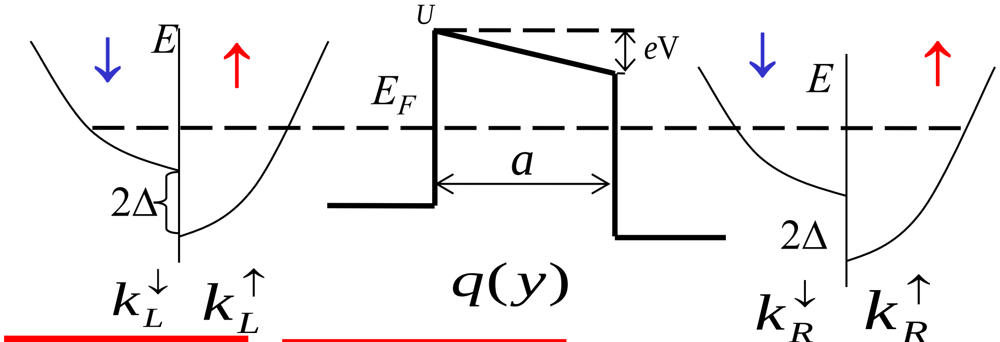
- Larmor spin precession length, λ_L
- Transverse spin decay length, λ_d
- Applied voltage dependent

M. Chshiev, A. Manchon, A. Kalitsov et al, Phys. Rev. B (2015)



$$E_n = \exp\left(\int_0^d q(y)dy\right)$$

Free electron model



$$P_i = \frac{k_i^\uparrow - k_i^\downarrow}{k_i^\uparrow + k_i^\downarrow}$$

$$\alpha_i = \frac{q_i^2 - k_i^\uparrow k_i^\downarrow}{q_i^2 + k_i^\uparrow k_i^\downarrow}$$

$$\eta_i = \frac{q_i(k_i^\uparrow + k_i^\downarrow)}{q_i^2 + k_i^\uparrow k_i^\downarrow}$$

Total torques:

→ Deviations from sine dependence in case of low/thin barrier

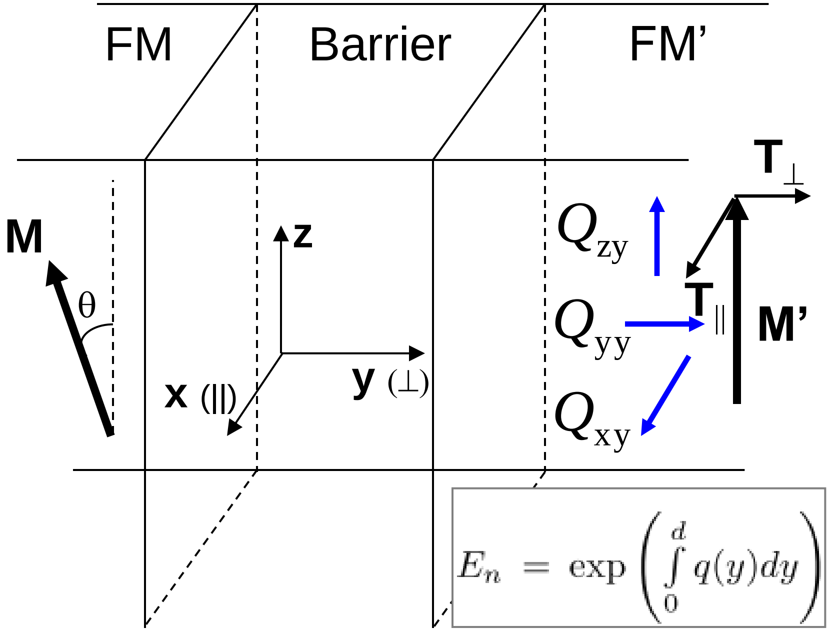
→ Eventually for metallic spin valves

$$T_{||} = \frac{4\sin\gamma}{|Den|^2} P_L\left(2\alpha_R - \alpha_L[E_n^2 - E_n^{-2}]\right)[f_L - f_R]$$

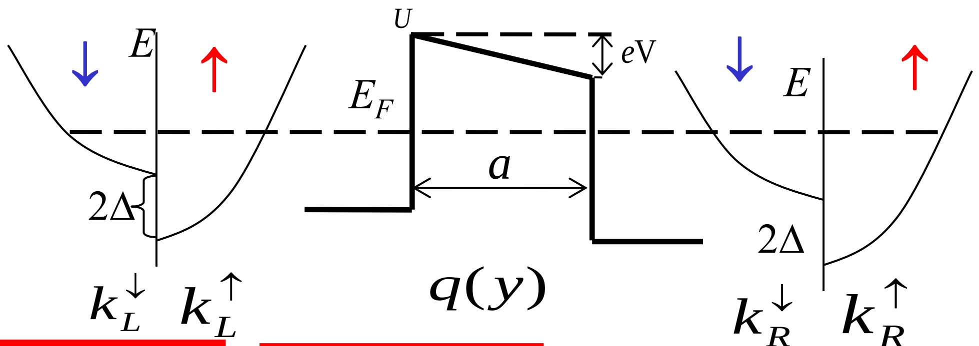
$$T_\perp = -\frac{4\sin\gamma}{|Den|^2} P_L P_R\left(\alpha_L\eta_R f_L + \alpha_R\eta_L f_R\right)[E_n^2 - E_n^{-2}]$$

$$|Den|^2 = \frac{1}{\eta_L\eta_R}\Big\{(\eta_L^2+\alpha_L^2)(\eta_R^2+\alpha_R^2)[E_n^4+E_n^{-4}] - 2(\eta_L\eta_R - \alpha_L\alpha_R)(1-\eta_L\eta_R P_L P_R\cos\gamma)[E_n^2+E_n^{-2}] + 2(\eta_L^2-\alpha_L^2)(\eta_R^2-\alpha_R^2) - 8\eta_L\eta_R\alpha_L\alpha_R + 4(1-\eta_L\eta_R P_L P_R\cos\gamma)^2\Big\}$$

Free electron model



$$E_n = \exp\left(\int_0^d q(y)dy\right)$$



$$P_i = \frac{k_i^\uparrow - k_i^\downarrow}{k_i^\uparrow + k_i^\downarrow} \qquad \alpha_i = \frac{q_i^2 - k_i^\uparrow k_i^\downarrow}{q_i^2 + k_i^\uparrow k_i^\downarrow} \qquad \eta_i = \frac{q_i(k_i^\uparrow + k_i^\downarrow)}{q_i^2 + k_i^\uparrow k_i^\downarrow}$$

Total torques:

→ Case of thick barrier

→ Parallel torque related to longitudinal spin current

$P_i^S = P_i\alpha_i$ - Slonczweski polarization

$P_i^\eta = P_i\eta_i$ - out-of-plane polarization

$T_i = \frac{\eta_i}{\alpha_i^2 + \eta_i^2}$ - Spin averaged interfacial transmission probability

$$T_{||} = -4T_L T_R P_L^S E_n^{-2}[f_L - f_R]\sin\gamma$$

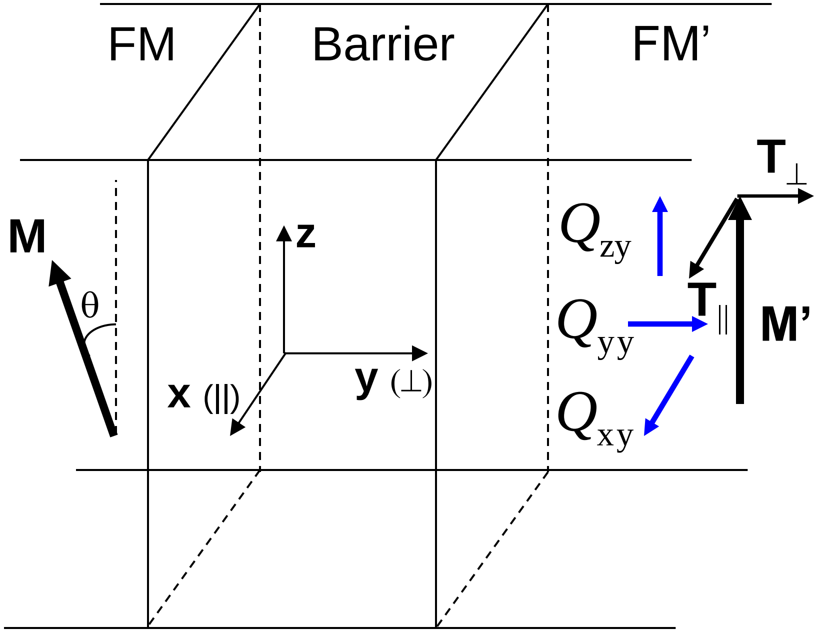
$$T_\perp = -4T_L T_R\left(P_L^S P_R^\eta f_L + P_R^S P_L^\eta f_R\right)E_n^{-2}\sin\gamma$$

$$J_e = -8T_L T_R\left(1 + P_L^S P_R^S\cos\gamma\right)[f_L - f_R]E_n^{-2}$$

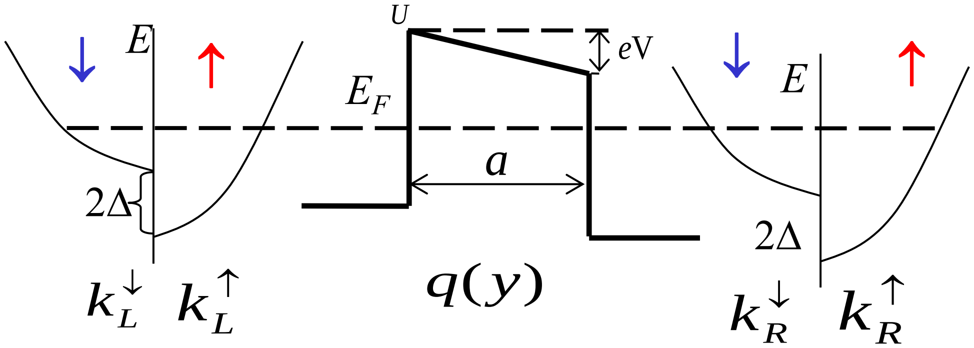
$$Q_z = -4T_L T_R\left(P_R^S + P_L^S\cos\gamma\right)[f_L - f_R]E_n^{-2}$$

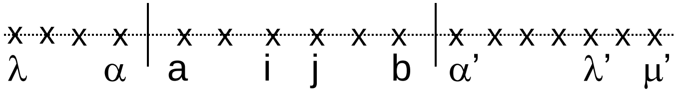
$$T_{||} = Q_x = \frac{Q_z(0) - Q_z(\pi)}{2}\mathbf{M}_R \times (\mathbf{M}_L \times \mathbf{M}_R)$$

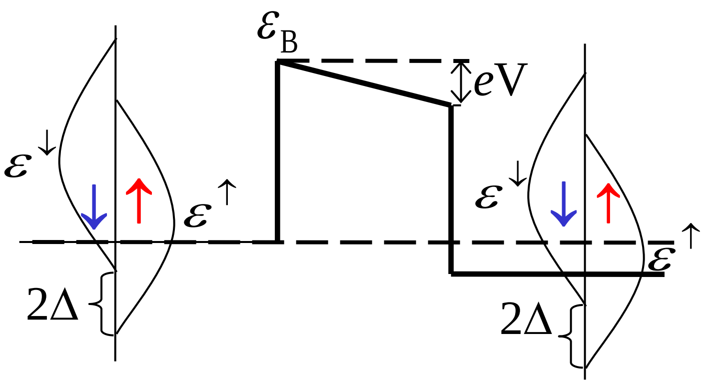
M. Chshiev, A. Manchon, A. Kalitsov et al, Phys. Rev. B (2015)



Free electron model







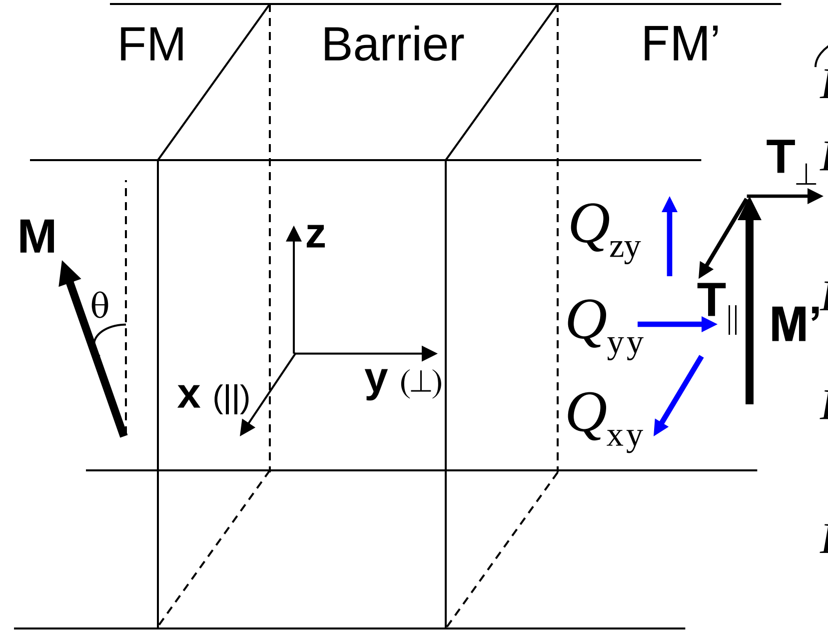
Tight-binding model

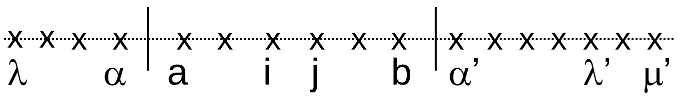
Model parameters:

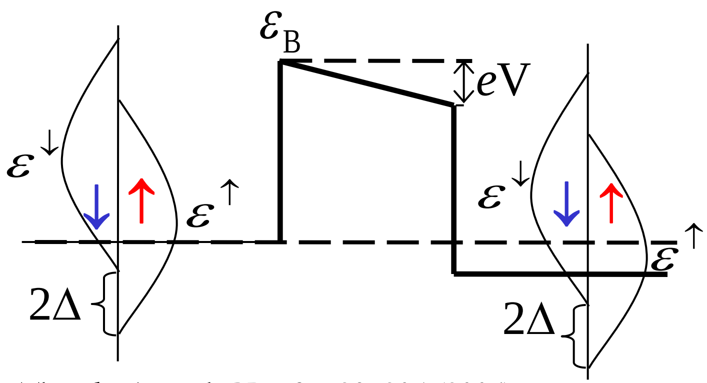
$\varepsilon^{\uparrow(\downarrow)}, \varepsilon^{B}$ - on-site energies

t, t^B – hopping

$t^{\alpha a}$, $t^{\alpha' b}$ – couplings







Hamiltonian

$$H = H_L + H_R + H_B + H_{LB} + H_{RB}$$

$$H_L^\sigma = \sum_\lambda \varepsilon^\sigma c_\lambda^+ c_\lambda + t \sum_{NN} c_\lambda^+ c_\mu$$

$$H_{L(R)} = \frac{H_{L(R)}^\uparrow + H_{L(R)}^\downarrow}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \frac{H_{L(R)}^\uparrow - H_{L(R)}^\downarrow}{2} \begin{pmatrix} \cos\gamma & \sin\gamma \\ \sin\gamma & -\cos\gamma \end{pmatrix}$$

$$H_R^\sigma = \sum_{\lambda'} (\varepsilon^\sigma + e\mathrm{V}) c_{\lambda'}^+ c_{\lambda'} + t \sum_{NN} c_{\lambda'}^+ c_{\mu'}$$

$$H_{LB} = t_{a\alpha} c_\alpha^+ c_a \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + h.c.$$

$$H_{RB} = t_{b\alpha'} c_{\alpha'}^+ c_b \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + h.c.$$

$$H_B = \Big(\sum_i \varepsilon_{\mathrm{B}}^i c_i^+ c_i + t_{\mathrm{B}} \sum_{NN} c_i^+ c_j\Big) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \qquad \varepsilon_{\mathrm{B}}^i = \varepsilon_B + \frac{i}{N} e\mathrm{V}$$

Tight-binding model

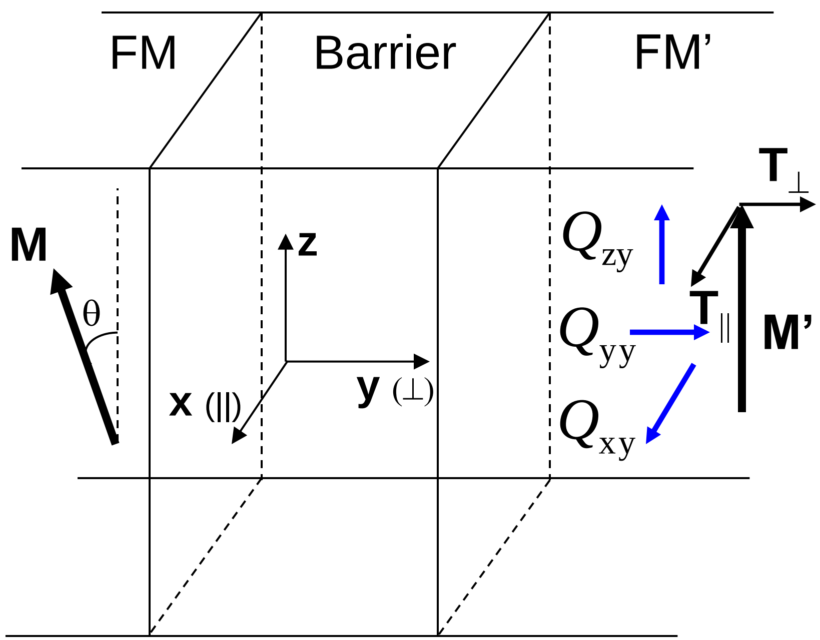
Model parameters:

$\varepsilon^{\uparrow(\downarrow)}, \varepsilon^B$ - on-site energies

t, t^{B} – hopping

$t^{\alpha a}$, $t^{\alpha' b}$ – couplings

I. Theodonis et al, PRL 97, 237205 (2006)
M. Chshiev et al, IEEE Trans. Mag. 44, 2543 (2008)
A. Kalitsov et al, PRB 79, 174416 (2009)



Keldysh formalism with non-equilibrium Green functions

$$G^{-+}_{\lambda'\mu'}(t,t') = -i\left\langle c^{\dagger}_{\mu'}(t')c_{\lambda'}(t)\right\rangle$$

Charge current:

$$\mathbf{J} = \frac{e}{8\pi^3 h}\int dE \int dk_\parallel Tr\left\{\left[G^{-+}_{\lambda'+1,\lambda'}T' - G^{-+}_{\lambda',\lambda'+1}T'^{+}\right]\right\}\hat{\mathbf{y}}$$

Spin current:

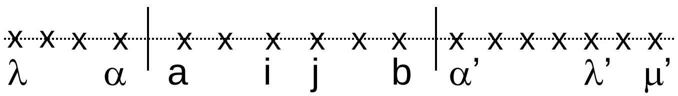
$$\mathbf{Q}_{\lambda'+1,\lambda'} = \frac{1}{16\pi^3}\int dE \int dk_\parallel Tr\left\{\left[G^{-+}_{\lambda'+1,\lambda'}T' - G^{-+}_{\lambda',\lambda'+1}T'^{+}\right]\boldsymbol{\sigma}\right\}$$

Torque: $\mathbf{T}_{\lambda'} = \mathbf{Q}_{\lambda'-1,\lambda'} - \mathbf{Q}_{\lambda',\lambda'+1}$

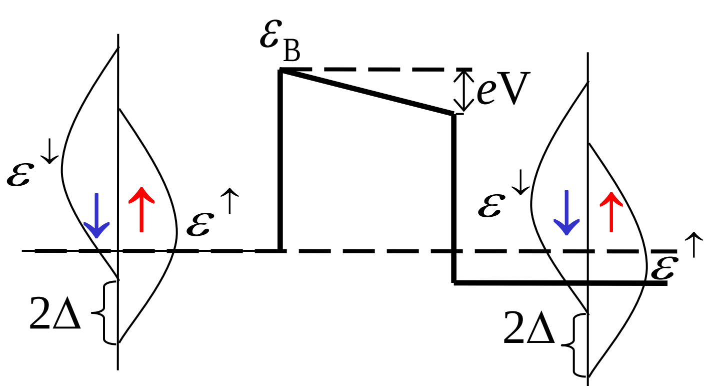
Total torque:

$$\mathbf{T} = \sum_{\lambda'=0}^{\Lambda}\mathbf{T}_{\lambda'} = \sum_{\lambda'=0}^{\Lambda}\left(\mathbf{Q}_{\lambda'-1,\lambda'} - \mathbf{Q}_{\lambda',\lambda'+1}\right) = \mathbf{Q}_{-1,0} - \mathbf{Q}_{\Lambda-1,\Lambda}$$

$\Lambda \to \infty$



Non-collinear **M** and **M’**



Tight-binding model

Model parameters:

$\varepsilon^{\uparrow(\downarrow)}, \varepsilon^{B}$ - on-site energies

t, t^{B} – hopping

$t^{\alpha a}, t^{\alpha' b}$ – couplings

2 x 2 matrices

$$G = \begin{pmatrix} G^{\uparrow\uparrow} & G^{\uparrow\downarrow} \\ G^{\downarrow\uparrow} & G^{\downarrow\downarrow} \end{pmatrix}$$

$$\langle O\rangle = -i\hbar\sum_{\sigma\sigma'}\hat{O}_{\sigma\sigma'}G^{-+\sigma'\sigma}$$

D. M. Edwards et al, PRB 71, 054407 (2005)
I. Theodonis et al, PRL 97, 237205 (2006)
M. Chshiev et al, IEEE Trans. Mag. 44, 2543 (2008)

Two ways to find spin torque in ballistic regime

In ballistic regime:

$$\mathbf{T} = \nabla \bullet \mathbf{Q}(r,t) = \frac{J_{sd}}{\hbar}\mathbf{S_d} \times \mathbf{s}(r,t)$$

1. Using divergence of spin current **Q**:

$$\mathbf{T} = \nabla \bullet \mathbf{Q} = \partial_k Q_{ik}$$

i=*x*, *y*, *z* in spin space and *k*=*x*, *y*, *z* in real space

Current flows in **y** direction →
$$\begin{cases} Q_{xy} \neq 0 \\ Q_{yy} \neq 0 \\ Q_{zy} \neq 0 \end{cases}$$

2. Using magnetic moment and exchange splitting:

$$\mathbf{T} = \frac{1}{\mu_B}\boldsymbol{\mu} \times \boldsymbol{\Delta}$$

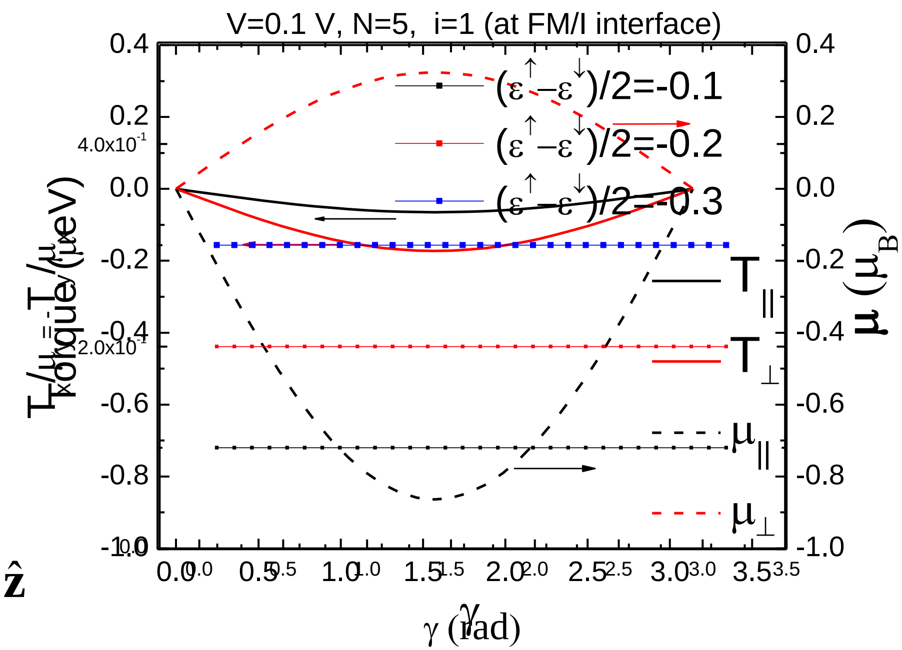
$$\boldsymbol{\Delta} = \frac{\varepsilon^{\downarrow} - \varepsilon^{\uparrow}}{2}\hat{\mathbf{z}}$$

Two ways to find spin torque in ballistic regime

Let's check relation between **T** and **μ** using its' angular dependence. Suppose they are related via unknown vector **a**. Then:

$$\mathbf{T} = \frac{1}{\mu_B}\boldsymbol{\mu}\times\mathbf{a} \qquad \mathbf{a}(0,0,a_z)$$

$$\Rightarrow \quad \begin{cases} T_\parallel = \mu_\perp a_z \\ T_\perp = -\mu_\parallel a_z \\ T_z = 0 \end{cases} \quad \Rightarrow \quad a_z = \frac{T_\parallel}{\mu_\perp} = -\frac{T_\perp}{\mu_\parallel}$$



$$\mathbf{a} = \boldsymbol{\Delta}$$

The two methods give quantitative agreement and are connected directly via exchange splitting

$$\mathbf{T} = \frac{1}{\mu_B}\boldsymbol{\mu}\times\boldsymbol{\Delta} = \nabla\bullet\mathbf{Q} \qquad \boldsymbol{\Delta} = \frac{\varepsilon^{\downarrow}-\varepsilon^{\uparrow}}{2}\hat{\mathbf{z}}$$

A. Kalitsov et al, JAP 99, 08G501 (2006)

Two ways to find spin torque in ballistic regime

In ballistic systems:

$$\mathbf{T} = \nabla \bullet \mathbf{Q}(r,t) = \frac{J_{sd}}{\hbar} \mathbf{S_d} \times \mathbf{s}(r,t)$$

The exchange interaction between spin-polarized s electrons and more localized d electrons is responsible for spin-transfer torque. This interaction yields a precessional motion of spin-density of s electrons around the local magnetization. In ballistic regime, the spin-transfer torque is also equal to the divergence of spin-current.

In diffusive systems:

$$\mathbf{T} = \nabla \bullet \mathbf{Q}(r,t) + \frac{\mathbf{s}}{\tau_{SF}} = \frac{J_{sd}}{\hbar} \mathbf{S_d} \times \mathbf{s}(r,t)$$

Takes into account the spin-memory loss by scattering with spin lifetime τ_{SF}

A. Manchon et al, JPCM 20 (2008) 145208

Local torques in the right FM at zero voltage

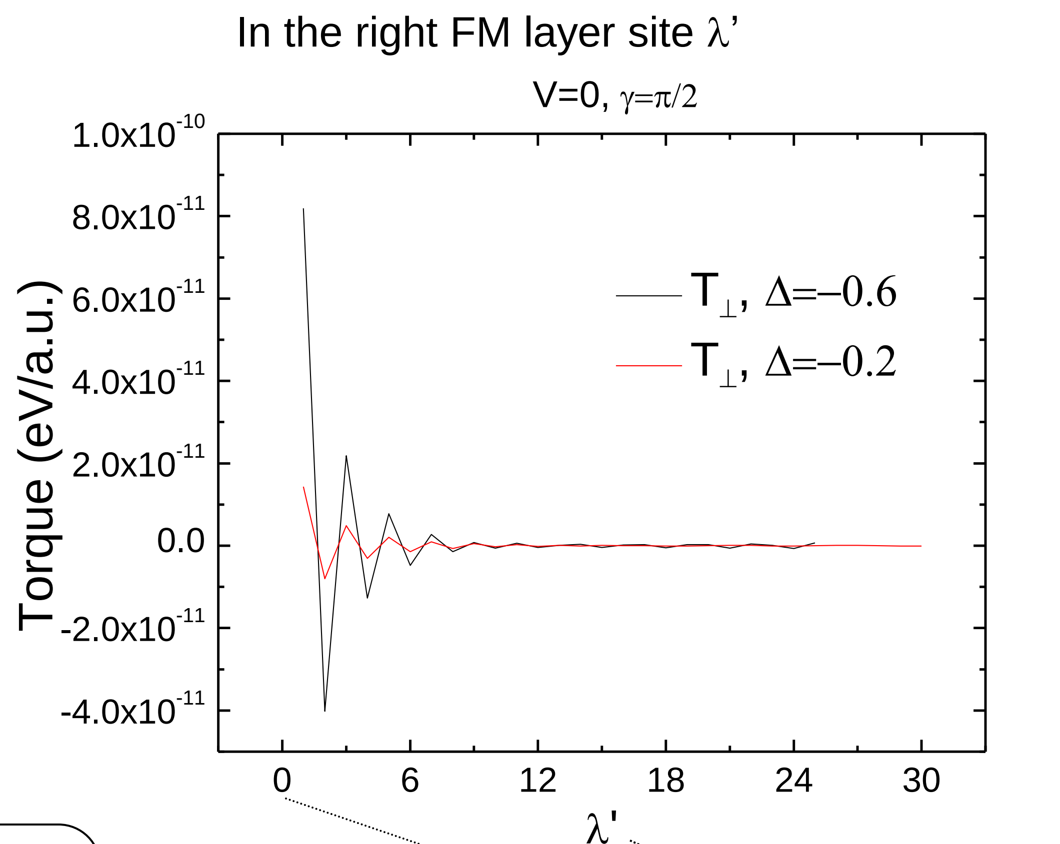
Period of oscillations is ~ $1/(k^{\uparrow} + k^{\downarrow})$

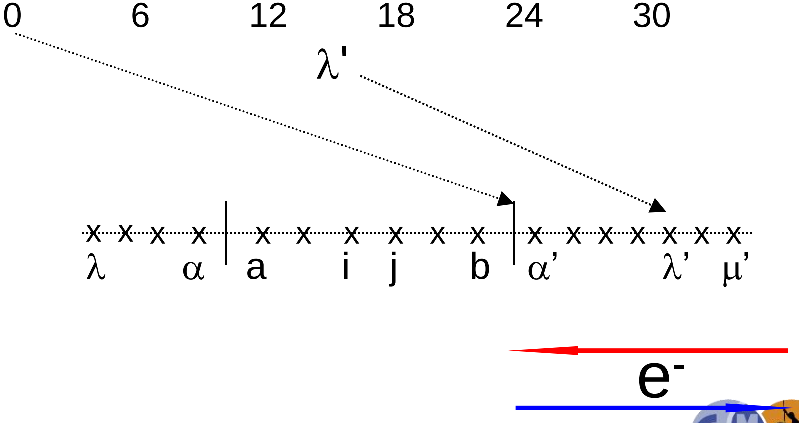
Note RKKY period (summation of k)

Coupling amplitude decreases with exchange splitting

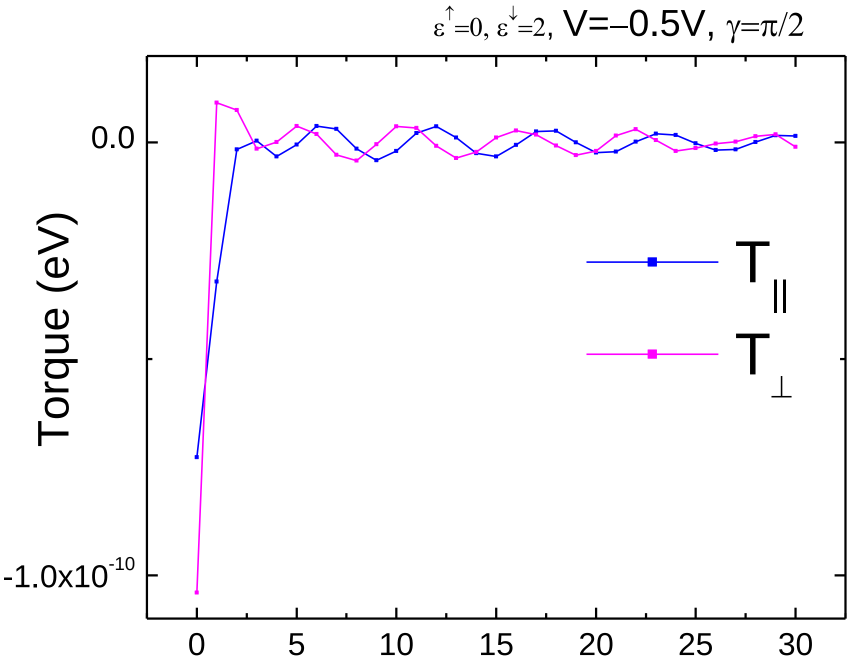
J. C. Slonczewski, Phys. Rev. B **39**, 6995 (1989); *ibid.***71**, 6995 (2005);
D. M. Edwards et al, Phys. Rev. B **71**, 024405 (2005)
A. Manchon et al, JPCM 20, 145208 (2008)

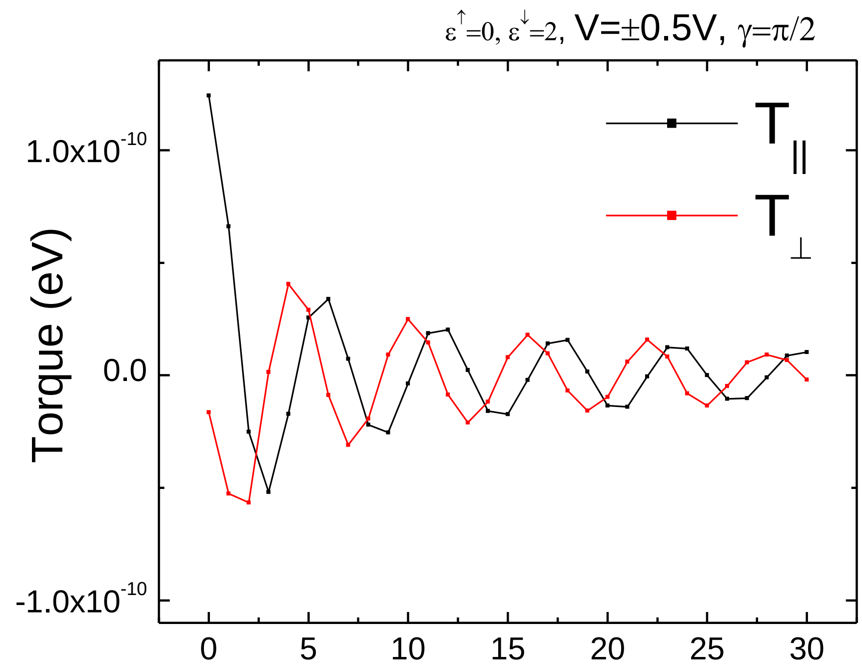
Perpendicular torque component $T_{\perp}$ is not zero @ zero bias describing exchange coupling between FM layers

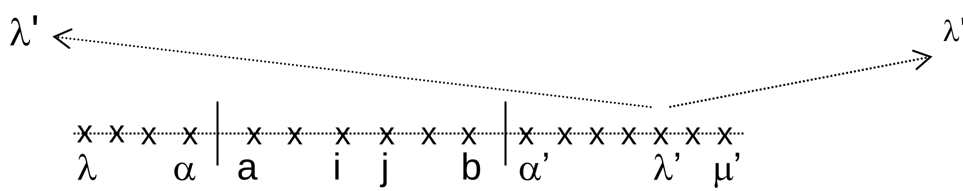




Local torques in the right FM at positive/negative bias







Period of oscillations is $\sim 1/(k^{\uparrow} - k^{\downarrow})$

A. Kalitsov et al., JAP 99, 08G501
A. Manchon et al, JPCM 20, 145208
M. Wilczyński et al., PRB 77, 054434
D. Ralph and M.Stiles, JMMM 320, 1190

Note voltage (current) induced STT period (difference of k)

e^-

Precession of spin state in exchange field of the magnet

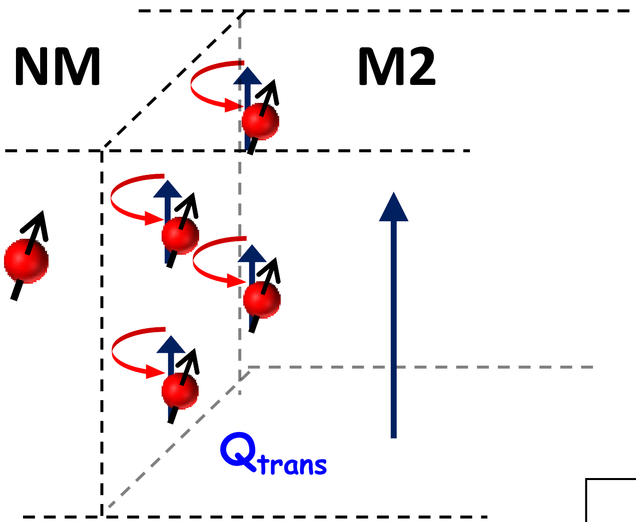
Case 1: insulating barrier (tunnel junctions)

→ precession period $2\pi/(k\uparrow + k\downarrow)$ for RKKY IEC

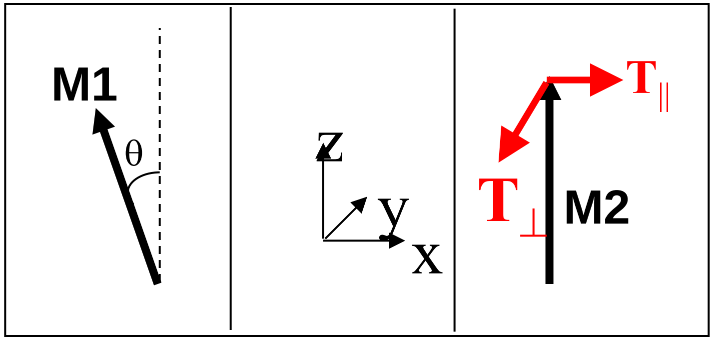
→ precession period $2\pi/(k\uparrow - k\downarrow)$ for STT voltage induced

→only electrons with $k\perp$ interface tunnel → selection of k-vectors

→integration over k-vectors does not average to zero



$$\mathbf{N}_{\rm st} = A\hat{\mathbf{x}}\cdot(\mathbf{Q}_{\rm in} + \mathbf{Q}_{\rm refl} - \mathbf{Q}_{\rm trans})$$
$$= \frac{A}{\Omega}\frac{\hbar^2 k}{2m}\sin(\theta)[1 - {\rm Re}(t_\uparrow t_\downarrow^* + r_\uparrow r_\downarrow^*)]\hat{\mathbf{x}}$$
$$- \frac{A}{\Omega}\frac{\hbar^2 k}{2m}\sin(\theta)\,{\rm Im}(t_\uparrow t_\downarrow^* + r_\uparrow r_\downarrow^*)\hat{\mathbf{y}}.$$



Non-zero X and Y – component of torque!!!

Difference with metallic structures for STT

Precession of spin state in exchange field of the magnet

Case 2: metallic structures

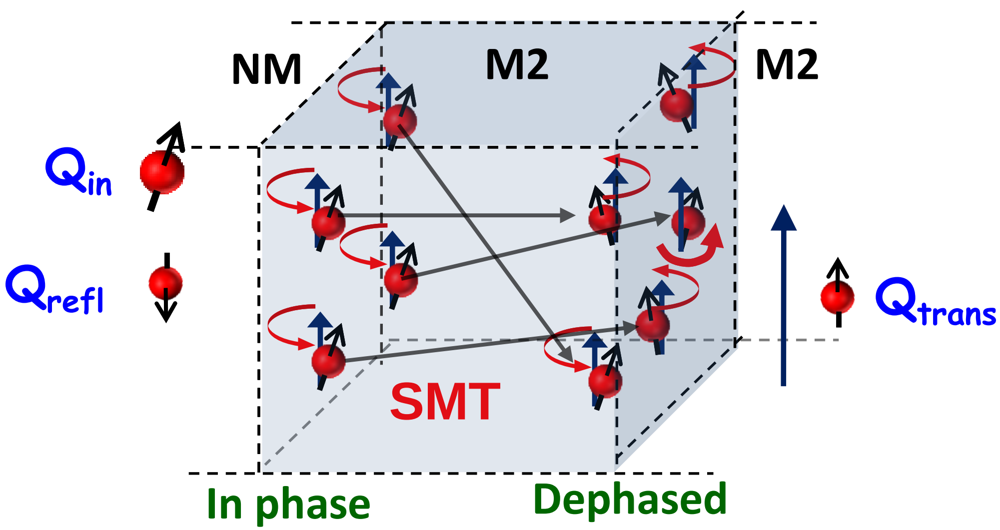
Consequence of dephasing

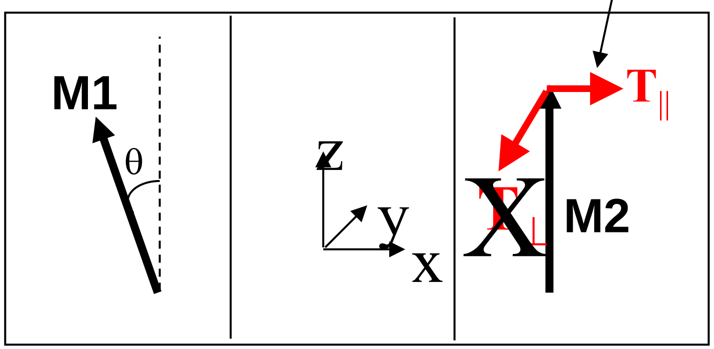
→ away from the interface, reflected and transmitted spin currents are collinear to M2

→ The entire transverse spin current is absorbed by M2 at interface

$$\mathbf{N}_{\mathrm{st}} = A\hat{\mathbf{x}} \cdot (\mathbf{Q}_{\mathrm{in}} + \mathbf{Q}_{\mathrm{refl}} - \mathbf{Q}_{\mathrm{trans}}) \approx A\hat{\mathbf{x}} \cdot \mathbf{Q}_{\mathrm{in}\perp}$$

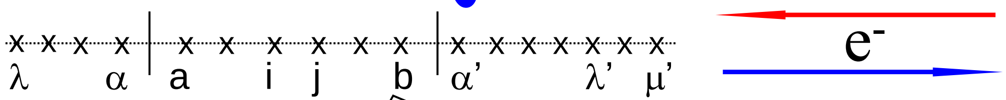
Only torque in x-direction





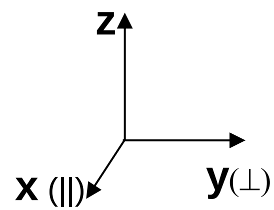
Spin current (total torque) on energy

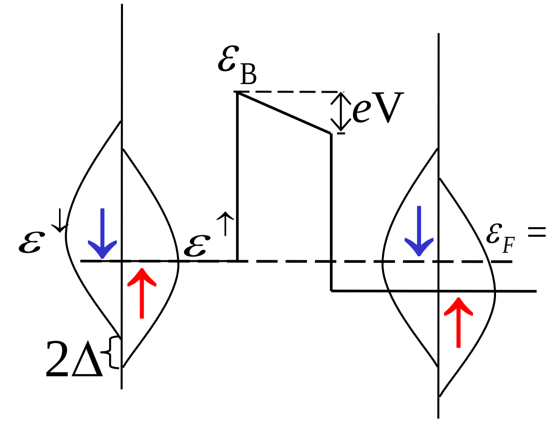
Back to tunnel junctions

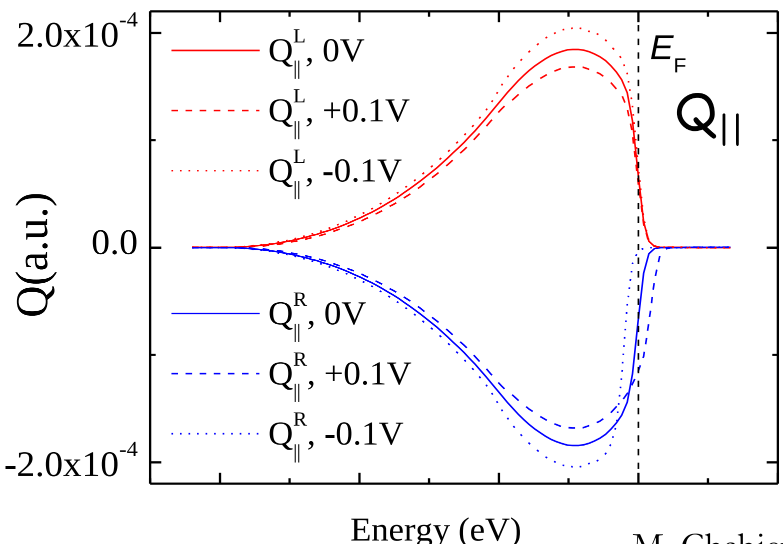


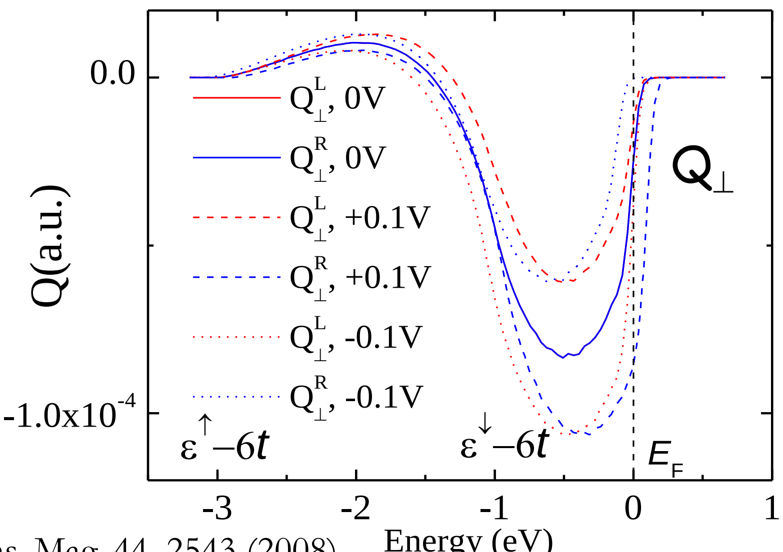
$$\mathbf{Q} = \mathbf{Q}^{\mathrm{L}} + \mathbf{Q}^{\mathrm{R}}$$

$$\mathbf{T} = \sum_{\lambda'=0}^{\infty} \mathbf{T}_{\lambda'} = \sum_{\lambda'=0}^{\infty} \mathbf{Q}_{\lambda'-1} - \mathbf{Q}_{\lambda'} = \mathbf{Q}_{-1} - \mathbf{Q}_{\infty} = \mathbf{Q}_{-1}$$







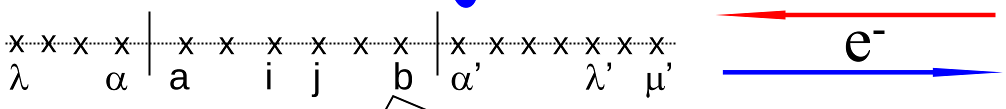


M. Chshiev et al, IEEE Trans. Mag. 44, 2543 (2008)

$$Q_{\parallel}^{L}(E) = -Q_{\parallel}^{R}(E)$$
$$E < \min\{f_L, f_R\}$$

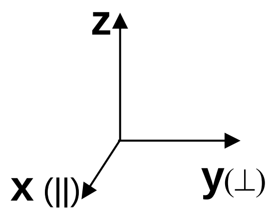
$$Q_{\perp}^{L(R)}(E)\Big|_{V>0} = Q_{\perp}^{R(L)}(E - eV)\Big|_{V<0}$$
$$Q_{\perp}(E)\Big|_{V>0} = Q_{\perp}(E - eV)\Big|_{V<0}$$

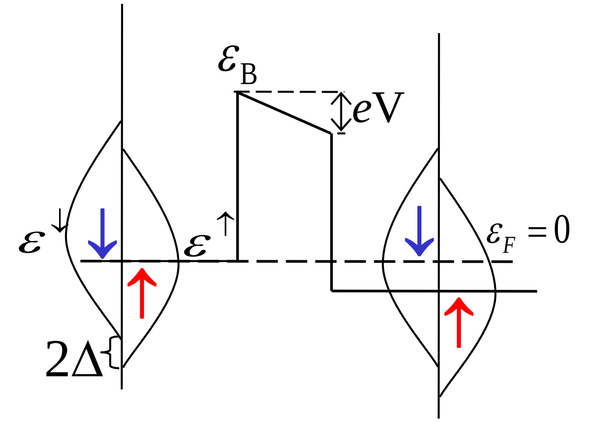
Back to tunnel junctions

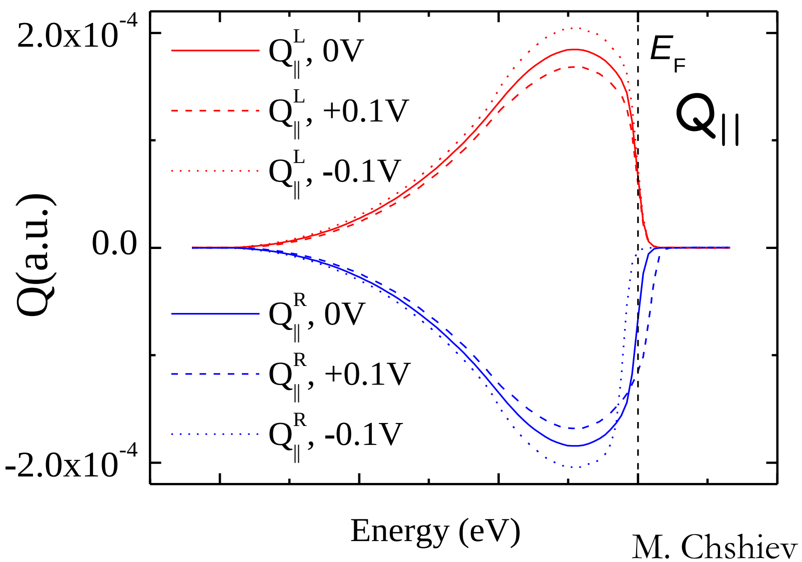


$$\mathbf{Q} = \mathbf{Q}^{\mathrm{L}} + \mathbf{Q}^{\mathrm{R}}$$

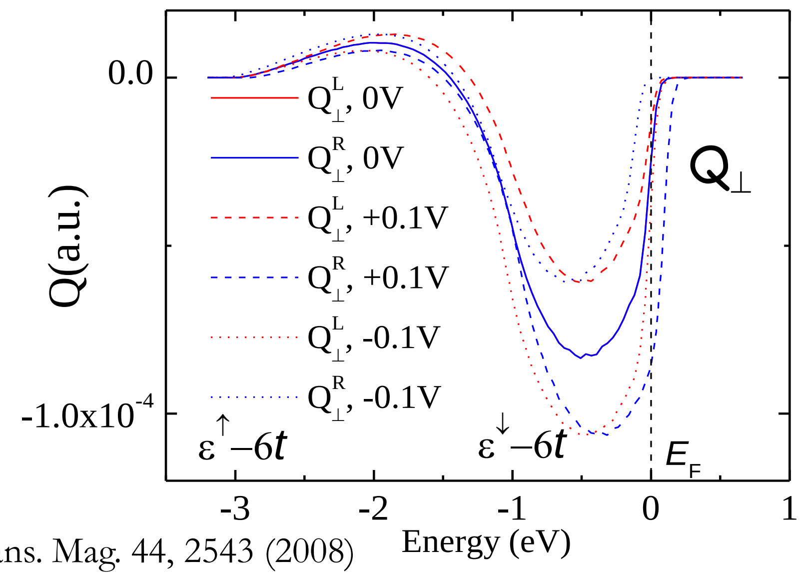
$$\mathbf{T} = \sum_{\lambda'=0}^{\infty} \mathbf{T}_{\lambda'} = \sum_{\lambda'=0}^{\infty} \mathbf{Q}_{\lambda'-1} - \mathbf{Q}_{\lambda'} = \mathbf{Q}_{-1} - \mathbf{Q}_{\infty} = \mathbf{Q}_{-1}$$







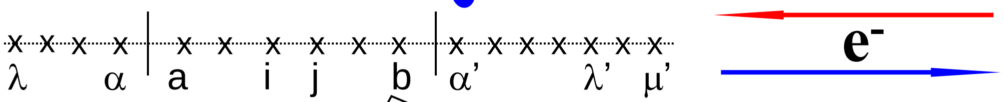
M. Chshiev et al, IEEE Trans. Mag. 44, 2543 (2008)



$$Q_{\parallel}^{L}(E) = -Q_{\parallel}^{R}(E)$$
$$E < \min\{ f_L, f_R \}$$

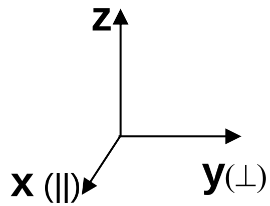
$$Q_{\perp}^{L(R)}(E)\Big|_{V>0} = Q_{\perp}^{R(L)}(E - eV)\Big|_{V<0}$$
$$Q_{\perp}(E)\Big|_{V>0} = Q_{\perp}(E - eV)\Big|_{V<0}$$

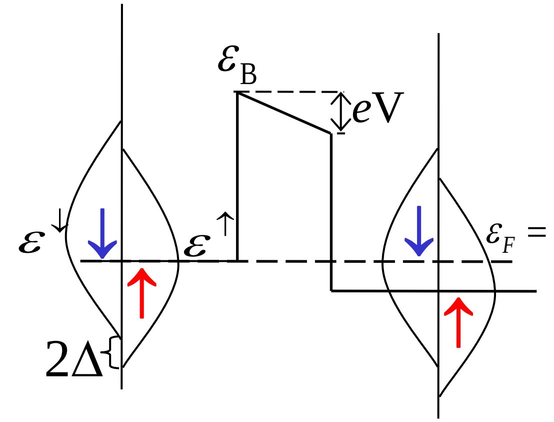
Back to tunnel junctions

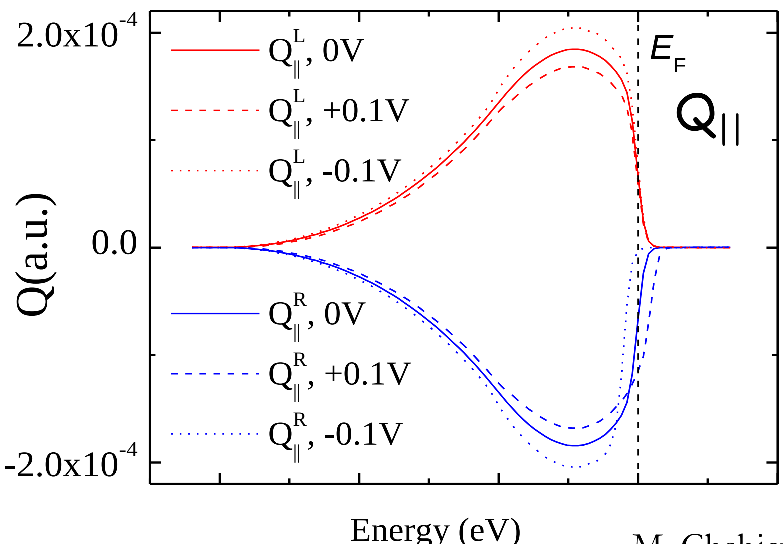


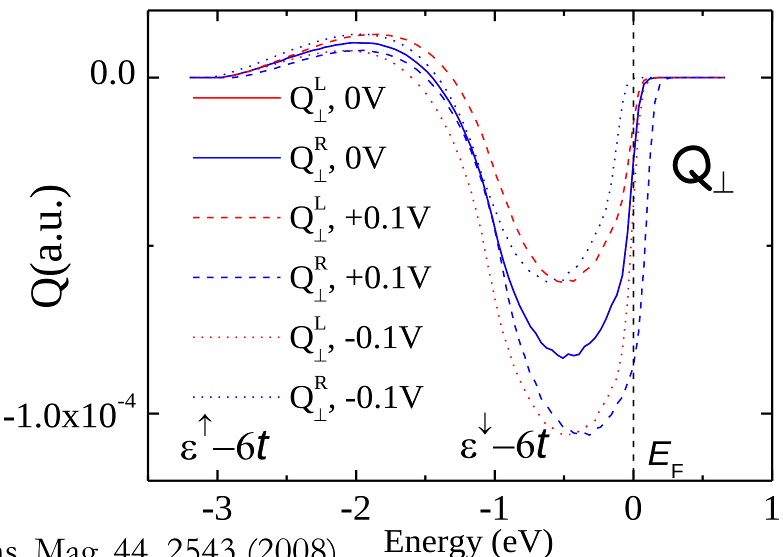
$$\mathbf{Q} = \mathbf{Q}^{L} + \mathbf{Q}^{R}$$

$$\mathbf{T} = \sum_{\lambda'=0}^{\infty} \mathbf{T}_{\lambda'} = \sum_{\lambda'=0}^{\infty} \mathbf{Q}_{\lambda'-1} - \mathbf{Q}_{\lambda'} = \mathbf{Q}_{-1} - \mathbf{Q}_{\infty} = \mathbf{Q}_{-1}$$







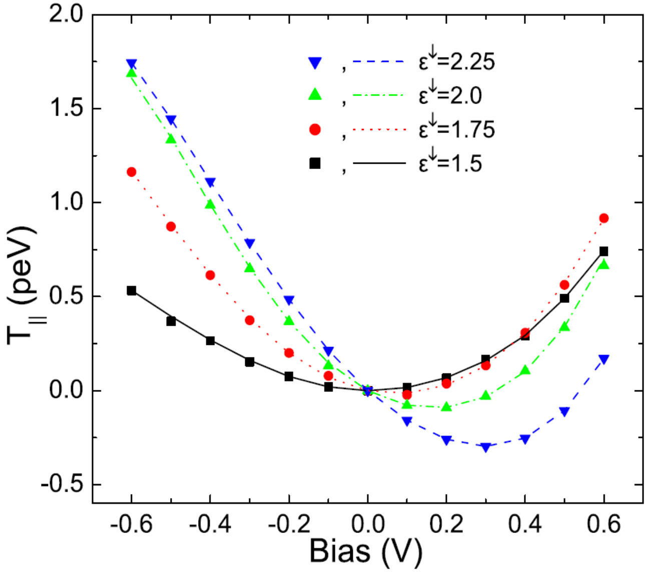


M. Chshiev et al, IEEE Trans. Mag. 44, 2543 (2008)
D. Ralph and M.Stiles, JMMM 320, 1190 (2008)

$T_{\parallel}$ is zero at zero voltage and is non monotonic function of applied voltage

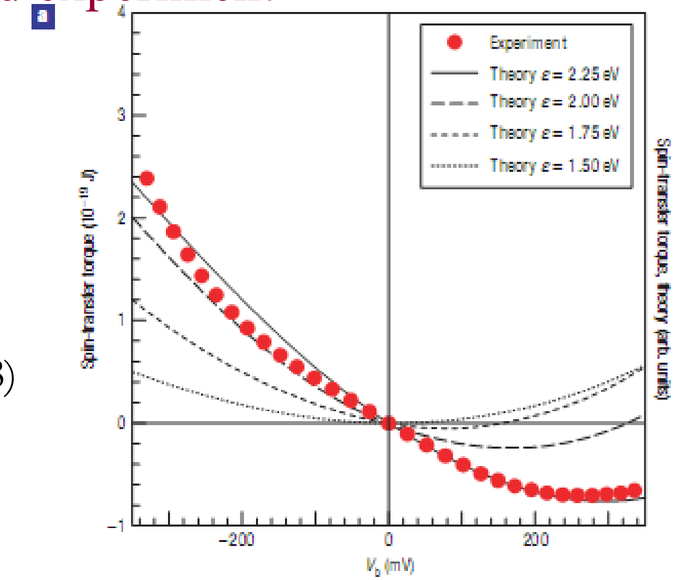
$T_{\perp}$ is an even parity function of applied voltage!

Total torques: Comparison of theory and experiment

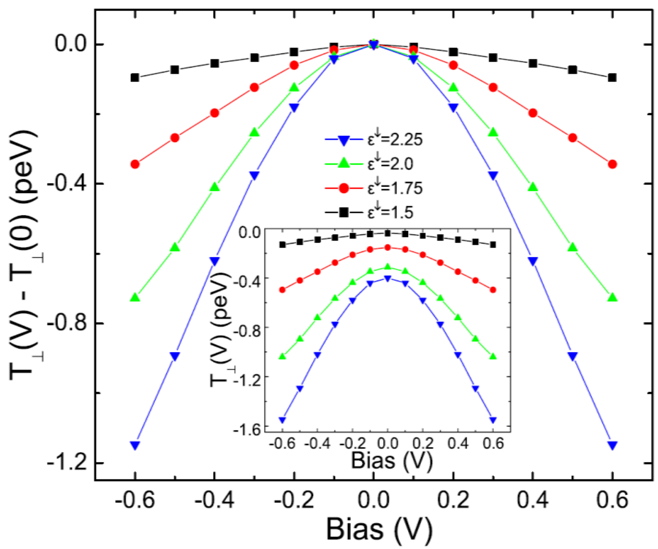


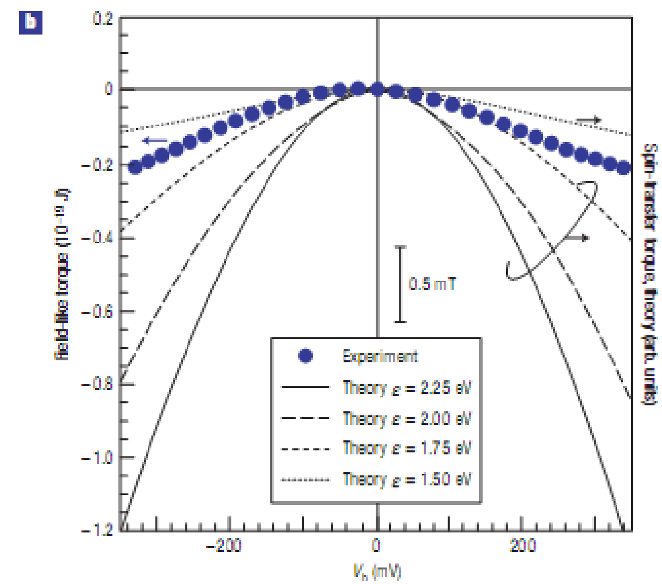
$T_{\parallel}$

theory
PRL 97, 237205 (2006)
IEEE Trans. Mag. 44, 2543 (2008)



H. Kubota et al,
Nature Physics 4, 37 (2008)



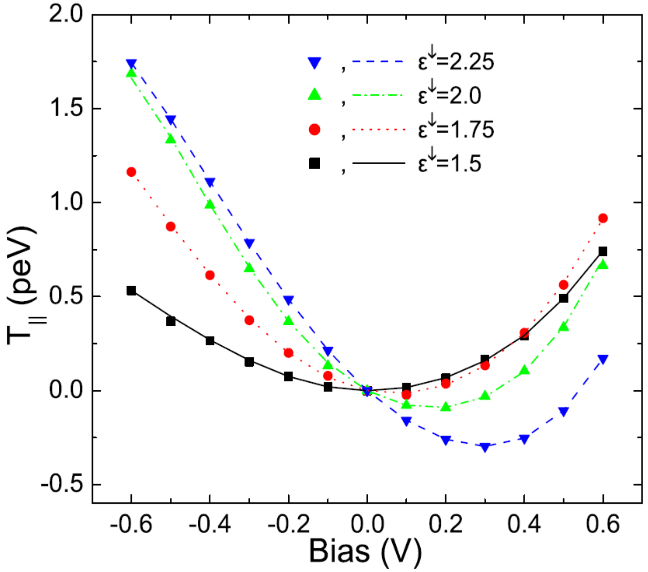


$T_{\perp}$

(field-like)

$$T_{\perp} = T_{\perp}^{0} + \sum C_{2i} V^{2i}$$

Total torques: Comparison of theory and experiment



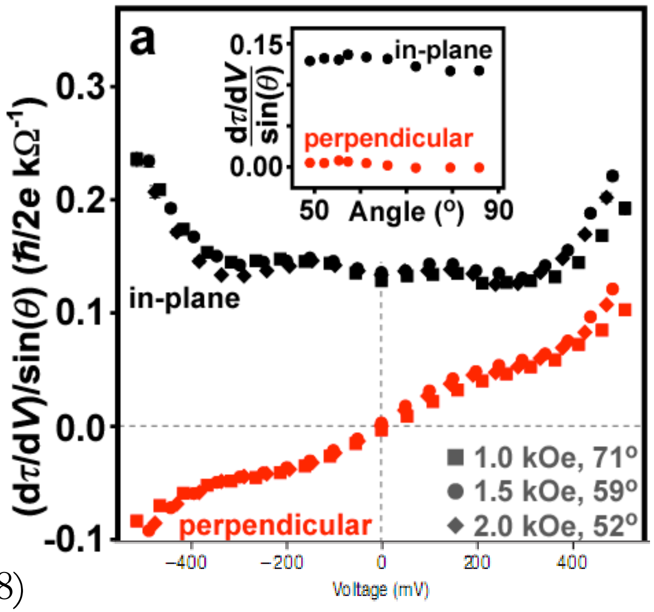
$T_{\parallel}$

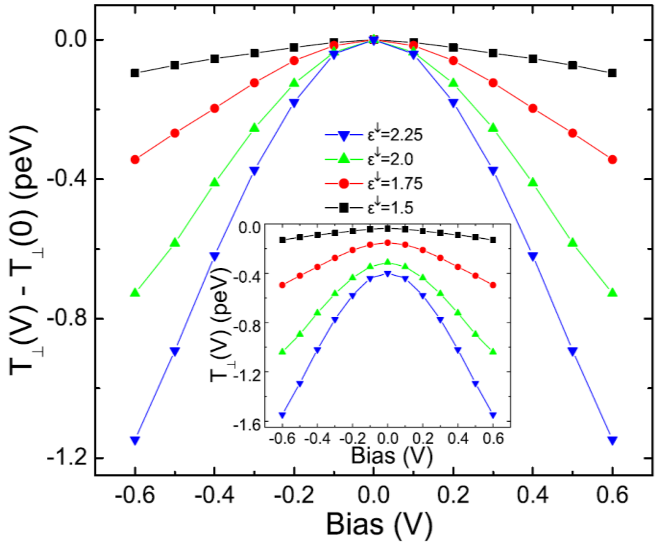
~V

theory
PRL 97, 237205 (2006)
IEEE Trans. Mag. 44, 2543 (2008)

H. Kubota et al,
Nature Physics 4, 37 (2008)

J. C. Sankey et al, *ibid.* 4, 67 (2008)





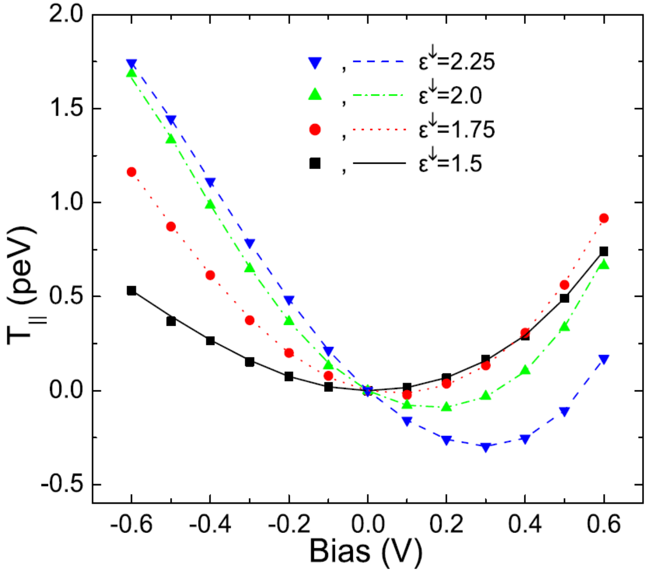
~V²

$T_{\perp}$

(field-like)

$$T_{\perp} = T_{\perp}^{0} + \sum C_{2i} V^{2i}$$

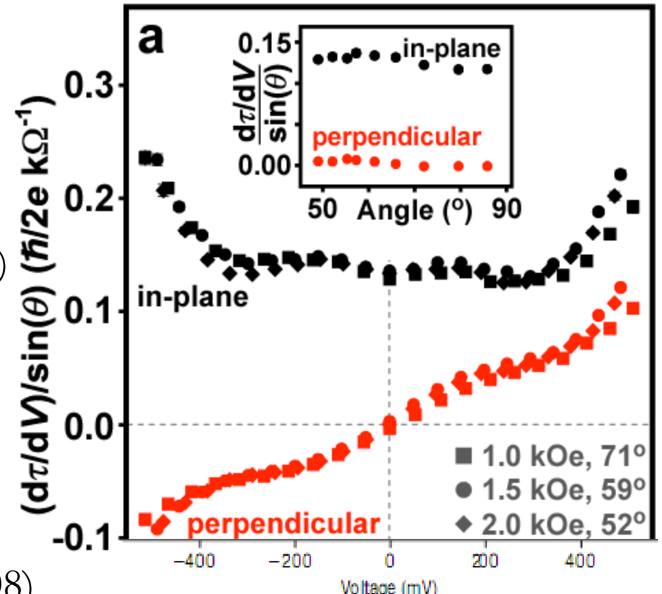
Total torques: Comparison of theory and experiment



$T_{\parallel}$

~V

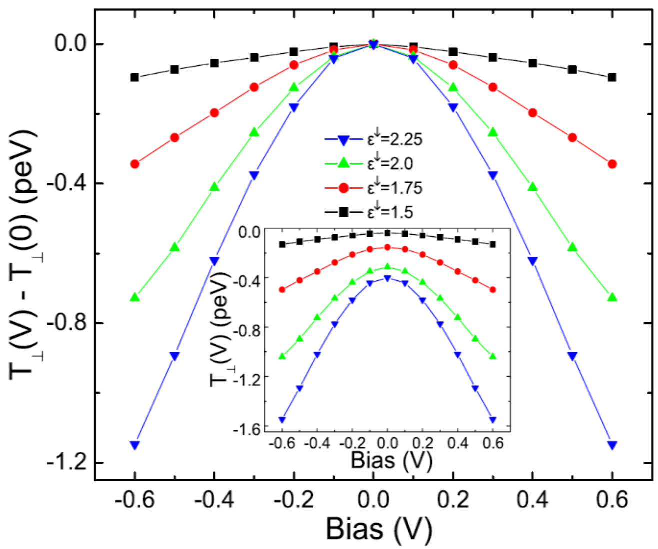
theory
I. Theodonis et al,
PRL 97, 237205 (2006)
IEEE Trans. Mag. 44, 2543 (2008)



H. Kubota et al,
Nature Physics 4, 37 (2008)

J. C. Sankey et al, *ibid.* 4, 67 (2008)

A. Deac, *ibid.* 4, 803 (2008)



C. Heiliger et al, PRL 100, 186805 (2008)
A. Manchon et al, JPCM 20, 145208 (2008)
M. Wilczyński et al., PRB 77, 054434 (2008)
J. Xiao et al., PRB 77, 224419 (2008)

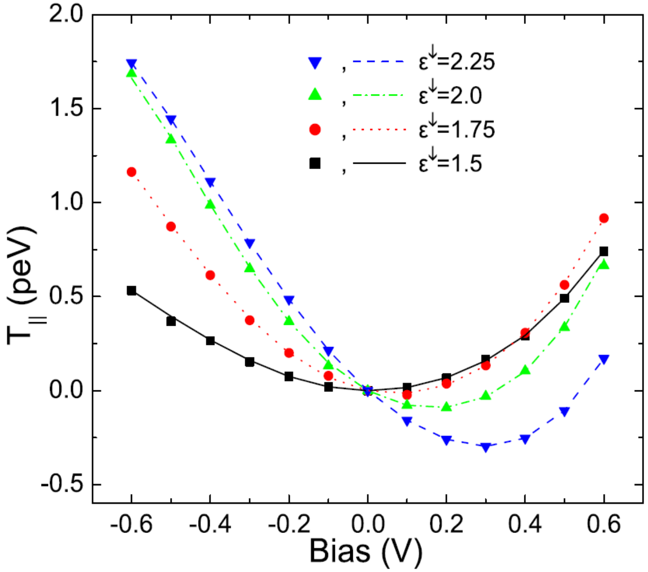
~V²

$T_{\perp}$

(field-like)

$$T_{\perp} = T_{\perp}^{0} + \sum C_{2i} V^{2i}$$

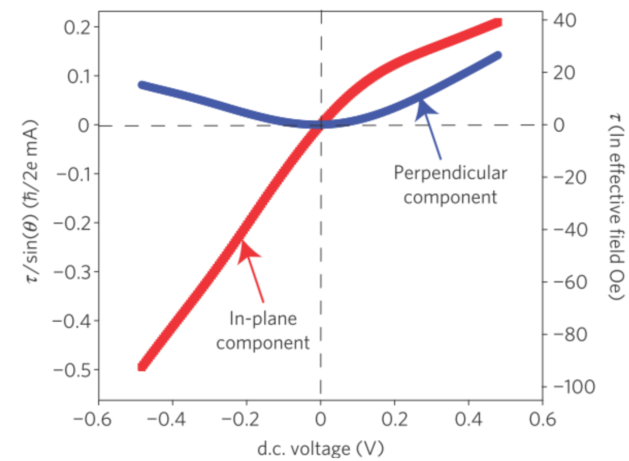
Total torques: Comparison of theory and experiment



$T_{\parallel}$

theory
I. Theodonis et al,
PRL 97, 237205 (2006)
IEEE Trans. Mag. 44, 2543 (2008)

C. Wang et al., Nature Phys. (2011)



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Nature Physics 4, 37 (2008)

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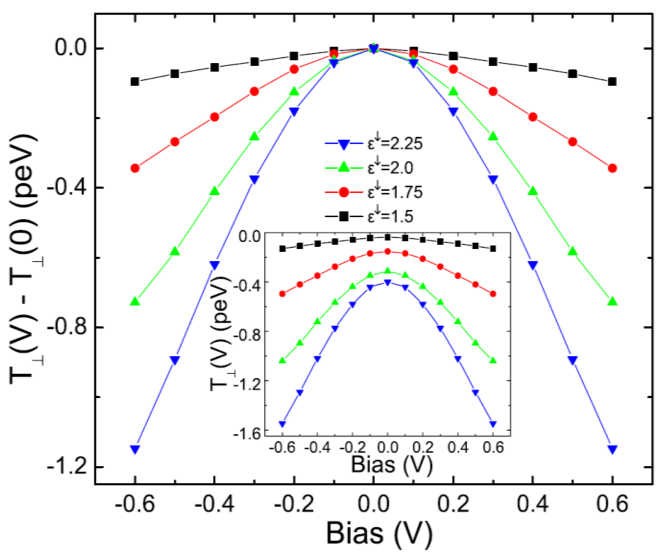
A. Deac, *ibid.* 4, 803 (2008)



C. Heiliger et al, PRL 100, 186805 (2008)
A. Manchon et al, JPCM 20, 145208 (2008)
M. Wilczyński et al., PRB 77, 054434 (2008)
J. Xiao et al., PRB 77, 224419 (2008)

$\sim V^2$

$T_{\perp}$
(field-like)

$$T_{\perp} = T_{\perp}^{0} + \sum C_{2i} V^{2i}$$

In-plane torque ($T_{||}$) for symmetric MTJ

The parallel (Slonczewski) torque $T_{||}$ may be found from collinear currents

$$T_{\|}(\gamma) = \frac{\hbar}{4e}\left[Q_z(\pi) - Q_z(0)\right]\mathbf{M}'\times(\mathbf{M}\times\mathbf{M}'); \quad Q_z(\gamma) = J^{\uparrow\uparrow}(\gamma) - J^{\downarrow\downarrow}(\gamma)$$

Brinkman model:

I. Theodonis et al, PRL 97, 237205, 2006

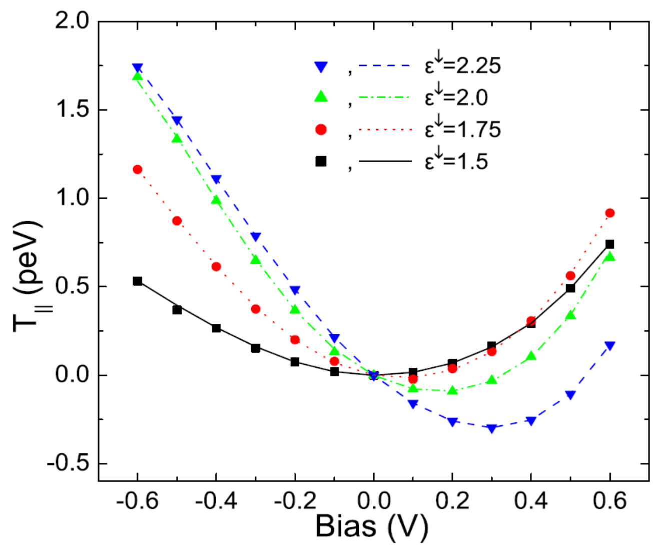
$$J^{\sigma}(V) = \xi_1(\overline{\Phi}^{\sigma})V - \xi_2(\overline{\Phi}^{\sigma})\Delta\Phi^{\sigma}V^2 + O(V^3), \text{where } \overline{\Phi}^{\sigma} = (\Phi_1^{\sigma} + \Phi_2^{\sigma})/2, \quad \Delta\Phi^{\sigma} = \Phi_1^{\sigma} - \Phi_2^{\sigma}$$

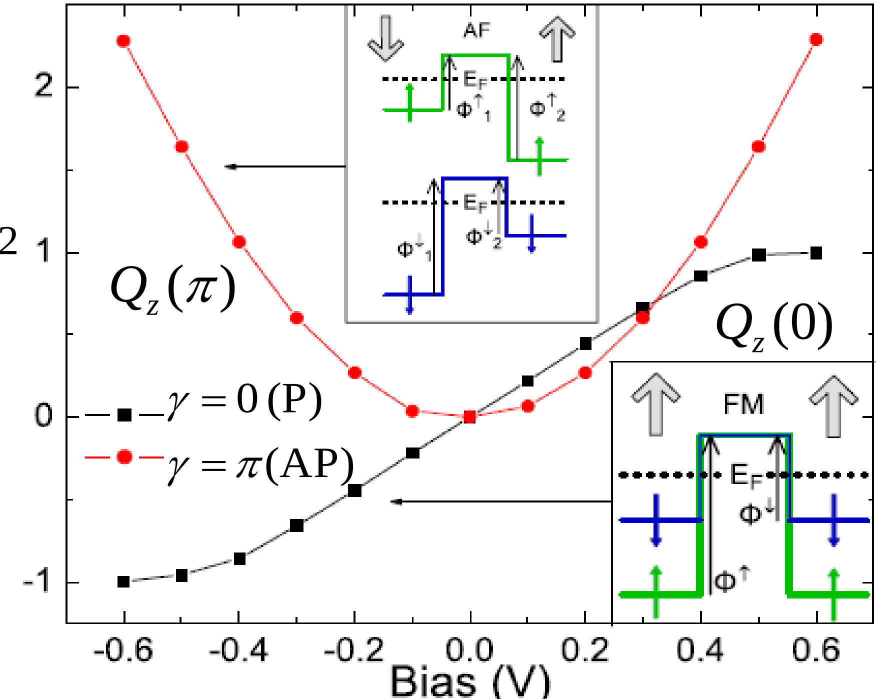
Parallel magnetizations:

$$\overline{\Phi}^{\uparrow} \neq \overline{\Phi}^{\downarrow}, \Delta\Phi^{\uparrow} = \Delta\Phi^{\downarrow} = 0 \Rightarrow Q_z(0) \propto V$$

Antiparallel magnetizations:

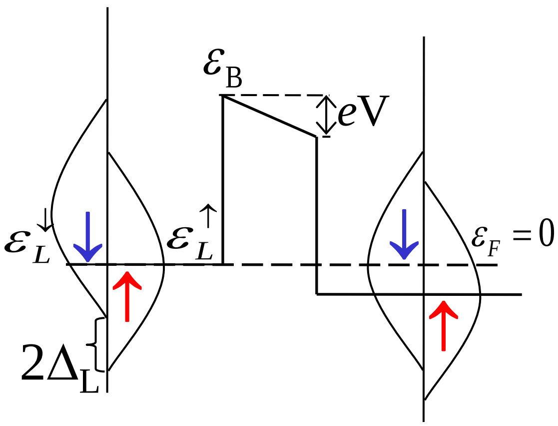
$$\overline{\Phi}^{\uparrow} = \overline{\Phi}^{\downarrow}, \Delta\Phi^{\uparrow} = -\Delta\Phi^{\downarrow} \Rightarrow Q_z(\pi) \propto V^2$$





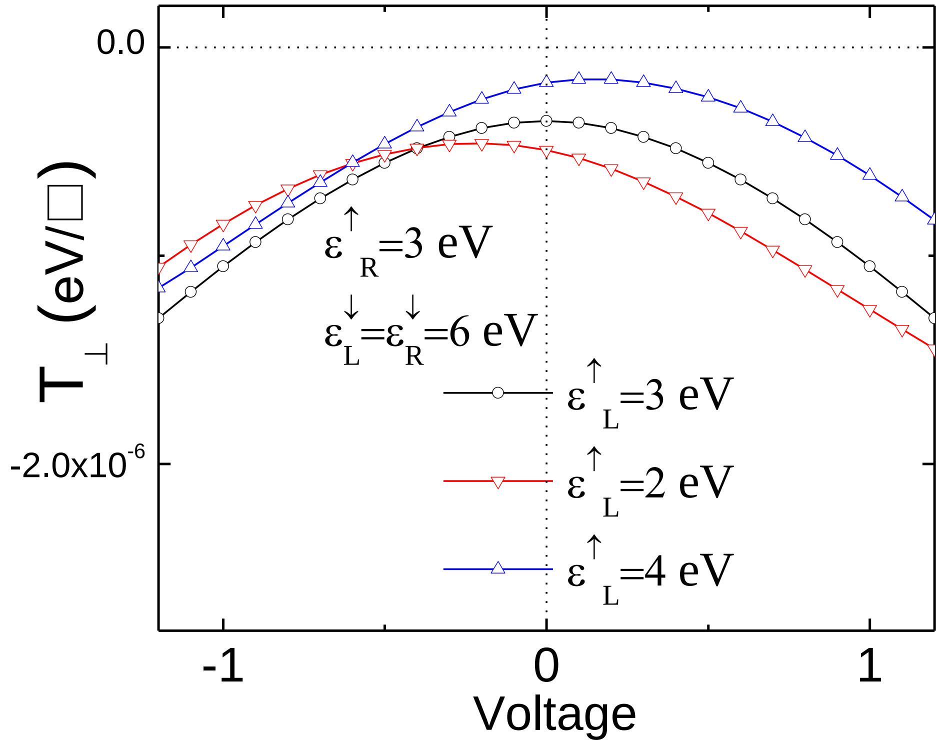
$Q_z(0)$ may vanish $\Rightarrow$ $T_{||}$ α V^2

Field-like torque ($T_\perp$) for (a)symmetric MTJ



$$\varepsilon^0_{L(R)} = \frac{\varepsilon^\uparrow_{L(R)} + \varepsilon^\downarrow_{L(R)}}{2}, \Delta_{L(R)} = \frac{\varepsilon^\downarrow_{L(R)} - \varepsilon^\uparrow_{L(R)}}{2}$$

$$\begin{cases} \varepsilon^\uparrow_{L(R)} = \varepsilon^0_{L(R)} - \Delta_{L(R)} \\ \varepsilon^\downarrow_{L(R)} = \varepsilon^0_{L(R)} + \Delta_{L(R)} \end{cases}$$



Symmetric MTJ:

$T_\perp$ is an even parity function of applied voltage:

$$T_\perp = \sum_i C_{2i} V^{2i}$$

(I. Theodonis et al, PRL 97, 237205 (2006); M. Chshiev et al, IEEE Trans. Mag. 44, 2543 (2008))

Asymmetric MTJ (deviations from V²):

$T_\perp$ with odd parity terms appeared :

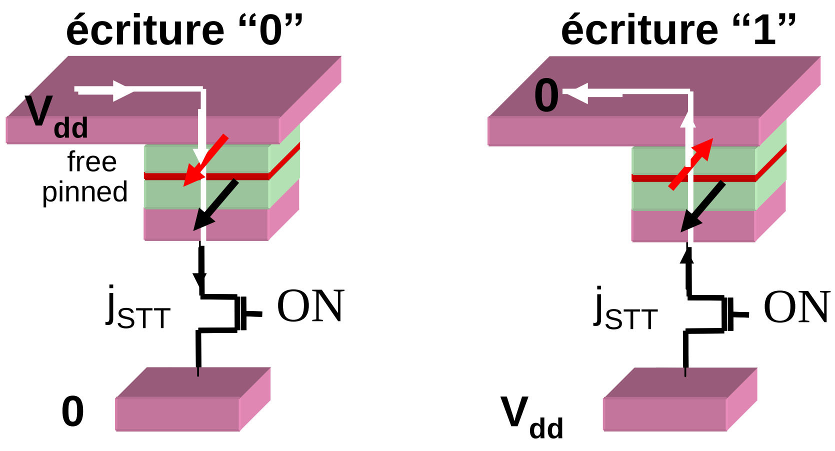
$$T_\perp = \sum_i C_i V^i$$

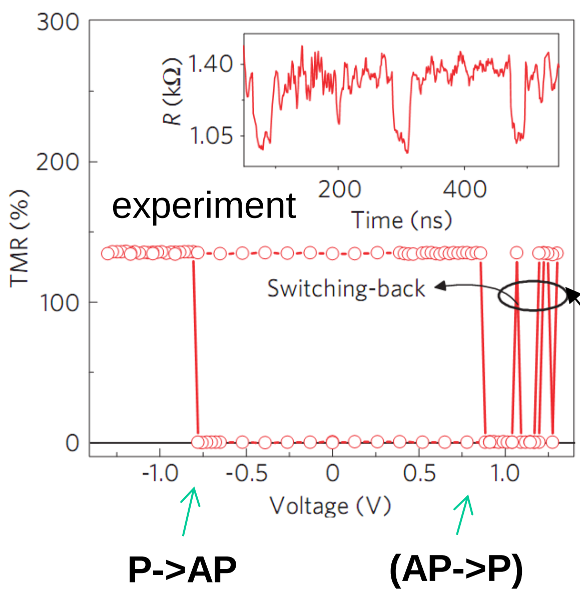
(C_1 in A. Manchon et al, JPCM 20, 145208 (2008); M. Wilczyński et al., PRB 77, 054434) ; Xiao et al., PRB 77, 224419 (2008); S.-C. Oh et al, Nature Physics 5, 898 (2009))

Spin Transfer Torques in Magnetic Tunnel Junctions

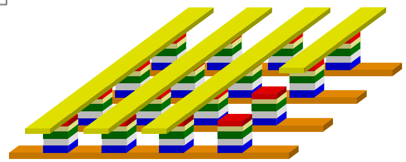
Uncontroled phenomenon during «bit» writing in STT-MRAMs: "back-switching"

Spin transfer MRAM: (STT-MRAM)





back switching is a problem for MRAM



Could theory help understanding a problem?

Yes!

2015 CLUJ-NAPOCA ROMANIA

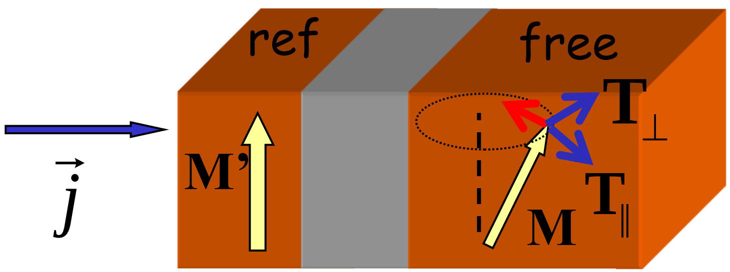
Spin Transfer Torques in Magnetic Tunnel Junctions

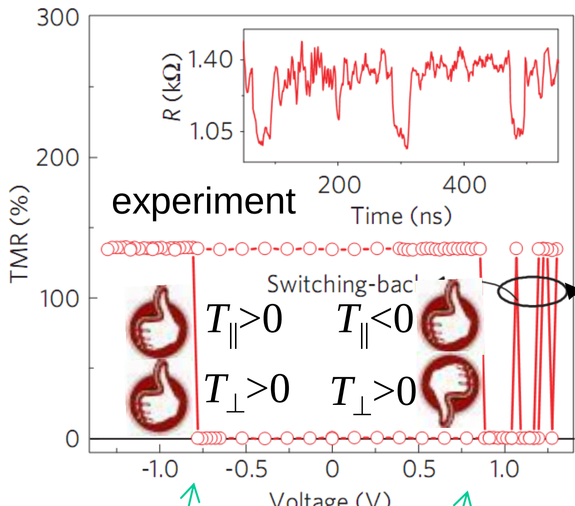
Landau-Lifshitz-Gilbert (LLG) equation:

precession — damping — Slonczewski — field-like

$$\frac{d\mathbf{M}}{dt} = -\gamma_0 \mathbf{M}\times\mathbf{H} + \frac{\alpha}{M_s}\mathbf{M}\times\frac{d\mathbf{M}}{dt} - \frac{|g_e|\mu_B}{\hbar}\left(T_{\parallel}\mathbf{M}\times\mathbf{M}\times\mathbf{M}' + T_{\perp}\mathbf{M}'\times\mathbf{M}\right)$$

STT: Current acts on Magnetization





P->AP **(AP->P)**

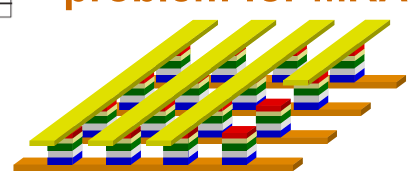
For symmetric MTJ theory predicted:

$$T_{\perp} \;\alpha\; V^2 \;;\; T_{//} \;\alpha\; -V$$

I. Theodonis et al, PRL 97, 237205 (2006)
M. Chshiev et al, IEEE Trans. Mag. 44, 2543 (2008)
A. Manchon et al, JPCM 20, 145208 (2008)
A. Kalitsov et al, PRB 79, 174416 (2009)

For V>0:
$T_{\perp}(V) = - T_{\parallel}(V)$

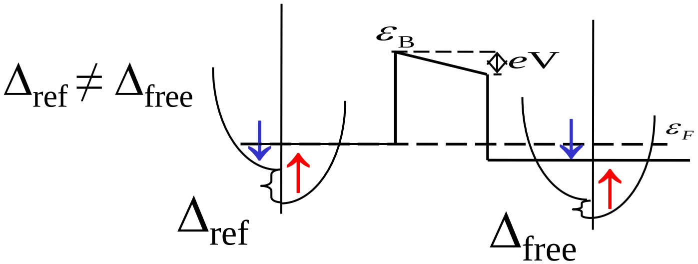
back switching is a problem for MRAM



Could theory provide a solution for backswitching?

Yes!

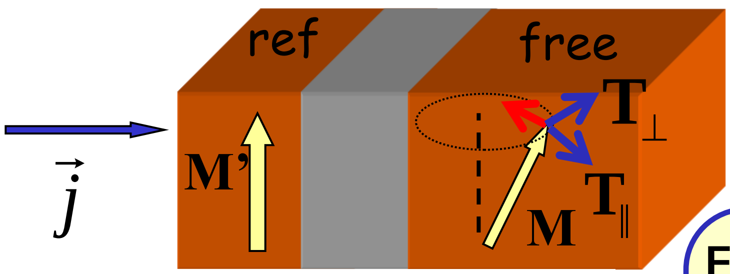
Spin Transfer Torques in Magnetic Tunnel Junctions

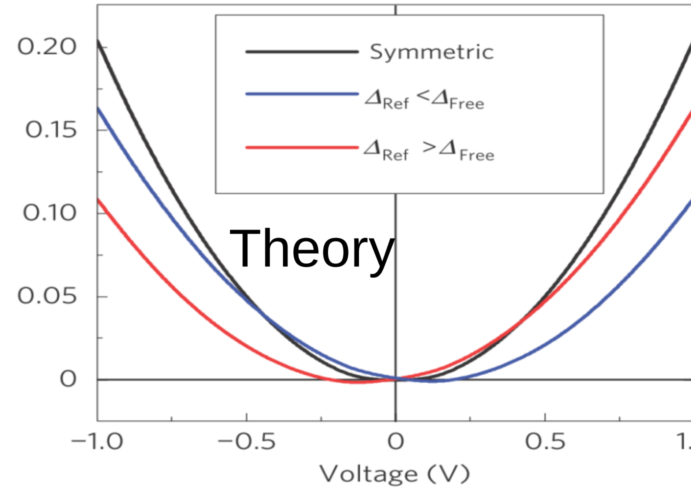


For asymmetric MTJ theory predicts linear term $T_\perp = \sum_i C_i V^i$ (which is also observed in experiment)

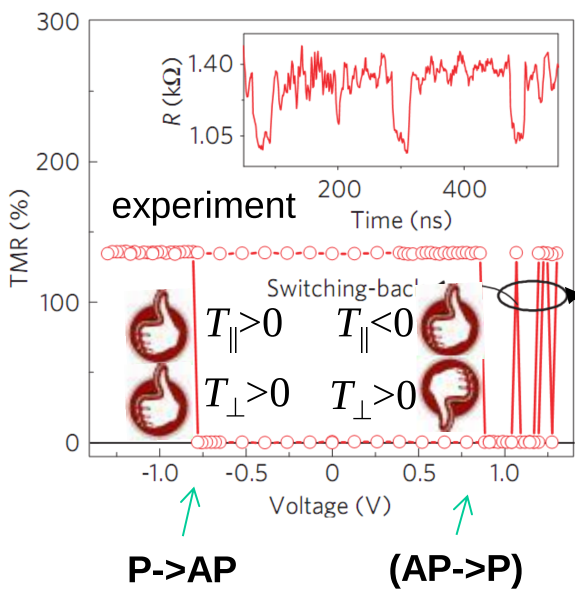
S.-C. Oh, S.-Y. Park, A. Manchon, M. Chshiev et al, ***Nature Physics*** 5, 898 (2009)

STT: Current acts on Magnetization

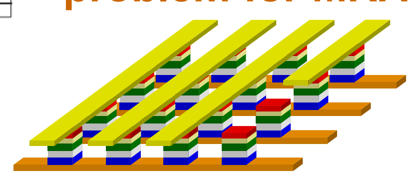


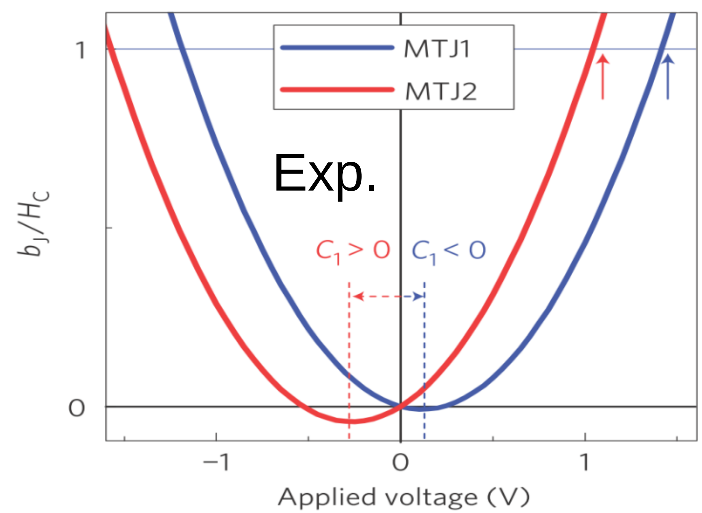


For asymmetric MTJs ($\Delta_{ref} < \Delta_{free}$) backswitching voltage can be shifted up (blue curves) away from writing voltage



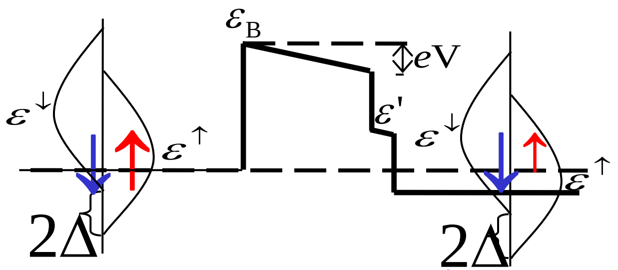
back switching is a problem for MRAM



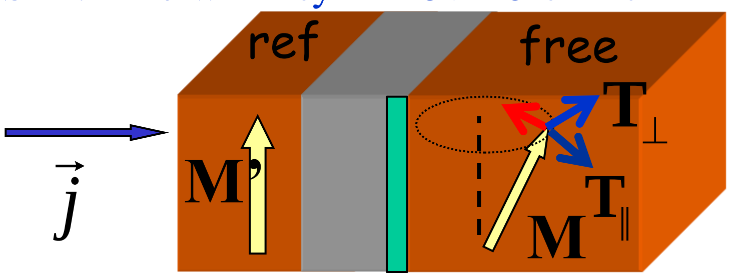


Spin Transfer Torques and TMR in Magnetic Tunnel Junctions

STT and TMR voltage dependence tuning by Interface engineering



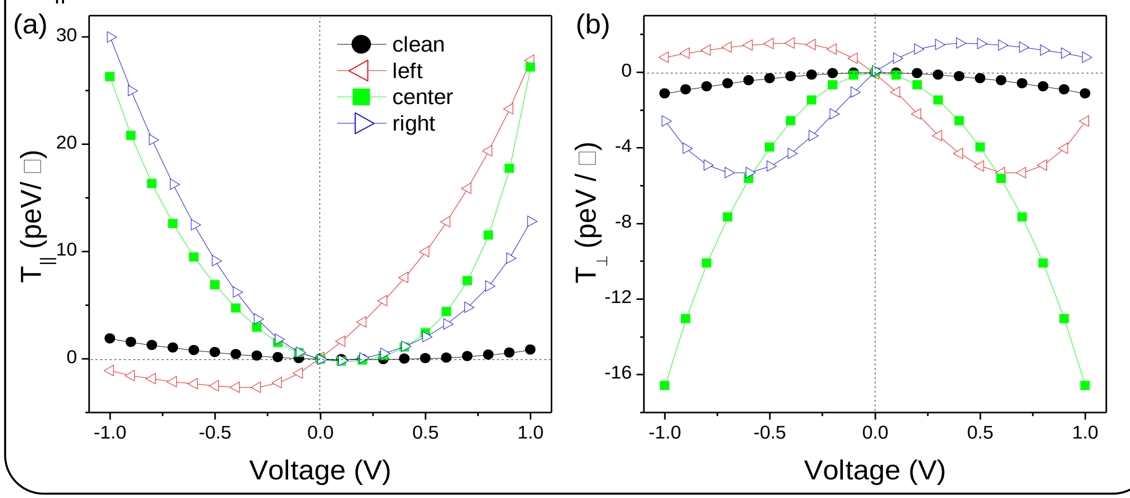
STT: MTJ with asymmetric barrier



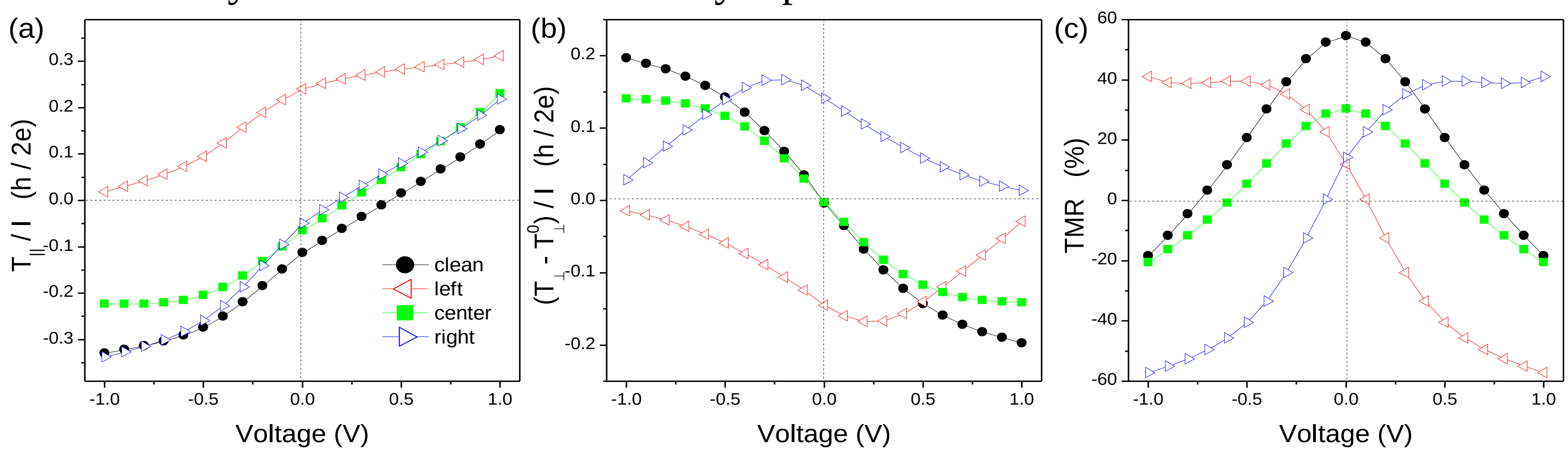
A. Kalitsov et al, PRB 88, 104430 (2013)

$\varepsilon' < \varepsilon_B - 6t$ **(resonant regime)** $\varepsilon' > \varepsilon_B - 6t$ (tunneling regime)

$T_\parallel(V)$ and $T_\perp(V)$ vs additional layer position in the barrier



STT efficiency and TMR vs additional layer position in the barrier



Spin Transfer Torques and TMR in Multiferroic Magnetic Tunnel Junctions

See lecture of A. Barthelemy

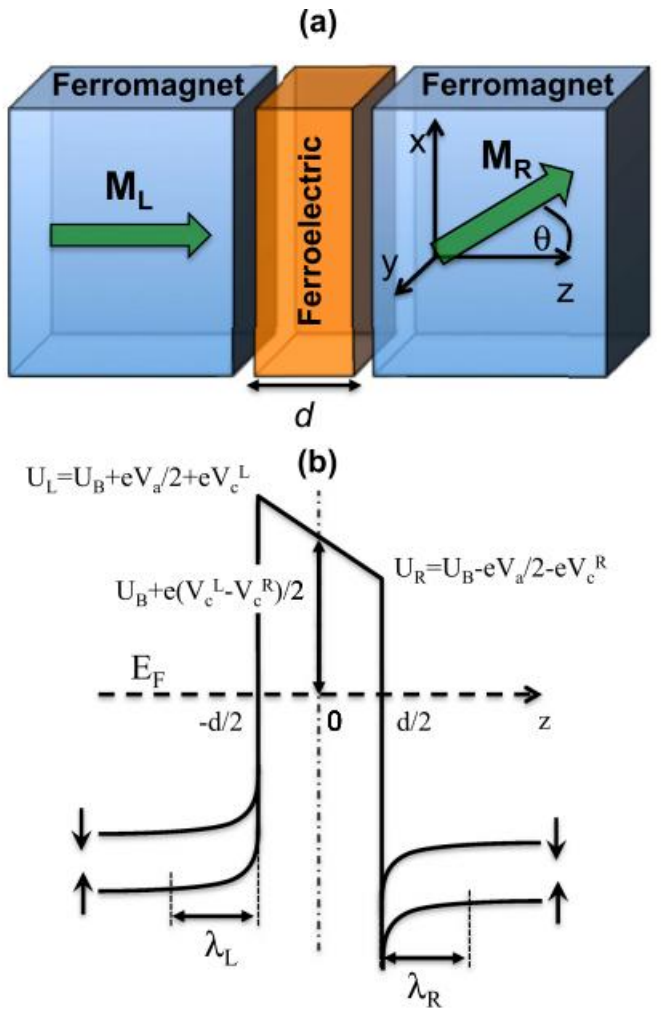


FIG. 1. (Color online) (a) Schematics of a magnetic tunnel junction comprising two ferromagnets and a ferroelectric insulator; (b) Potential profile of the junction with positive polarization (screening) and applied voltage V_a.

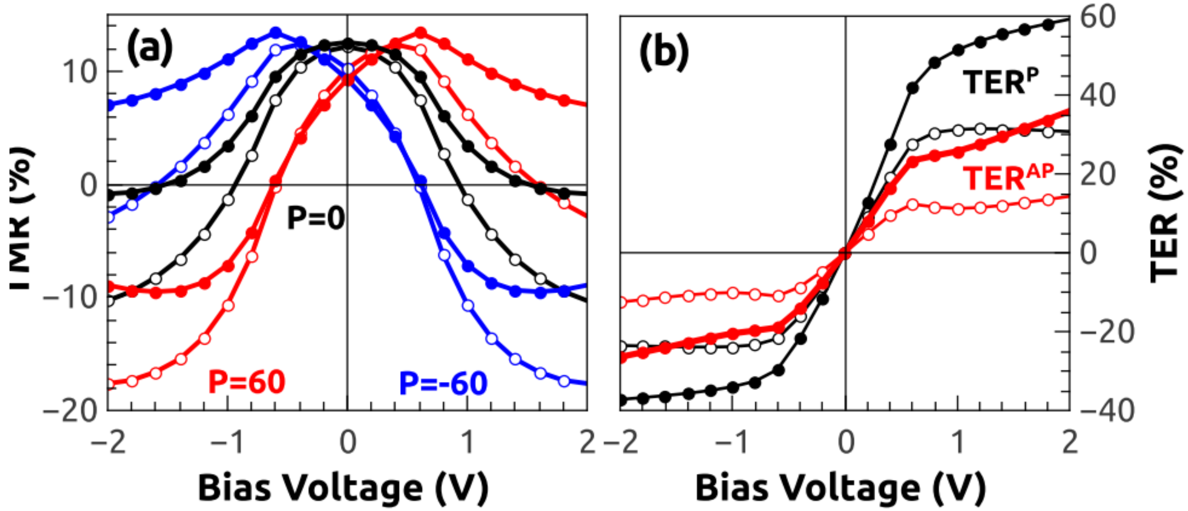


FIG. 2. (Color online) Voltage dependence of (a) TMR for zero (black symbols), positive (red symbols), and negative (blue symbols) FEP and (b) TER for P (black symbols) and AP (red symbols) configurations. The parameters are the same as in the text, with $U_B = 2$ eV, $P = 0, \pm 60\,\mu C/cm^2$, and $d = 1$ nm (open symbols) or 1.5 nm (filled symbols), corresponding to $V_c^{L,R} \approx 0.35$ V and 0.5 V, respectively.

A. Useinov, M. Chshiev and A. Manchon, ***Phys. Rev. B*** 91, 064412 (2015)

Spin Transfer Torques and TMR in Multiferroic Magnetic Tunnel Junctions

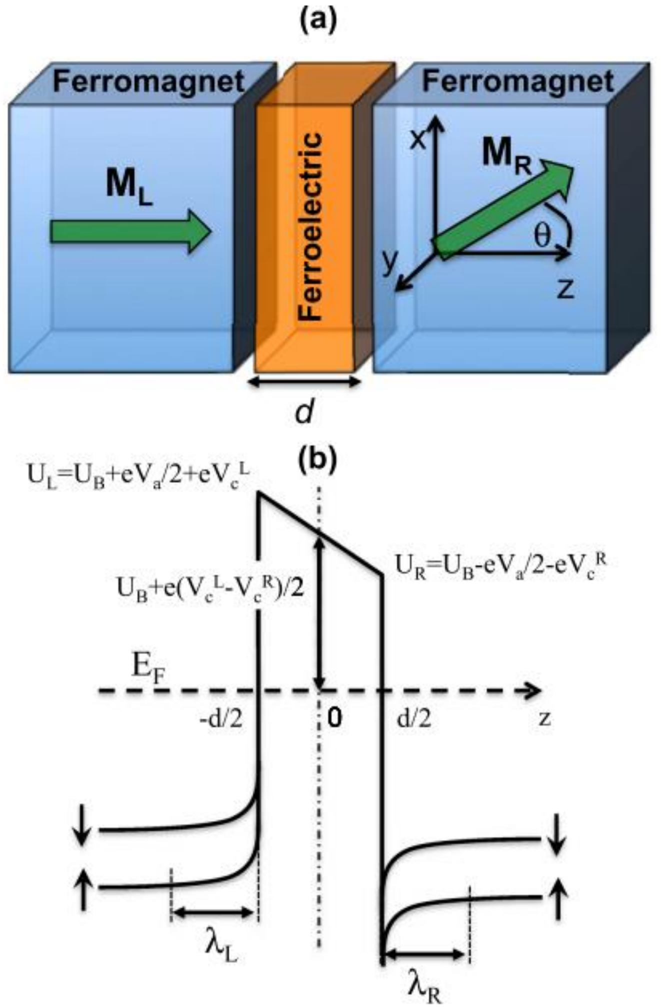


FIG. 1. (Color online) (a) Schematics of a magnetic tunnel junction comprising two ferromagnets and a ferroelectric insulator; (b) Potential profile of the junction with positive polarization (screening) and applied voltage V_a.

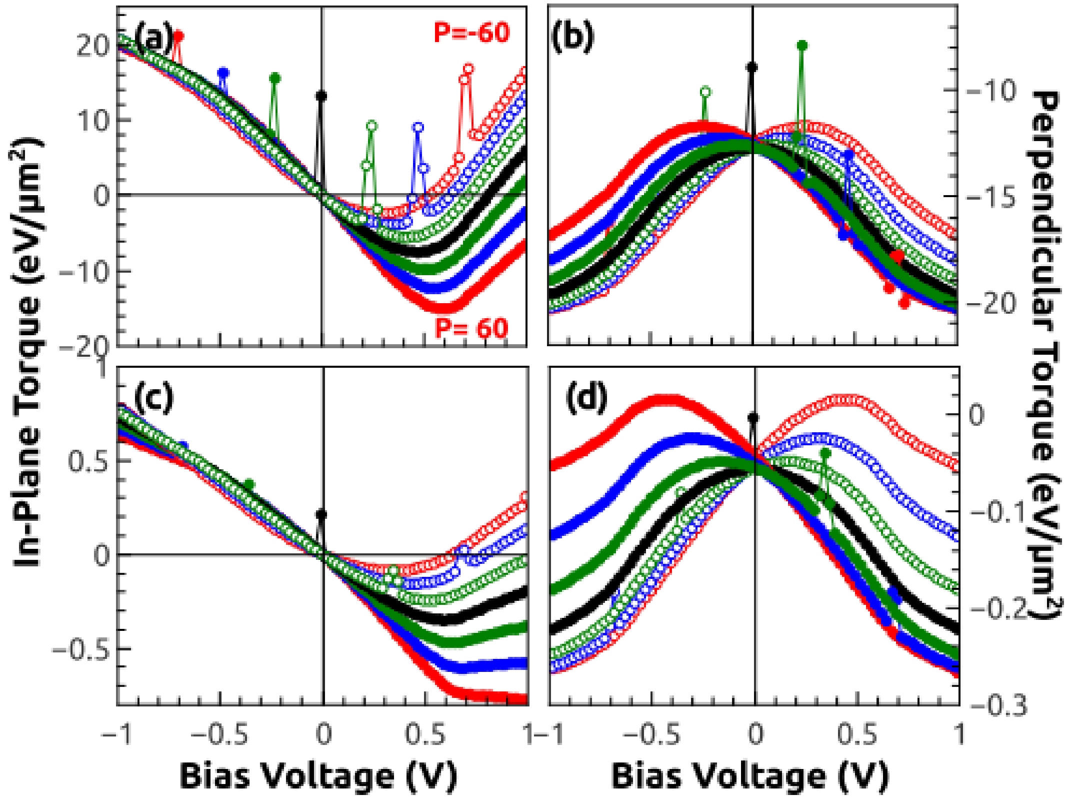


FIG. 3. (Color online) Voltage dependence of the (a,c) in-plane and (b,d) out-of-plane torques exerted on the right layer for $P = 0\ \mu C/cm^2$ (black symbols), $P = \pm 20\ \mu C/cm^2$ (green symbols), $P = \pm 40\ \mu C/cm^2$ (blue symbols), and $P = \pm 60\ \mu C/cm^2$ (red symbols). The parameters are $U_B = 2$ eV (a,b) $d = 1$ nm and (c,d) $d = 1.5$ nm, with $\theta = \pi/2$. The filled and open symbols refer to positive and negative FEP, respectively.

A. Useinov, M. Chshiev and A. Manchon, ***Phys. Rev. B*** 91, 064412 (2015)

Spin Filtering (SF) based on magnetic insulators (EuO, EuS, ferrites, etc.)

See lecture of S. Valenzuela

PHYSICAL REVIEW B **69**, 241203(R) (2004)

Observation of spin filtering with a ferromagnetic EuO tunnel barrier

Tiffany S. Santos* and Jagadeesh S. Moodera

Francis Bitter Magnet Laboratory, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA

(Received 19 April 2004; published 25 June 2004)

PHYSICAL REVIEW B **72**, 020406(R) (2005)

Spin filtering through ferromagnetic $BiMnO_3$ tunnel barriers

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[2]*Institut de Ciència de Materials de Barcelona, CSIC, Campus de la UAB, 08193 Bellaterra, Spain*

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[4]*Université d'Evry, rue du Père Jarlan, 91025 Evry, France*

[5]*Departamento de Física Aplicada i Òptica, Universitat de Barcelona, Diagonal 647, 08028 Barcelona, Spain*

(Received 19 April 2005; published 18 July 2005)

PHYSICAL REVIEW B **76**, 134412 (2007)

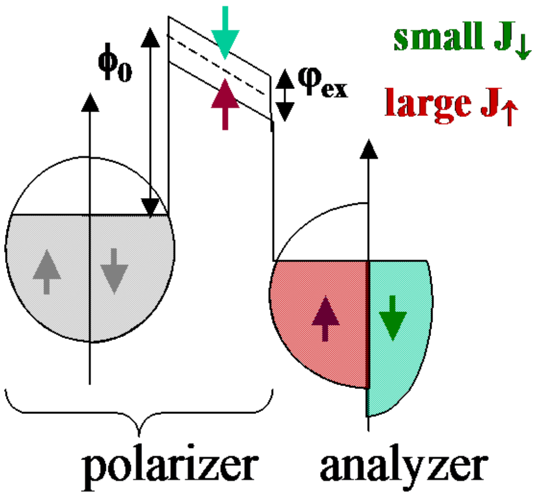
Bias dependence of tunnel magnetoresistance in spin filtering tunnel junctions: Experiment and theory

U. Lüders,[1] M. Bibes,[2] S. Fusil,[3] K. Bouzehouane,[3] E. Jacquet,[3] C. B. Sommers,[4] J.-P. Contour,[3] J.-F. Bobo,[1] A. Barthélémy,[3] A. Fert,[3] and P. M. Levy[3,5,*]

APPLIED PHYSICS LETTERS **91**, 122107 (2007)

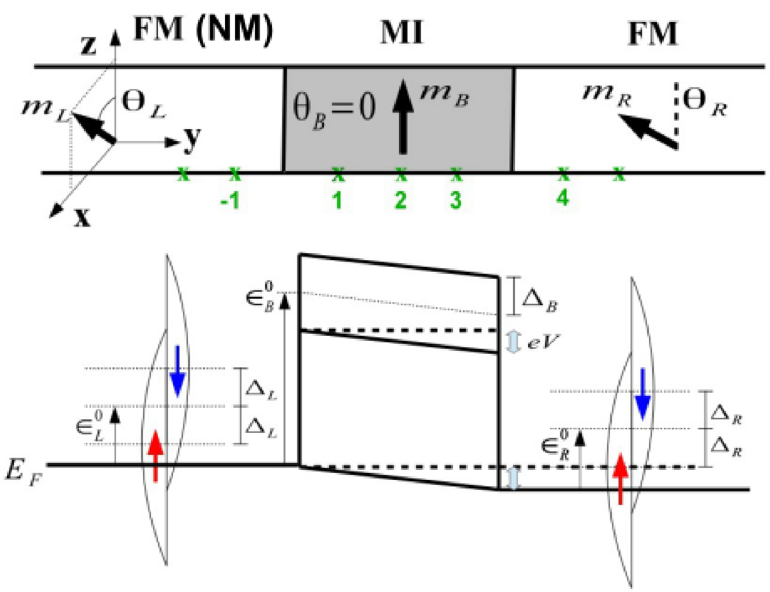
Room temperature spin filtering in epitaxial cobalt-ferrite tunnel barriers

A. V. Ramos[1], M.-J. Guittet[1], J.-B. Moussy[1], R. Mattana[2], C. Deranlot[2], F. Petroff[2], and C. Gatel[3]



STT in SFTJ and Tight Binding Model

Methodology: Semi-infinite leads separated by a finite barrier



$$H = H_L + H_R + H_B + H_{B|L} + H_{B|R}$$

$$H_L = \sum_{\sigma,\lambda} \epsilon_\lambda^\sigma c_\lambda^{\sigma\dagger} c_\lambda^\sigma + \sum_{\sigma,\lambda,\mu} t c_\lambda^{\sigma\dagger} c_\mu^\sigma \qquad H_{B|R} = \sum_\sigma t c_b^{\sigma\dagger} c_{\alpha'}^\sigma$$

$$H_R = \sum_{\sigma,\lambda'} \epsilon_{\lambda'}^\sigma c_{\lambda'}^{\sigma\dagger} c_{\lambda'}^\sigma + \sum_{\sigma,\lambda',\mu'} t c_{\lambda'}^{\sigma\dagger} c_{\mu'}^\sigma \qquad H_{B|L} = \sum_\sigma t c_a^{\sigma\dagger} c_\alpha^\sigma$$

$$H_B = \sum_i \epsilon_i^\sigma c_i^{\sigma\dagger} c_i^\sigma + \sum_{i,j} t c_i^{\sigma\dagger} c_j^\sigma$$

$$\epsilon_i^\sigma = \epsilon_B^\sigma - eV \frac{i-1}{N-1}$$

Isolated retarded Green functions:

⇩

Coupled retarded Green functions using Dyson equation:

⇩

Keldysh function using kinetic equation:

⇩

$$Q_R^{jy} = \frac{et}{2\pi\hbar} \int \mathrm{Tr}[(\hat{G}_{43}^{<} - \hat{G}_{34}^{<})\sigma_j] dE d\mathbf{k}_{||},$$

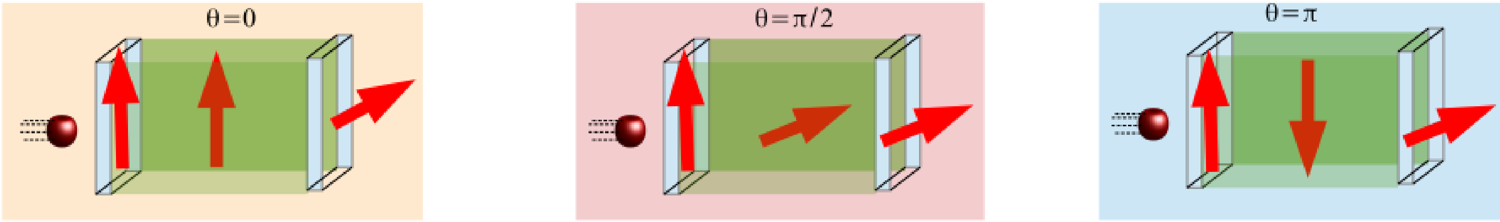
We adopt the following convention:

$$T_{||} \equiv Q_R^{xy} \cos\theta_R - Q_R^{zy} \sin\theta_R$$

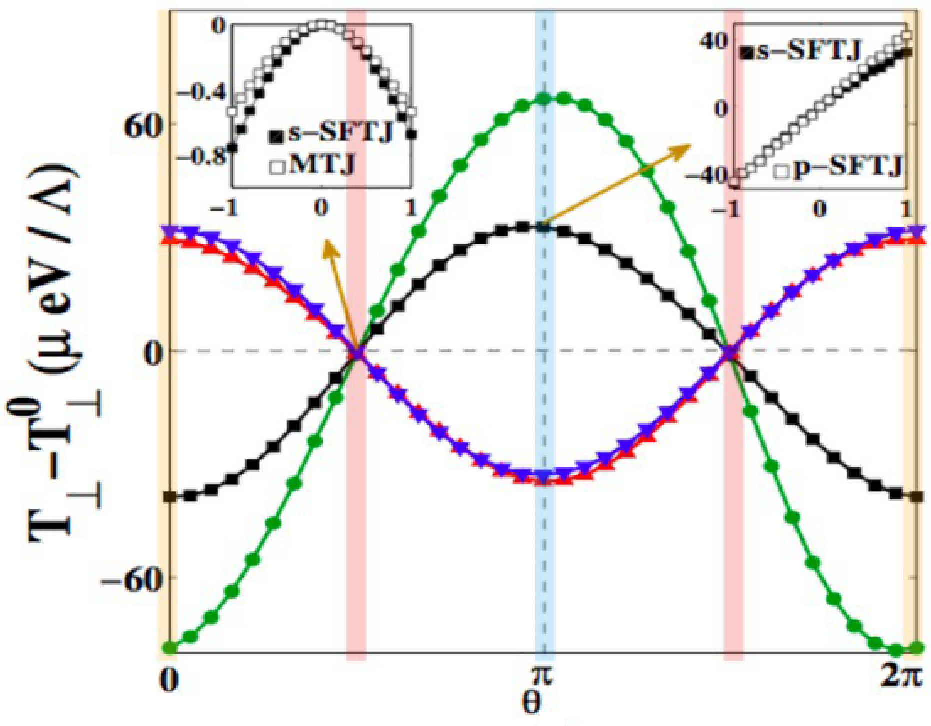
$$T_\perp \equiv Q_R^{yy}$$

C. Ortiz Pauyac et al, ***Phys. Rev. B*** 90, 235417 (2014)

Symmetric Spin Filter Tunnel Junction (1)



rotation of the magnetic insulating layer only



⇒

For all Band filling values, the perpendicular STT as a function of bias exhibits a quadratic behavior (red shadowed region) similar to MTJs when left lead perpendicular to MI, and a linear behavior (blue and orange shadowed regions), similar to p-SFTJ, when right lead is perpendicular to MI.

C. Ortiz Pauyac et al, ***Phys. Rev. B*** 90, 235417 (2014)

Spin Transfer Torques and TMR in Magnetic Tunnel Junctions

Spin filtering in crystalline MTJs (Fe|MgO|Fe)

W. H. Butler et al, PRB 63, 054416 (2001); IEEE Trans. Mag. 41 (2005) 2645

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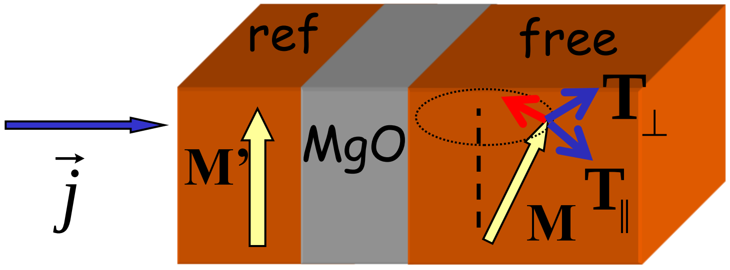

Models seems to be ok

Spin Transfer Torque (STT)

I. Theodonis et al, PRL 97, 237205 (2006)
A. Manchon et al, JPCM 20, 145208 (2008)
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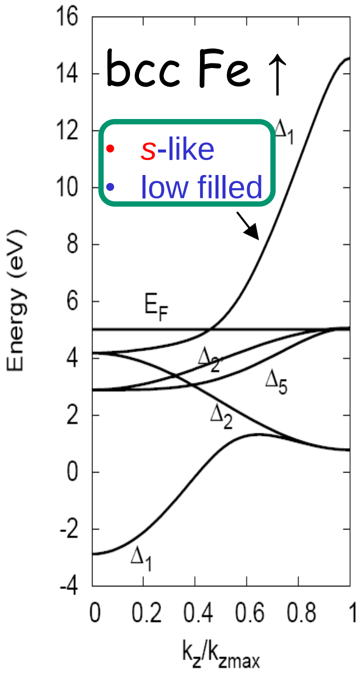
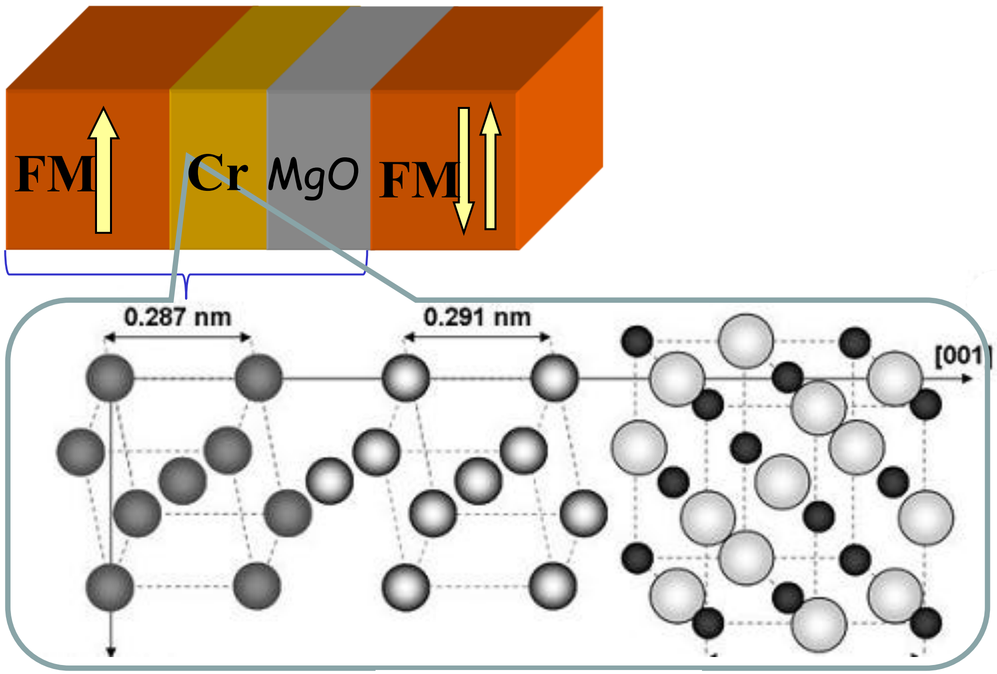
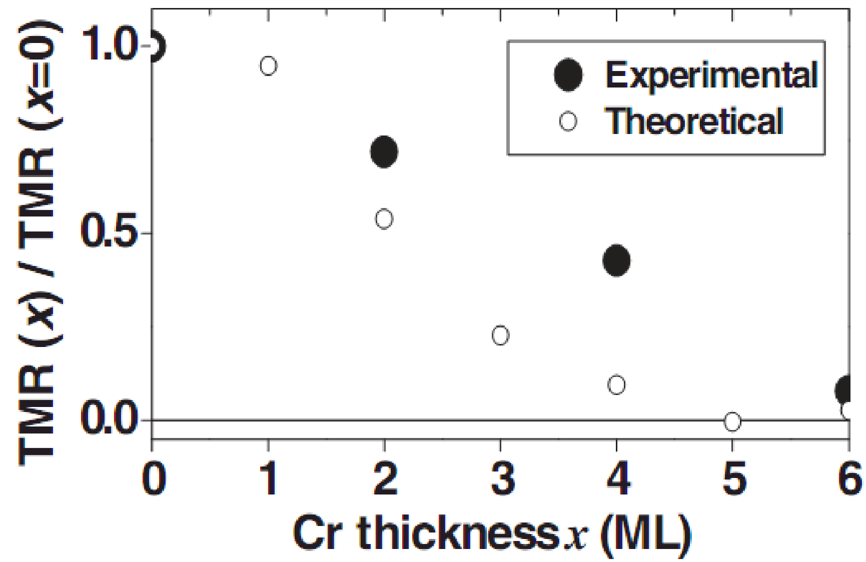
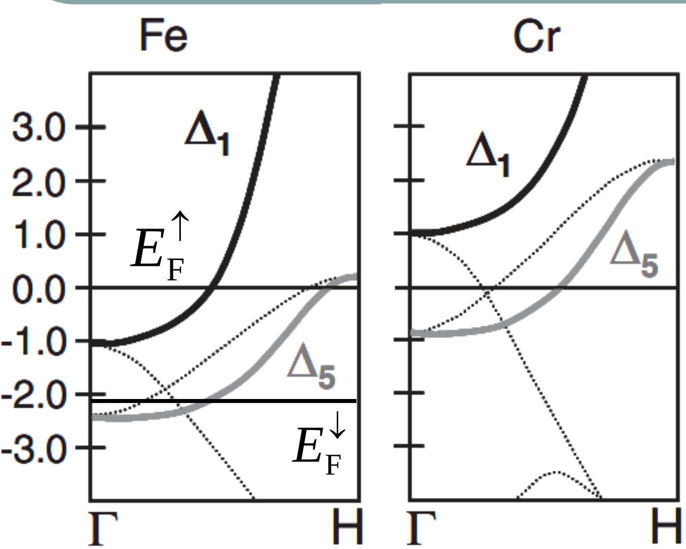


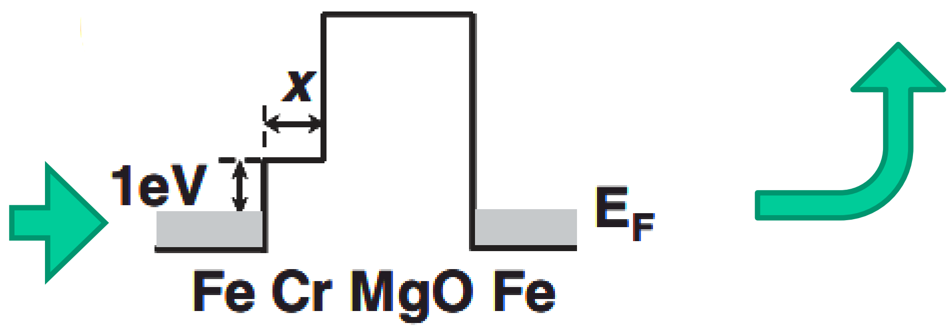
TMR in Fe|Cr|MgO|Fe Magnetic Tunnel Junctions



F. Greullet et al, PRL 99, 187202 (2007)



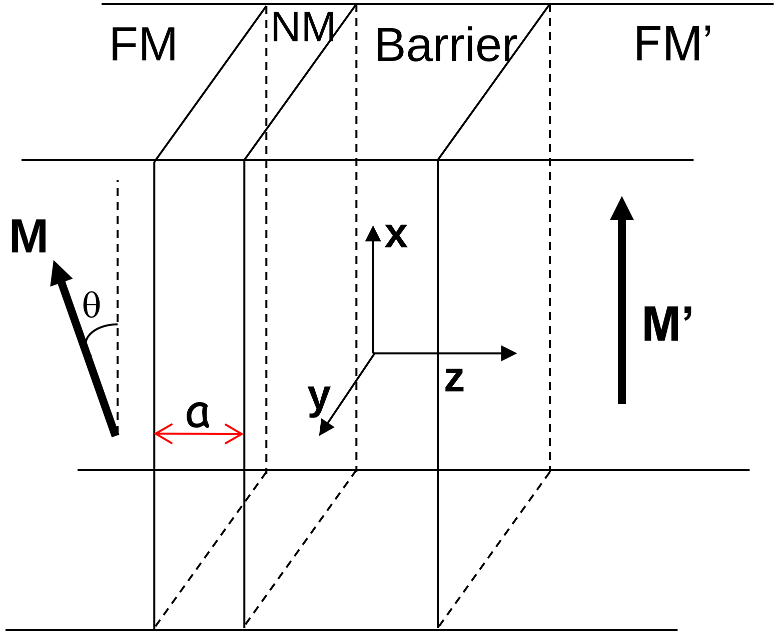




What about effect of Cr on STT?

Model (NEGF):

A. Manchon et al, JPCM, 20, 145208 (2008)



Charge current:

$$J \propto \iiint \kappa d\kappa dE \sum_{\sigma} \left(\frac{\partial}{\partial z'} - \frac{\partial}{\partial z} \right) G^{-+}_{\sigma\sigma}(z,z')\Big|_{z=z'}$$

Spin current:

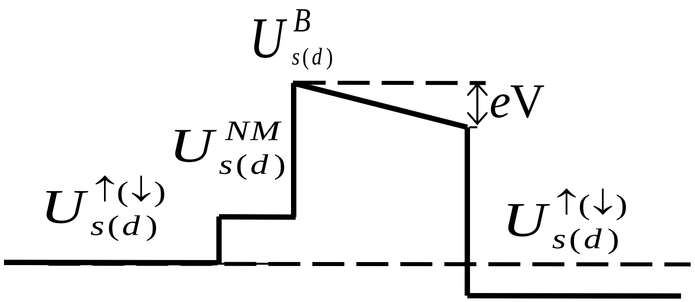
$$\mathbf{J}^{spin} \propto \iiint \kappa d\kappa dE \sum_{\sigma\sigma'} \mathbf{s}_{\sigma\sigma'} \otimes \left(\frac{\partial}{\partial z'} - \frac{\partial}{\partial z} \right) G^{-+}_{\sigma'\sigma}(z,z')\Big|_{z=z'}$$

Spin torque:

$$\mathbf{T} = -\nabla \bullet \mathbf{J}^{spin}$$

Current matrix:

$$\begin{pmatrix} J^{\uparrow\uparrow}_{s(d)} & J^{\uparrow\downarrow}_{s(d)} \\ J^{\downarrow\uparrow}_{s(d)} & J^{\downarrow\downarrow}_{s(d)} \end{pmatrix}$$



$$J_{s(d)}(\theta) = \frac{\hbar}{2e}\left(J^{\uparrow\uparrow}_{s(d)}(\theta) + J^{\downarrow\downarrow}_{s(d)}(\theta)\right)$$

Effective mass:

$$m^{\uparrow(\downarrow)}_{s(d)}, m^{NM}_{s(d)}, m^{b}_{s(d)}$$

$$\mathrm{TMR} = \frac{J(0) - J(\pi)}{J(\pi)}$$

M. E. Eames et al, APL, 88, 252511 (2006)
J. Callaway et al, PRB **16**, 2095 (1977)
J. Schäfer et al, *ibid.* **72**, 155115 (2005)
A. H. Davis et al, JAP **87**, 5224 (2000)
W. H. Butler, et al. PRB **63**, 054416 (2001)

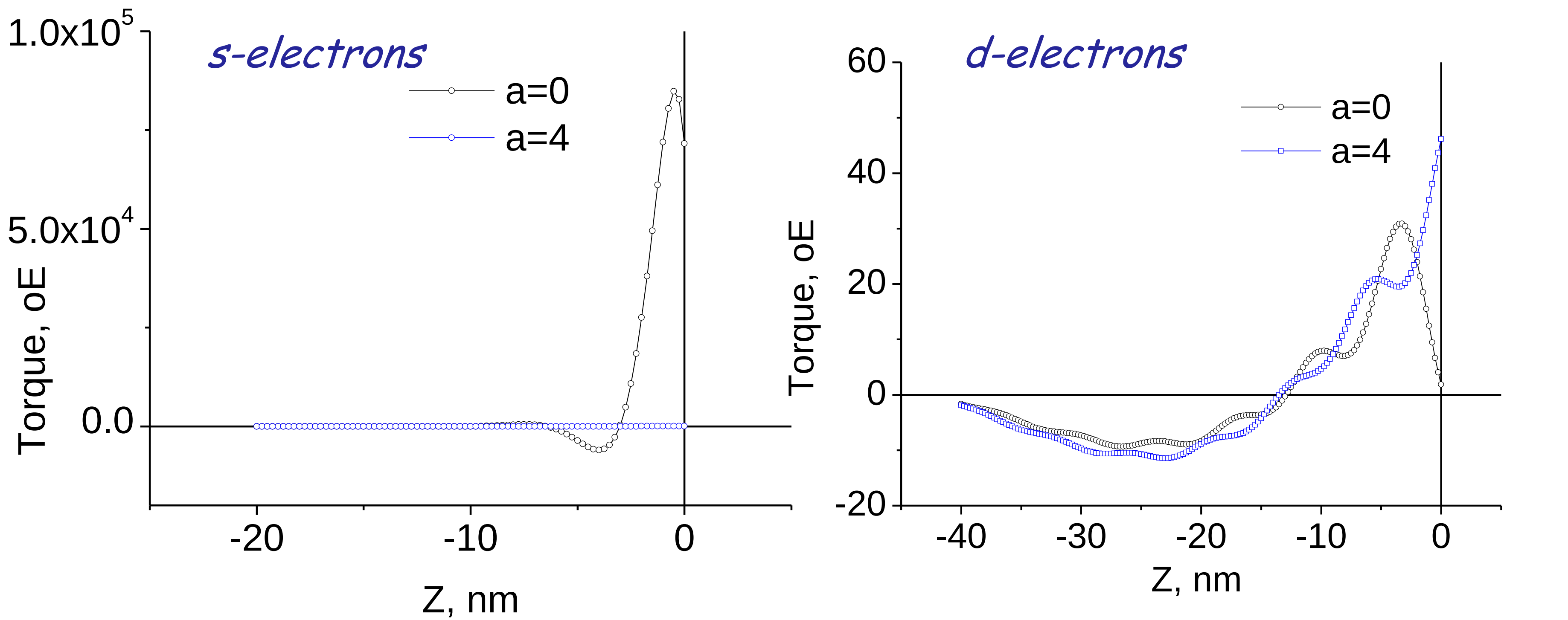
} Refs for parameters

$$'s' \equiv \Delta_1$$
$$'d' \equiv \Delta_5$$

A. Vedyaev et al, ***J. Appl. Phys.*** 107, 09C720 (2010)

Results for Fe|Cr(a)|MgO|Fe

Torque distribution in the left Fe layer



- Torque is mainly due to *s*-electrons
- It almost vanishes when Cr is inserted

(Cr acts as barrier for *s*-electrons, i.e. Δ_1)

- Torque due to *d*-electrons is weak and almost insensitive in value to Cr insertion
- Phase of oscillations is affected

Interlayer Exchange Coupling in Magnetic Tunnel Junctions

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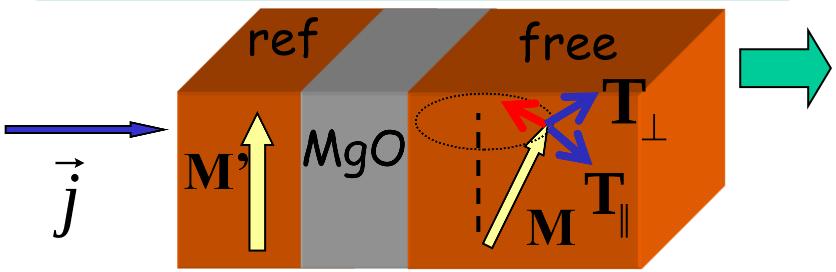

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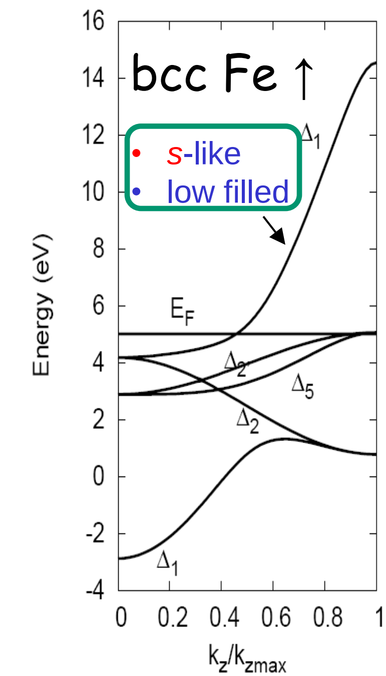
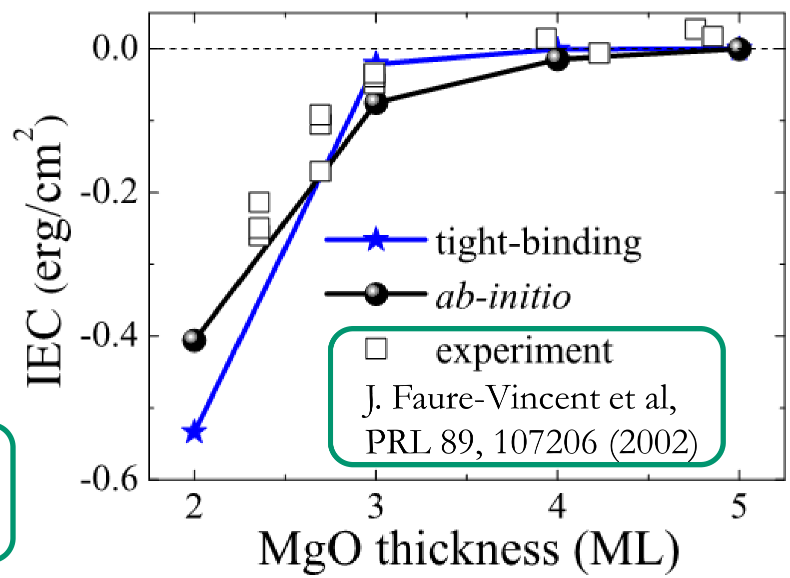


Interlayer Exchange Coupling (IEC)

H. X. Yang et al, APL 96, 262509 (2010)

- DFT with GGA for V_{xc}
- PAW pseudopotentials
- VASP



Tight-binding results with a choice of parameters used successfully for STT behaviour

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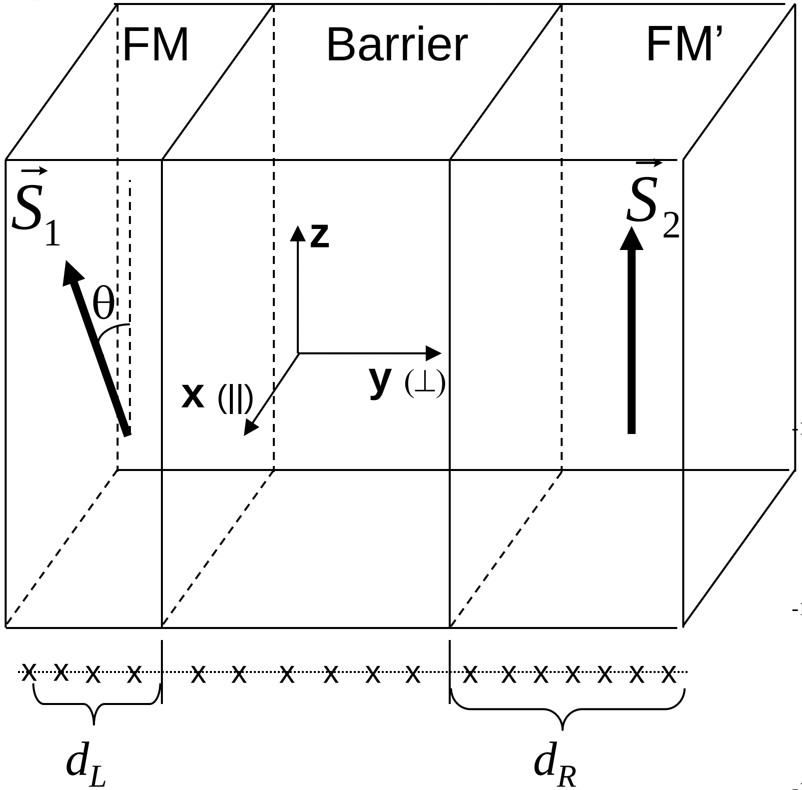
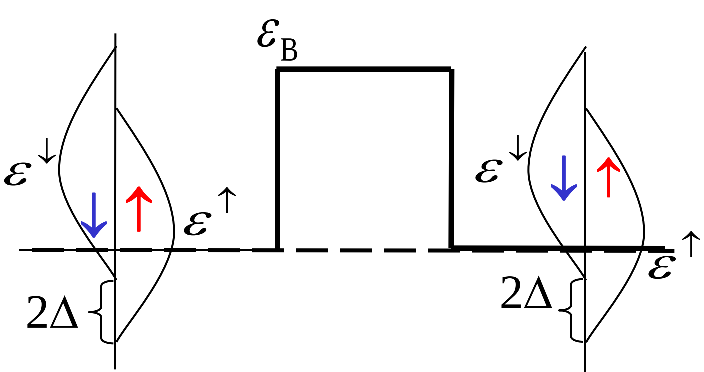
Equilibrium IEC on FM layers thickness



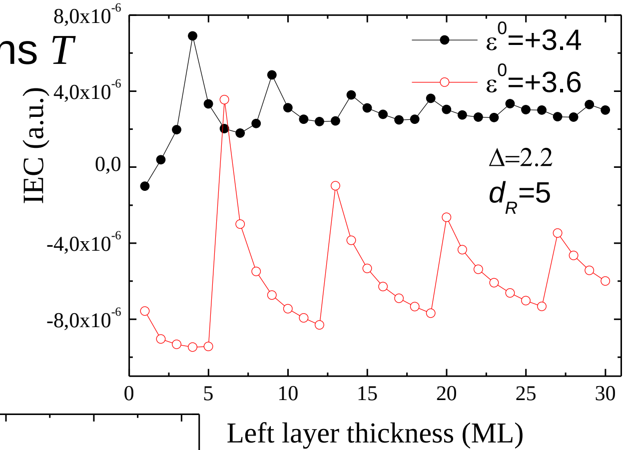


Total energy differences for P and AP

Period of oscillations T

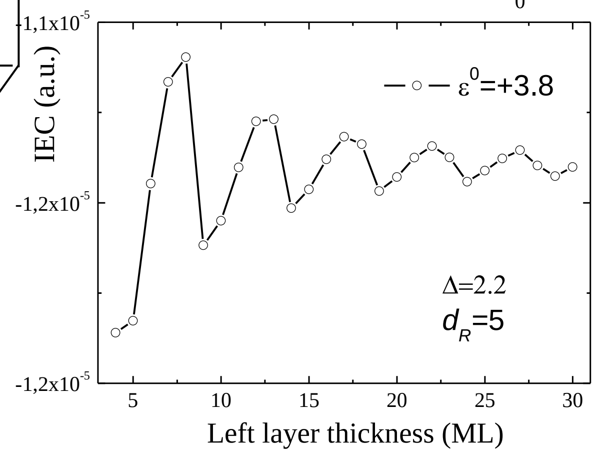
T~5 ML

T~7 ML



P.Bruno, PRB 52, 411 (1995)

L.E.Nistor et al, PRB 81, 220407 (2010)



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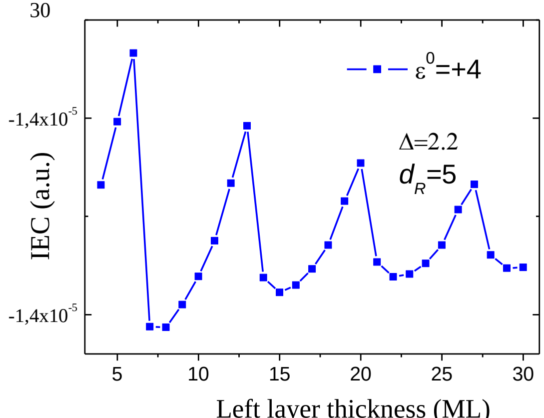


- **IEC period and amplitude are nonmonotonic functions of the Fermi level**

Interlayer Exchange Coupling in Magnetic Tunnel Junctions

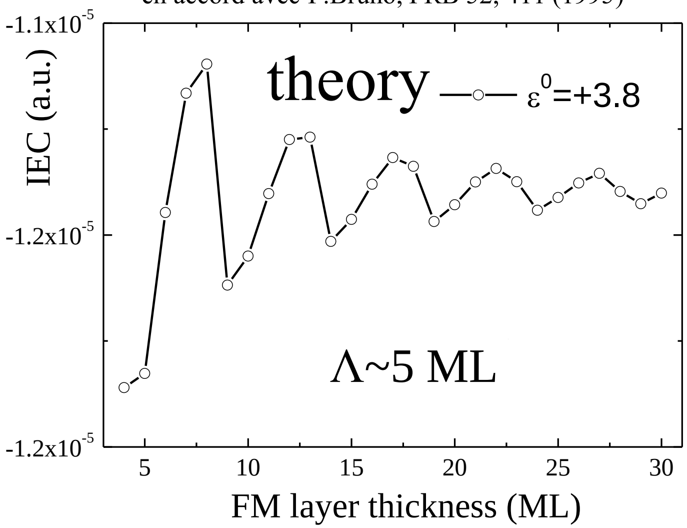
FM layers thickness dependence in MTJ with PMA (pMTJ)

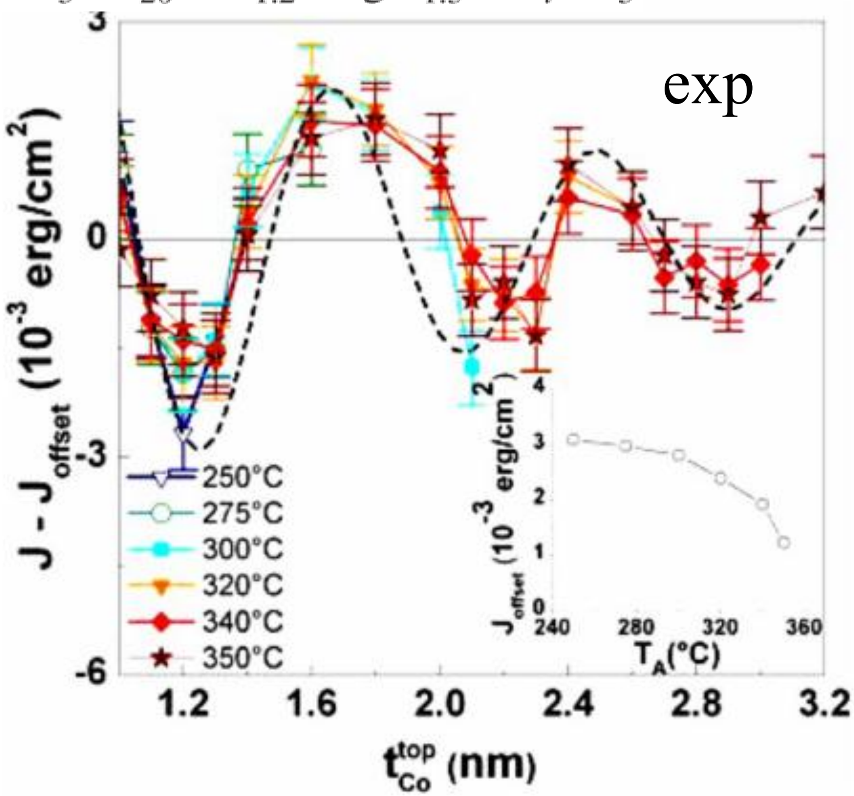
First observation of oscillatory AF IEC in perpendicular MTJs (pMTJ)

MTJ with perpendicular magnetic anisotropy (**pMTJ**)

$Si/SiO_2 \| Ta_3/Pt_{20}/Co_{1.2}/MgO_{1.3}/Co_t/Pt_3$

en accord avec P.Bruno, PRB 52, 411 (1995)





$$J = A/C^2 \sin(2\pi t/\Lambda + \Phi)$$

with $C = 1 + (k_F t)/(k_F^{\downarrow} D)$

$\Lambda = 0.85$ nm

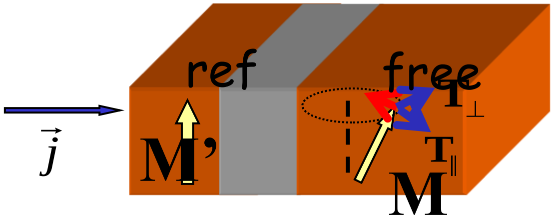
$\Phi = 0.6\pi$, and $k_F = 5$ nm^{-1}

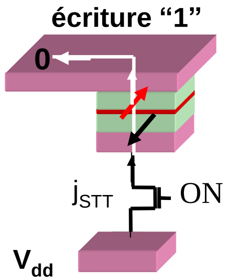
4.2 monolayers (MLs) for (111) fcc and (0001) hcp Co

~~4.9 ML for (001) fcc Co~~

L.E.Nistor et al,
Phys. Rev. B 81, 220407 (2010)

Summary





- Spin Transfer Torques and TMR:
    - Free electron and a tight-binding descriptions
    - Theory predicted STT voltage dependences in MTJs
    - Field-like torque is an even-parity function of applied voltage for symmetric MTJs
    - Linear term appears in case of asymmetric MTJs
    - provides with a solution for "back-switching" problem
    - Models are satisfactory for TMR, STT and IEC

Acknowledgments:
A. Manchon, A. Kalitsov, H.-X. Yang, A. Schuhl, B. Dieny, W. H. Butler, K.-J. Lee, C. Ortiz Pauyac, I. Theodonis, J. Velev, L. Nistor, N. Kioussis, A. Vedyayev, N. Strelkov, N. Ryzhanova and all colleagues

Thank you!