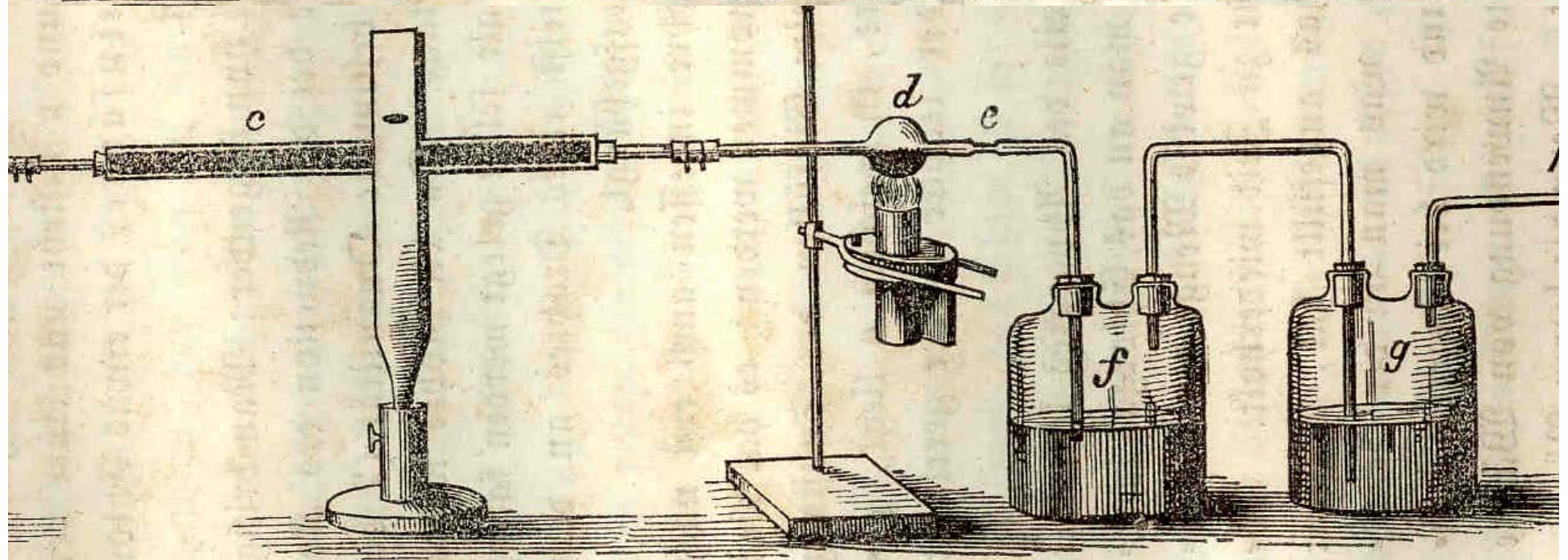


I mean the quantum mechanical spin



# PML 70 ???



New York, February 18, 2003

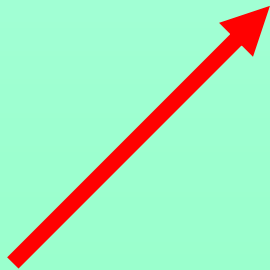
# PML 70 ???

A ten year old collaboration (1996 – 2006)  
and battle about:

- where is the spin ?
- what is spin polarization ?

This is the only classical spin I will show in the following!

But first on what we agreed. Actually a lot!



# 1998

PHILOSOPHICAL MAGAZINE B, 1998, VOL. 78, NOS. 5/6, 549–555

## **Giant magnetoresistance of repeated multilayers of $\text{Cu}_3\text{Ni}_3$ embedded in Cu(100)**

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### ABSTRACT

The resistivity and giant magnetoresistance (GMR) of  $(\text{Cu}_3\text{Ni}_3)_n$  embedded in Cu(100), for  $n \leq 11$ , that originates from the electronic structure of these finite, yet otherwise perfect, systems is calculated for currents in the plane of the layers (CIP) by using the Kubo–Greenwood formula for semi-infinite systems and the fully relativistic, spin-polarized screened Korringa–Kohn–Rostoker method. We find that for this particular type of repeated structure the CIP resistivity decreases from about 6 to  $2 \mu\Omega \text{ cm}$  as the number of repeats increases from 2 to 11, and the CIP-GMR while starting out at 4% for  $n=2$  goes up to 16% at  $n=11$ .

# 1999

Eur. Phys. J. B **9**, 245–250 (1999)

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**THE EUROPEAN  
PHYSICAL JOURNAL B**

EDP Sciences  
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Springer-Verlag 1999

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## On the orientational dependence of giant magnetoresistance

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Received 30 November 1998

**Abstract.** The functional dependence of the giant magnetoresistance (GMR) with respect to the relative angle between the orientations of the magnetization in the magnetic slabs of a trilayer system is calculated by using the Kubo-Greenwood formula for electrical transport together with the fully-relativistic spin-polarized screened Korringa-Kohn-Rostoker method for semi-infinite systems and the coherent potential approximation. It is found that the functional dependence of the GMR is essentially of the form  $(1 - \cos \varphi)$ .

**PACS.** 71.20.Be Transition metals and alloys – 72.15-v Electronic conduction in metals and alloys – 75.30.Et Exchange and superexchange interactions

# 1999

PHYSICAL REVIEW B

VOLUME 60, NUMBER 1

1 JULY 1999-I

## ***Ab initio* calculations of magnetotransport for magnetic multilayers**

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(Received 8 February 1999)

We have used the spin-polarized relativistic screened Korringa-Kohn-Rostoker method for layered systems together with the Kubo-Greenwood formalism and the coherent-potential approximation to describe electrical transport properties of magnetic multilayers. We are able to calculate resistivities and magnetoresistance of model structures with no adjustable parameters by simultaneously determining contributions to the giant magnetoresistance of multilayers coming from both the electronic structure and spin-dependent scattering off impurities. [S0163-1829(99)05125-5]

# 2001

PHYSICAL REVIEW B, VOLUME 63, 224408

## **Electrical transport properties of bulk $\text{Ni}_c\text{Fe}_{1-c}$ alloys and related spin-valve systems**

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(Received 31 July 2000; revised manuscript received 19 December 2000; published 18 May 2001)

Within the Kubo-Greenwood formalism we use the fully relativistic, spin-polarized, screened Korringa-Kohn-Rostoker method together with the coherent-potential approximation for layered systems to calculate the resistivity for the permalloy series  $\text{Ni}_c\text{Fe}_{1-c}$ . We are able to reproduce the variation of the resistivity across the entire series; notably the discontinuous behavior in the vicinity of the structural phase transition from bcc to fcc. The absolute values for the resistivity are within a factor of 2 of the experimental data. Also the giant magnetoresistance of a series of permalloy-based spin-valve structures is estimated; we are able to reproduce the trends observed on prototypical spin-valve structures.

DOI: 10.1103/PhysRevB.63.224408

PACS number(s): 75.30.Gw, 75.70.Ak, 75.70.Cn

# 2002

PHYSICAL REVIEW B, VOLUME 65, 134427

## **Theoretical evaluation of magnetotransport properties in Co/Cu/Co-based spin valves**

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(Received 12 September 2001; published 22 March 2002)

The current-in-plane resistivities and corresponding magnetoresistance ratios are calculated for realistic Co/Cu/Co-based spin-valve samples by applying the Kubo-Greenwood approach together with the fully relativistic, spin-polarized, screened Korringa-Kohn-Rostoker method for layered structures. We study the effects of both alloying in the spacer layers with a selection of  $3d$ ,  $4d$ , and  $5d$  elements as well as different profiles for interdiffusion at the Co/Cu interfaces. On comparing our results to available experimental data we find that both interdiffusion and confinement effects, due to the finite overall thickness of the spin valve, strongly influence the magnetoresistance of spin-valve structures.

DOI: 10.1103/PhysRevB.65.134427

PACS number(s): 75.30.-m, 75.70.Ak, 75.70.Cn

# 2003

PHYSICAL REVIEW B **68**, 054406 (2003)

## ***Ab initio* description of domain walls in Permalloy: Energy of formation and resistivities**

S. Gallego,<sup>1,2</sup> P. Weinberger,<sup>1</sup> L. Szunyogh,<sup>1,3</sup> P. M. Levy,<sup>4</sup> and C. Sommers<sup>5</sup>

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(Received 18 March 2003; revised manuscript received 22 May 2003; published 7 August 2003)

To determine the formation energy and resistivity for domain walls in permalloy (fcc-Ni<sub>85</sub>Fe<sub>15</sub>) we use the fully relativistic spin-polarized screened Korringa-Kohn-Rostoker method for layered systems and the corresponding Kubo-Greenwood equation in the context of the (inhomogeneous) coherent potential approximation. We find that the difference in formation energy between 90° and 180° domains becomes very small if the domain wall width increases. Furthermore, we show that regardless of the configuration within a domain wall the in-plane components of the resistivity are larger than in a single domain and, in particular, that the anisotropic magnetoresistance ratio within the domain wall vanishes.

DOI: 10.1103/PhysRevB.68.054406

PACS number(s): 75.30.Hx, 73.22.-f, 75.30.Gw



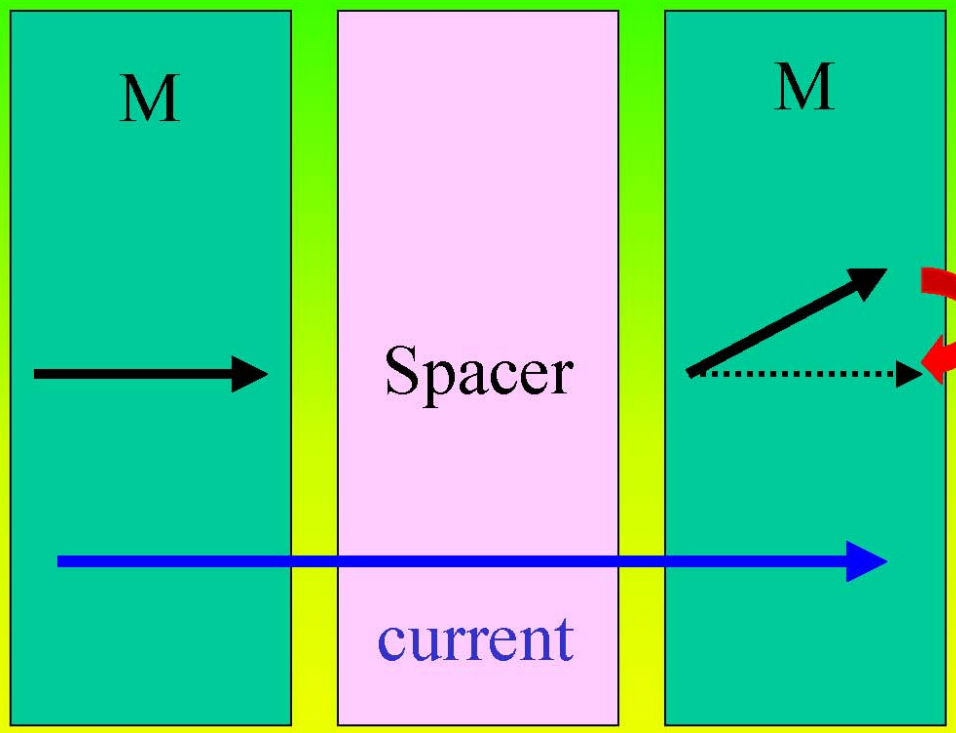
**Our everlasting topic:**

Spins, spin-polarization & currents

**or (at least at present):**

An ab-initio theory of current-induced switching

„Thin layer“



# Non-relativistic phenomenological set of Landau-Lifshitz & transport equations

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

$$\vec{j} = \vec{\sigma} \vec{E} - D \vec{\nabla} \delta n - \vec{\Lambda} \cdot (\vec{\nabla} \otimes \delta \vec{m})$$

$$\frac{\partial \vec{m}}{\partial t} + \vec{\nabla} \cdot \overleftrightarrow{\mathbf{J}}_{\text{spin}} = \vec{m} \times \vec{B}_{\text{eff}}$$

$$\overleftrightarrow{\mathbf{J}}_{\text{spin}} = \vec{\sigma}_{\text{spin}} \otimes \vec{E} - D_{\text{spin}} (\vec{\nabla} \otimes \delta \vec{m})^t - \vec{\Lambda}_{\text{spin}} \otimes \vec{\nabla} n$$

$$\overleftrightarrow{\mathbf{J}}_{\text{spin}} \simeq (\sigma_{\uparrow} - \sigma_{\downarrow}) \frac{\vec{m}}{m} \otimes \vec{E}$$

$\sigma_{\uparrow(\downarrow)}$  : "spin" up (down) conductivity

$n \equiv n(\vec{r}, t)$  : charge density

$\delta n = n - n_{\text{eq}}$

$\vec{j}$  : current density

$\vec{m} \equiv \vec{m}(\vec{r}, t)$  : magnetization density

$\delta \vec{m} = \vec{m} - \vec{m}_{\text{eq}}$

$\overleftrightarrow{\mathbf{J}}_{\text{spin}}$  : "spin" current density

$\vec{B}_{\text{eff}}$  : internal exchange field

$\vec{E}$  : external electric field

$\vec{\sigma}, D, \vec{\Lambda}$  : charge transport coefficients

$\vec{\sigma}_{\text{spin}}, D_{\text{spin}}, \vec{\Lambda}_{\text{spin}}$  : "spin" transport coefficients

$\otimes$  : tensorial product

$t$  : transposed

### ۳. محاسبه فرکانس امواج اسپین

برای محاسبه فرکانس امواج اسپین در یک فرومغناطیس، معادله لاندو-لیفشیتز را بر حسب زمان و مختصات فضایی مغناطش  $M$  می توان به صورت زیر نوشت:

$$\frac{\partial \vec{M}}{\partial t} = \gamma \vec{M} \times \vec{H}_{eff} \quad (1)$$

$\gamma$  ضریب ژیرومغناطیسی و  $H_{eff}$  میدان مؤثر است.  $H_{eff}$  شامل میدانهای مختلف اعمال شده بر روی اسپینهای اتمهاست. این میدانها ناشی از انرژی مبادله‌ای به علت تغییرات فضایی مغناطش، ناهمسانگردیهای مرتبه دوم و چهارم، ناهمسانگردی تک جهتی ناشی از انرژی مبادله‌ای در سطح تماس دولایه‌ای، و انرژی زیمن است. در واقع میدان مؤثر به صورت زیر تعریف می شود:

$$\vec{H}_{eff} = zH_0 - \frac{1}{M_S} \nabla_u F_{ani} + \frac{\gamma A}{M_S^2} \nabla^2 \vec{M} + \vec{h}_d \quad (2)$$

در این رابطه  $H_0$  میدان خارجی است که در جهت  $z$  بر نمونه اعمال می شود،  $M_S$  مغناطش اشباع،  $F_{ani}$  انرژی ناهمسانگردی

This is **not** from  
Mainmonides' famous  
*Guide for the Perplexed*

but Landau-Lifshitz in Pharsi

$$i\hbar \frac{\partial \psi(\vec{r}, t)}{\partial t} = \mathcal{H}_D \psi(\vec{r}, t)$$

$$\mathcal{H}_D = c\vec{\alpha} \cdot [\vec{p} - e\vec{A}(\vec{r}, t)] + \beta m_e c^2 + eV(\vec{r}, t)$$

$\vec{A}(\vec{r}, t)$	vector potential
$V(\vec{r}, t)$	scalar potential
$c$	speed of light
$e$	electron charge
$m_e$	electron mass
$\vec{p} = -i\hbar\vec{\nabla}$	momentum
$\alpha_\mu, \beta$	Dirac matrices

Time-dependent  
Dirac  
equation

# Fully relativistic coupled Landau-Lifshitz & transport equations for a single particle

$$\left\{ \begin{array}{l}
 \underbrace{\frac{d}{dt}(\psi^+ \mathbf{T} \psi)}_{LL-1} + \underbrace{c \nabla \circ [\psi^+ (\boldsymbol{\alpha} \otimes \mathbf{T}) \psi]}_{LL-2} = \underbrace{\frac{e}{m_e} \psi^+ (\boldsymbol{\Sigma} \times \mathbf{B}) \psi}_{LL-3} - \underbrace{\frac{e}{m_e c} \mathbf{E} \psi^+ \gamma_5 \psi}_{LL-4} \\
 \underbrace{\frac{d}{dt}(\psi^+ T_4 \psi)}_{T-1} + \underbrace{c \nabla \circ [\psi^+ (\boldsymbol{\alpha} \otimes T_4) \psi]}_{T-2} = \underbrace{\frac{ie}{m_e} \psi^+ (\boldsymbol{\Sigma} \cdot \mathbf{E}) \psi^+}_{T-3}
 \end{array} \right.$$

$$\mathbf{T} = \beta \boldsymbol{\Sigma} - \gamma_5 \frac{\boldsymbol{\pi}}{m_e c}$$

$$\boldsymbol{\pi} = \mathbf{p} - e\mathbf{A}$$

$$T_4 = \frac{i}{m_e c} \sum_{\mu} \Sigma_{\mu} \pi_{\mu}$$

**Polarization operator**

## Some definitions:

$$(\boldsymbol{\alpha} \otimes \mathbf{T}) = \begin{pmatrix} \alpha_x T_x & \alpha_x T_y & \alpha_x T_z \\ \alpha_y T_x & \alpha_y T_y & \alpha_y T_z \\ \alpha_z T_x & \alpha_z T_y & \alpha_z T_z \end{pmatrix}, \quad \boldsymbol{\alpha} \otimes T_4 = \begin{pmatrix} \alpha_x T_4 \\ \alpha_y T_4 \\ \alpha_z T_4 \end{pmatrix}$$

$$\boldsymbol{\alpha} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix}, \gamma_5 = \begin{pmatrix} 0 & -I_2 \\ -I_2 & 0 \end{pmatrix}, \boldsymbol{\beta} = \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix}, \boldsymbol{\Sigma} = \begin{pmatrix} \boldsymbol{\sigma} & 0 \\ 0 & \boldsymbol{\sigma} \end{pmatrix}$$

$$\psi(\mathbf{r}, t) = \langle \mathbf{r} | \psi(t) \rangle = \begin{pmatrix} \phi(\mathbf{r}, t) \\ \chi(\mathbf{r}, t) \end{pmatrix}$$

$$\chi(\mathbf{r}, t) = \frac{1}{2m_e c} \boldsymbol{\sigma} \cdot \boldsymbol{\pi} \phi(\mathbf{r}, t)$$

## Bispinor representation

$$\psi(\vec{r}, t) = \begin{pmatrix} \phi(\vec{r}, t) \\ \chi(\vec{r}, t) \end{pmatrix}$$
$$\chi(\vec{r}, t) = \frac{1}{2m_e c} (\vec{\sigma} \cdot \vec{\pi}) \phi(\vec{r}, t)$$

Fully relativistic Landau-Lifshitz equation

$$\frac{d}{dt} \left[ \vec{m}_1(\vec{r}, t) + \vec{m}_2(\vec{r}, t) + \frac{1}{m_e c} \vec{m}_3(\vec{r}, t) \right] + c \vec{\nabla} \cdot \left( \mathcal{J}^{(1)}(\vec{r}, t) + \frac{1}{m_e c} \mathcal{J}^{(2)}(\vec{r}, t) \right)$$
$$= \frac{e}{m_e} \vec{m}_1(\vec{r}, t) \times \vec{B}(\vec{r}, t) + \frac{1}{m_e c} \vec{e}(\vec{r}, t)$$

$$\vec{m}_1(\vec{r}, t) = [\phi^+(\vec{r}, t) \vec{\sigma} \phi(\vec{r}, t) + \chi^+(\vec{r}, t) \vec{\sigma} \chi(\vec{r}, t)]$$

$$c^{-1} : \mathcal{J}^{(1)}(\vec{r}, t) \quad , \quad \vec{e}(\vec{r}, t)$$

$$c^{-2} : \vec{m}_2(\vec{r}, t) = -2\chi^+(\vec{r}, t) \vec{\sigma} \chi(\vec{r}, t)$$

# LL-equation

Omitting all terms of the order of  $c^{-2}$

$$\frac{d}{dt} [\vec{m}_1(\vec{r}, t)] + \vec{\nabla} \cdot \left( \mathcal{J}^{(1)}(\vec{r}, t) + \frac{1}{m_e} \mathcal{J}^{(2)}(\vec{r}, t) \right) \simeq \frac{e}{m_e} \vec{m}_1(\vec{r}, t) \times \vec{B}(\vec{r}, t)$$

Non-relativistic limit,  $c \rightarrow \infty$ ,

$$\frac{d}{dt} [\vec{m}(\vec{r}, t)] + \frac{1}{m_e} \vec{\nabla} \cdot \left( \mathcal{J}^{(1)}(\vec{r}, t) + \mathcal{J}^{(2)}(\vec{r}, t) \right) = \frac{e}{m_e} \vec{m}(\vec{r}, t) \times \vec{B}(\vec{r}, t)$$

$$e.g. : \vec{m}(\vec{r}, t) = \varphi^+(\vec{r}, t) \vec{\sigma} \varphi(\vec{r}, t)$$

## Fully relativistic transport equation

$$\frac{d}{dt} \left\{ \sum_{\mu} \frac{1}{m_e c} [\phi^+(\vec{r}, t) \sigma_{\mu} (p_{\mu} - e A_{\mu}(\vec{r}, t)) \phi(\vec{r}, t) + \chi^+(\vec{r}, t) \sigma_{\mu} (p_{\mu} - e A_{\mu}(\vec{r}, t)) \chi(\vec{r}, t)] \right\}$$

$$= c \vec{\nabla} \cdot \mathcal{J}^{(4)}(\vec{r}, t) - \frac{ie}{m_e} \sum_{\mu} [\phi^+(\vec{r}, t) \sigma_{\mu} E_{\mu}(\vec{r}, t) \phi(\vec{r}, t) + \chi^+(\vec{r}, t) \sigma_{\mu} E_{\mu}(\vec{r}, t) \chi(\vec{r}, t)]$$

$$\mathcal{J}^{(4)}(\vec{r}, t) = \left\{ \mathcal{J}_{\mu\nu}^{(4)}(\vec{r}, t) \right\}, \quad \mathcal{J}_{\mu\nu}^{(4)}(\vec{r}, t) = \sum_v [\chi^+(\vec{r}, t) \sigma_{\mu} \sigma_{\nu} [p_{\nu} - e A_{\nu}(\vec{r}, t)] \phi(\vec{r}, t) + \phi^+(\vec{r}, t) \sigma_{\mu} \sigma_{\nu} [p_{\nu} - e A_{\nu}(\vec{r}, t)] \chi(\vec{r}, t)]$$

$$\lim_{c \rightarrow \infty} c \vec{\nabla} \cdot \mathcal{J}^{(4)}(\vec{r}, t) = \frac{ie}{m_e} [\varphi^+(\vec{r}, t) (\vec{\sigma} \cdot \vec{E}(\vec{r}, t)) \varphi(\vec{r}, t)]$$

Non-relativistic limit

# Schematic Landau-Lifshitz & transport equations

$$\frac{\partial \vec{m}}{\partial t} + \vec{\nabla} \cdot \vec{J} = \vec{m} \times \vec{B}_{\text{eff}}$$

„Spin torque term“

Effective field

# Effective field:

$$\vec{B}_{\text{eff}} = -\mu_0 \nabla_{\vec{M}} (\Delta E_b + F_J)$$

$$F_J(t) \simeq - \sum_{k,k'=\text{con,int}} \int d^3r d^3r' \int dt' \vec{j}_k(\vec{r}, t) \tilde{\chi}_{k,k'}(\vec{r} - \vec{r}'; t - t') \vec{j}_{k'}(\vec{r}', t')$$

# Twisting energy & Kubo equation

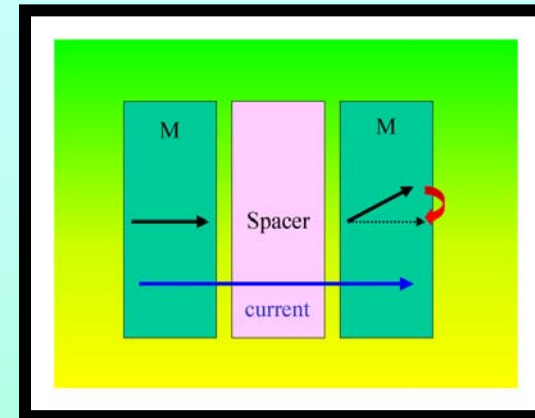
**Twisting energy:**

$$\Delta E(\Theta; \mathbf{x}, m) = E(\Theta; \mathbf{x}, m) - \min[E(\Theta; \mathbf{x}, m)]$$

$E(\Theta; \mathbf{x}, m)$  grand potential  
 $m$  number of spacer layers  
 $\mathbf{x}$  vector of concentrations in case of inhomogeneous alloying

**Expansion:**

$$\Delta E^{(k)}(\Theta; \mathbf{x}, m) = \sum_{s=0}^k a_s(\mathbf{x}, m) (\cos(\Theta))^s$$



$$\sigma_{\mu\mu} = \frac{\hbar}{\pi N_0 \Omega_{at}} \text{Tr} \langle J_\mu \text{Im} G^+(\epsilon_F) J_\mu \text{Im} G^+(\epsilon_F) \rangle$$

$\mu \in \{x, y, z\}$   
 $N_0$  number of atoms  
 $\Omega_{at}$  atomic volume  
 $J_\mu$  representation of the  $\mu$ -th component of the current operator  
 $G^+(\epsilon_F)$  (one-particle) Green's function  
 $\epsilon_F$  Fermi energy

# Mapping on a classic Ohms law

## Current

$$\begin{aligned} I(\Theta; \mathbf{x}, m) &= \sqrt{\frac{A_0 \Delta E(\Theta; \mathbf{x}, m)}{\tau(\Theta; \mathbf{x}, m) r(\Theta; \mathbf{x}, m)}} \\ &= \sqrt{\frac{\langle A_0 \rangle}{\langle \tau(\Theta; \mathbf{x}, m) \rangle}} I_0(\Theta; \mathbf{x}, m) \end{aligned}$$

$A_0$	unit area
$\tau(\Theta; \mathbf{x}, m)$	(minimal) switching time
$I_0(\Theta; \mathbf{x}, m)$	reduced current

$\tau$  : Landau-Lifshitz-Gilbert equation for layered systems

$$\begin{aligned} \frac{d\vec{n}}{dt} &= -\gamma \vec{n} \times \vec{H}^{eff}(\mathbf{x}, m) \\ &\quad + \alpha \vec{n} \times (\vec{n} \times \vec{H}^{eff}(\mathbf{x}, m)) \\ \vec{n} &= n_x \vec{e}_x + n_y \vec{e}_y + n_z \vec{e}_z \end{aligned}$$

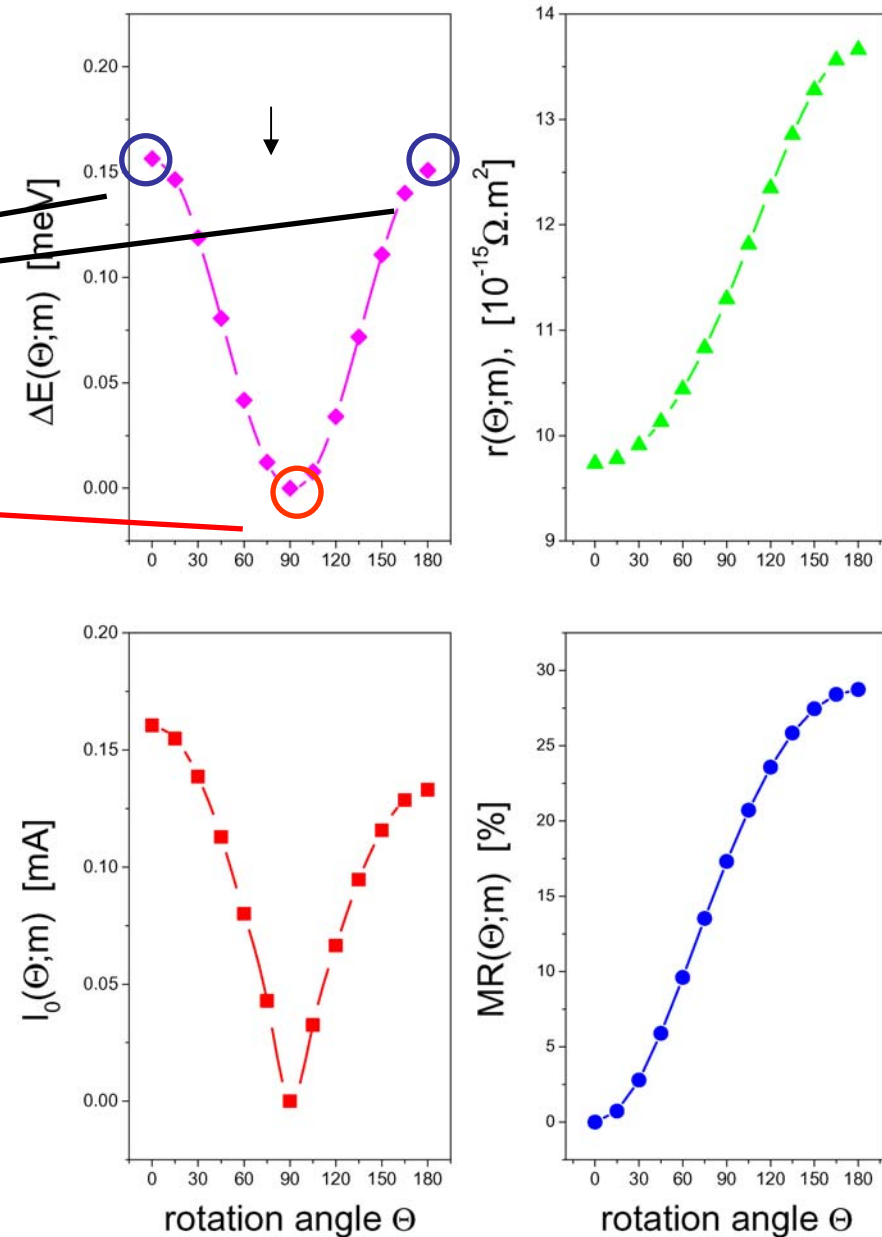
$\vec{n}$	orientation of the magnetization in the
$\vec{H}^{eff}(\mathbf{x}, m)$	internal effective field
$\vec{e}_x, \vec{e}_y, n_z \vec{e}_z$	unit vectors

**Cu/Py<sub>m</sub>/Cu<sub>20</sub>/Py<sub>n</sub>/Cu**  
**m >> n**

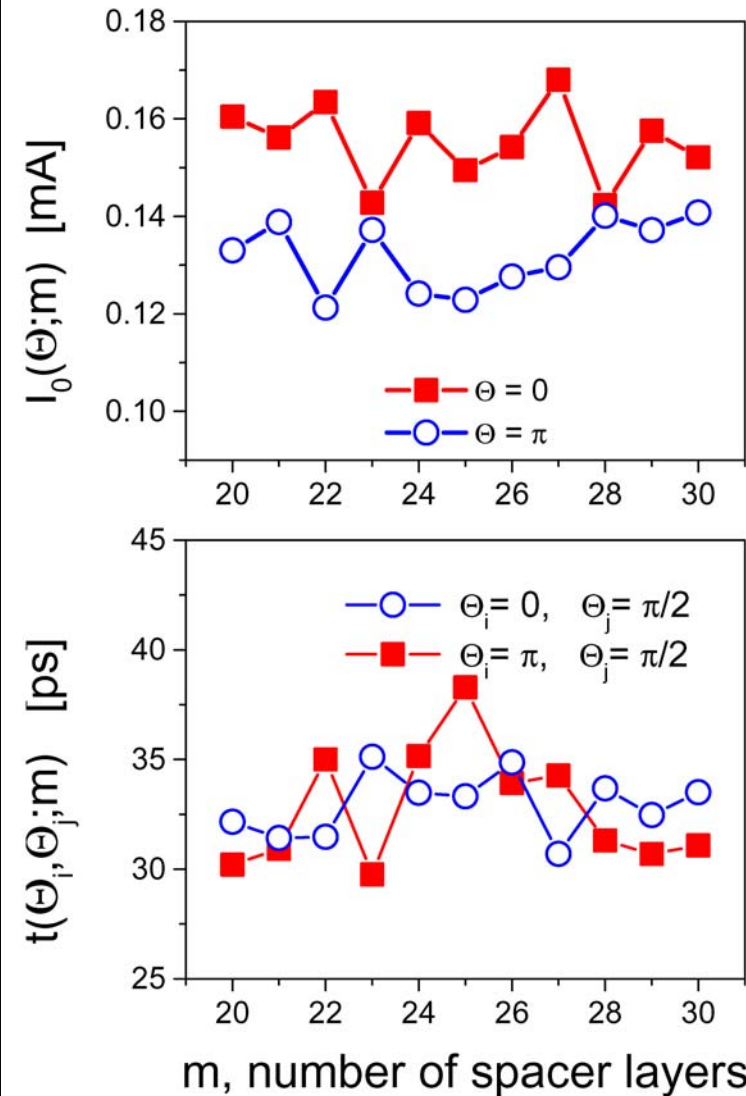
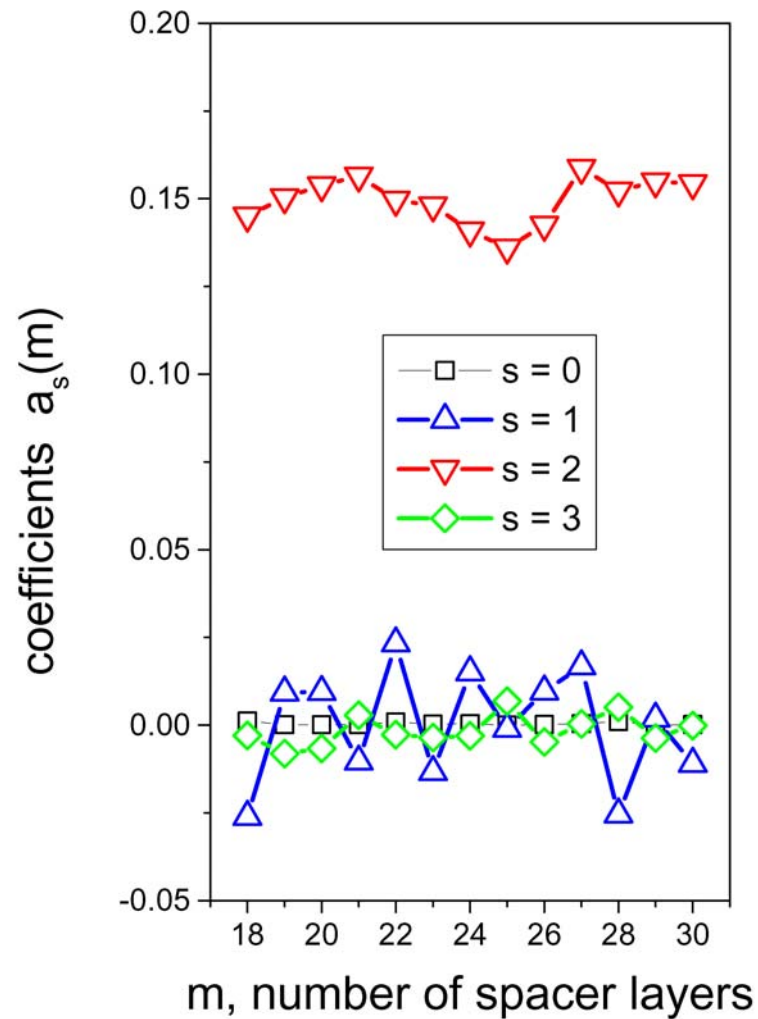
**final state**

**ground state**

**Reduced current:  
Mapping on a classical  
Ohms Law**



# Expansion coefficients & switching times



# Resume

- Sorry, there is still no trace of a classical spin
- if we speak about „spin polarization“, hopefully we now agree on what is meant with this term
- „spin torque“ does have a quantum mechanical counterpart, even in a non-relativistic description
- I think, it is about time for another Pastrami sandwich at Katz!



So then:

... till 120 !!!

(or integer multiples thereof)

New York, February 18, 2003