Spin excitations and spin dynamics in nanoscopic systems

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FAPESP, 23/06/2017

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Collaborators

Theory

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- Marcio Costa (LNNano)
- Mauro Ferreira (TCD)
- Roberto Bechara Muniz (UFF)
- Filipe Guimarães (FZ Jülich)
- Samir Lounis (FZ Jülich)

Experiments

- Harald Ibach (FZ Jülich)
- Alex Khajetoorians (Radboud University, Nijmegen)
- Jens Wiebe (Hamburg University)

Why spin dynamics (excitations)?

“Static” (ground state) properties provide only a small fraction of the available information

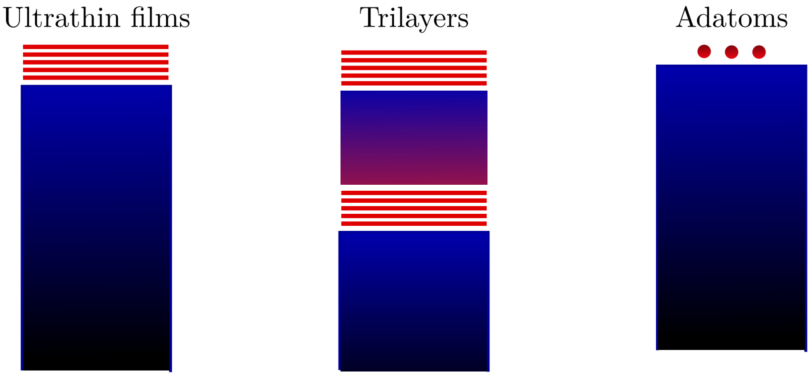
Dynamic properties are related to how the system

- behaves at different temperatures,
- relax towards equilibrium,
- absorbs and emits energy,
- interacts with external probes,
- converts charge currents into spin currents and vice-versa,
- etc.

Experimental techniques

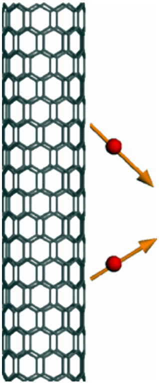
- Ferromagnetic resonance (FMR) – bulk; $\lambda \to \infty$.
- Neutron scattering – bulk; resolves λ.
- Electron energy loss spectroscopy (EELS) – surface sensitive; resolves λ.
- Inelastic scanning tunneling spectroscopy – localized excitations.
- Spin-Hall effects (direct and inverse) – transport experiments.

Typical Systems – metallic substrates

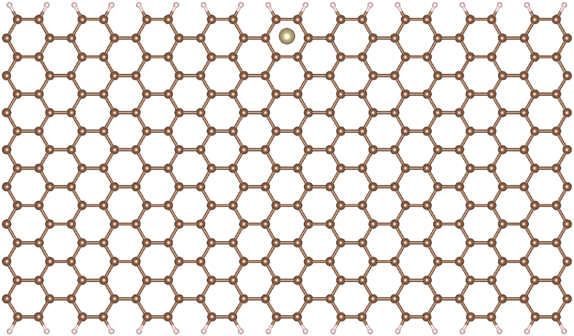


Typical Systems – low-dimensional substrates

Adatoms on carbon nanotubes



Adatoms on graphene nanoribbons and topological insulators



Model

- LCAO description of the electronic structure.

$$H = H_0 + H_U + H_{\text{SO}}$$

$$H_0 = \sum_{l,l';\mu,\nu;\sigma} T_{ll'}^{\mu\nu} a_{l\mu\sigma}^{\dagger} a_{l'\nu\sigma}$$

$$H_U = \sum_{l} \sum_{\mu,\nu,\mu'\nu} \sum_{\sigma,\sigma'} U_l^{\mu\nu\mu'\nu'} a_{l\mu\sigma}^{\dagger} a_{l\nu\sigma'}^{\dagger} a_{l\nu'\sigma'} a_{l\mu'\sigma}$$

$$H_{\text{SO}} = \sum_{l} \sum_{\mu\nu} \frac{\xi_l}{2} \left[L_{\mu\nu}^{z} (c_{l\mu\uparrow}^{\dagger} c_{l\nu\uparrow} - c_{l\mu\downarrow}^{\dagger} c_{l\nu\downarrow}) + L_{\mu\nu}^{+} c_{l\mu\downarrow}^{\dagger} c_{l\nu\uparrow} + L_{\mu\nu}^{-} c_{l\mu\uparrow}^{\dagger} c_{l\nu\downarrow} \right]$$

- $T_{ll'}^{\mu\nu}$ obtained from DFT calculations [PRB **88**, 165127 (2013)].

What I talk about when I talk about spin dynamics

- Spin excitation spectra from the electronic structure alone:

$$\chi_{ll'}^{+-}(t) = -i\theta(t)\left\langle\left[S_l^{+}(t), S_{l'}^{-}(0)\right]\right\rangle$$

$$S_l^{-} \equiv a_{l\downarrow}^{\dagger} a_{l\uparrow}$$

- All damping mechanisms (except for magnon-magnon scattering) are inherent to this approach:
  - spin-orbit coupling damping,
  - spin pumping damping,
  - damping via Stoner excitations.
- SOC $\Rightarrow$ Magnetocrystalline anisotropy $\Rightarrow$ gap in the spin wave spectrum.

Spin dynamics in the presence of SOC

SOC couples transverse spin excitations, given by

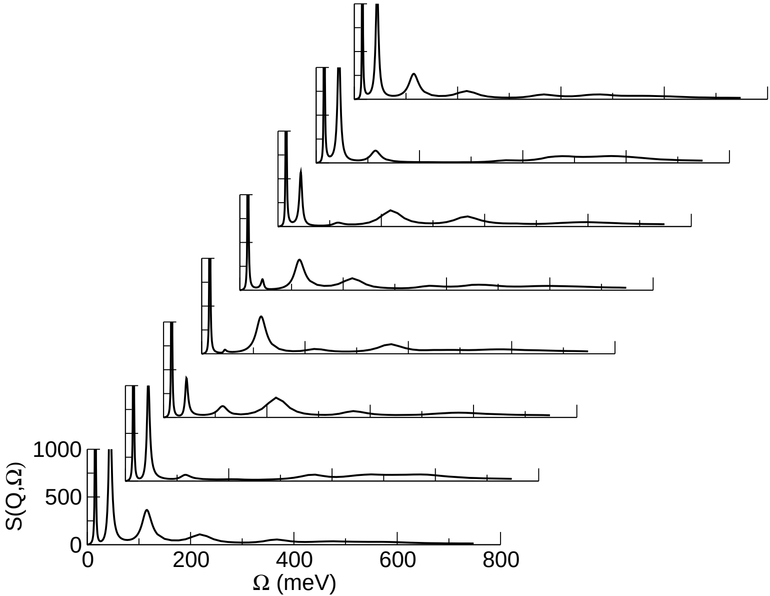
$$\chi_{ll'}^{+-}(t) = -i\theta(t)\left\langle\left[S_l^+(t), S_{l'}^-(0)\right]\right\rangle$$

to longitudinal spin excitations and charge excitations,

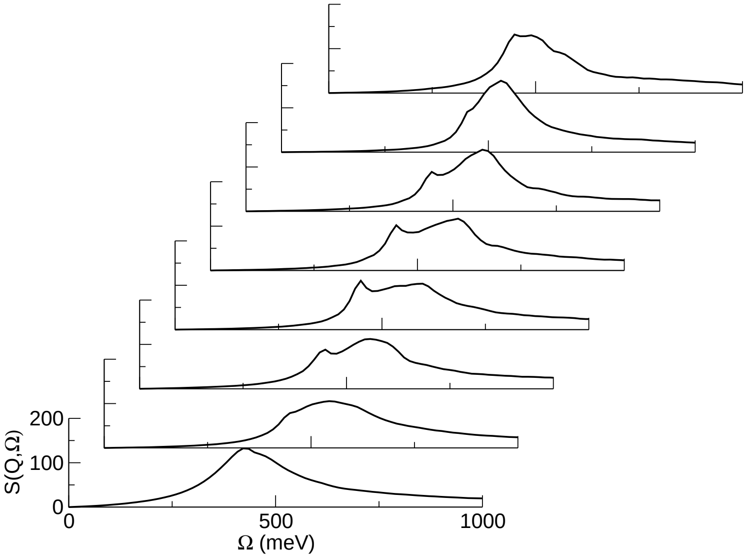
$$\chi_{ll'}^{\uparrow -}(t) = -i\theta(t)\left\langle\left[n_l^\uparrow(t), S_{l'}^-(0)\right]\right\rangle$$
$$\chi_{ll'}^{\downarrow -}(t) = -i\theta(t)\left\langle\left[n_l^\downarrow(t), S_{l'}^-(0)\right]\right\rangle$$
$$\chi_{ll'}^{--}(t) = -i\theta(t)\left\langle\left[S_l^-(t), S_{l'}^-(0)\right]\right\rangle$$

PRB **82**, 014428 (2010)

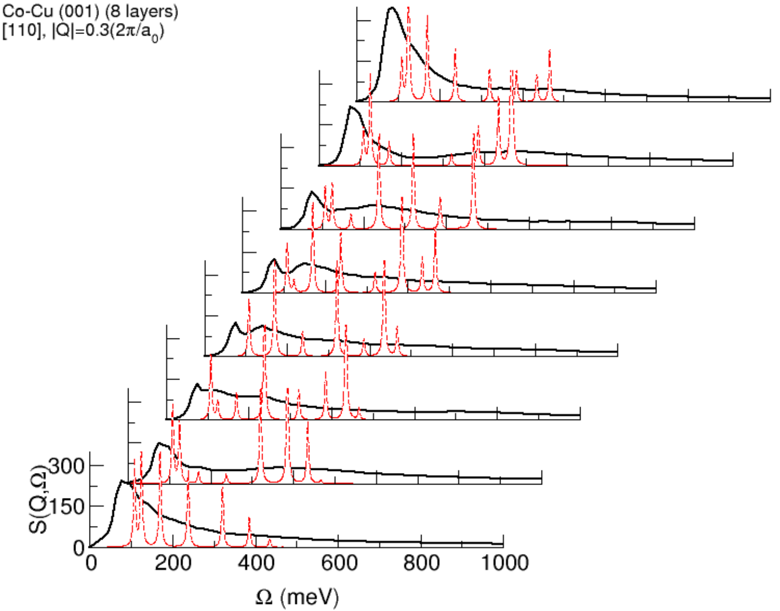
SW spectrum: 8Co/Cu(001), long wavelength



SW spectrum: 8Co/Cu(001), short wavelength

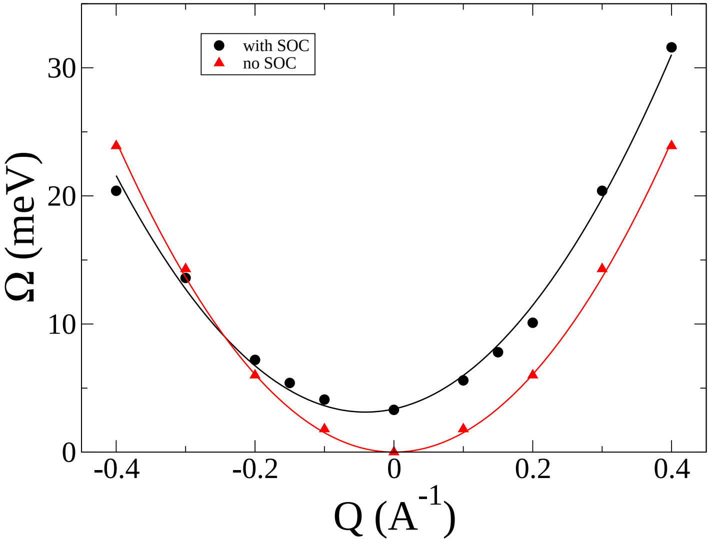


SW spectrum: 8Co/Cu(001), intermediate wavelength



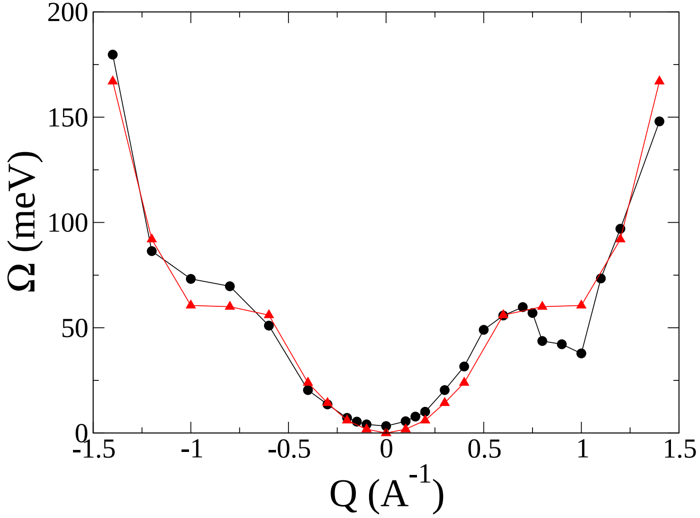
SW dispersion relation - Fe/W(110)

Magnetocrystalline anisotropy gap.

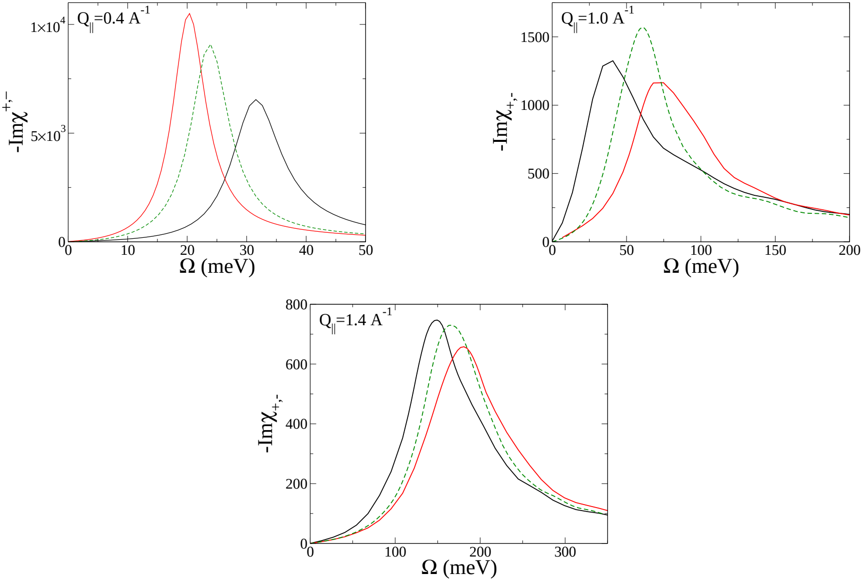


SW dispersion relation - Fe/W(110)

Dzyaloshiskii-Moriya coupling - left-right asymmetry.

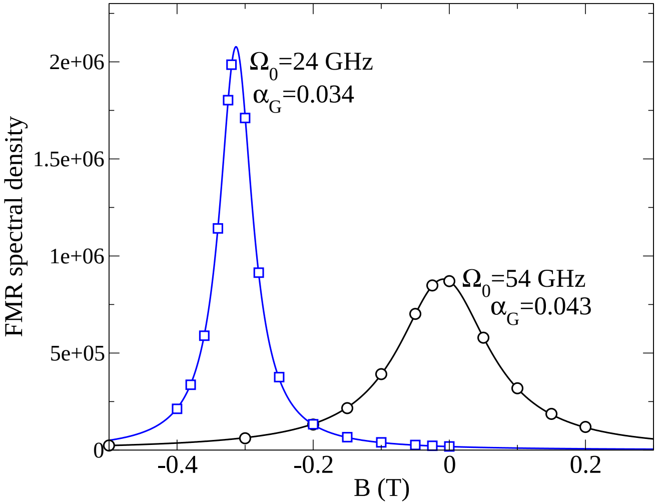


Magnon spectral density



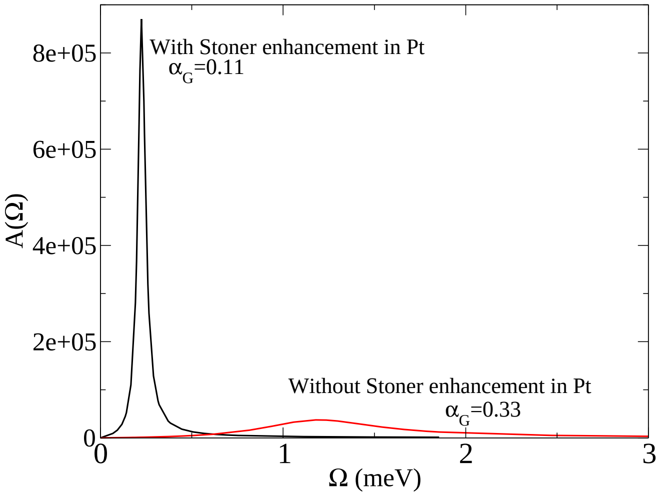
Frequency-dependent Gilbert damping - 2Co/2Pt(001)

FMR sweeping Zeeman field.



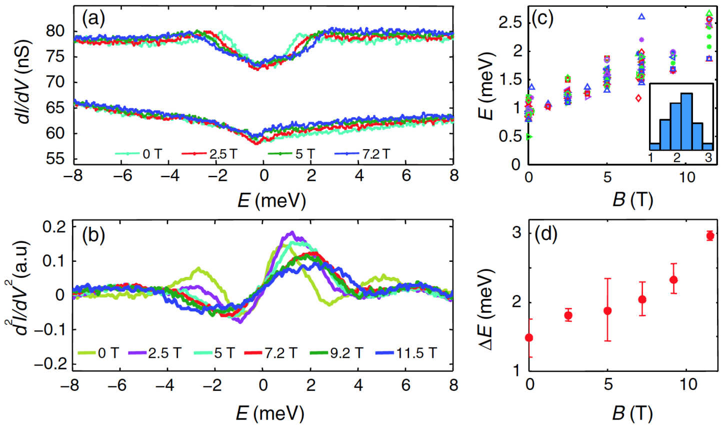
PRB **92**, 014419 (2015).

Gilbert damping and Stoner enhancement - 2Co/2Pt(001)



PRB **92**, 014419 (2015).

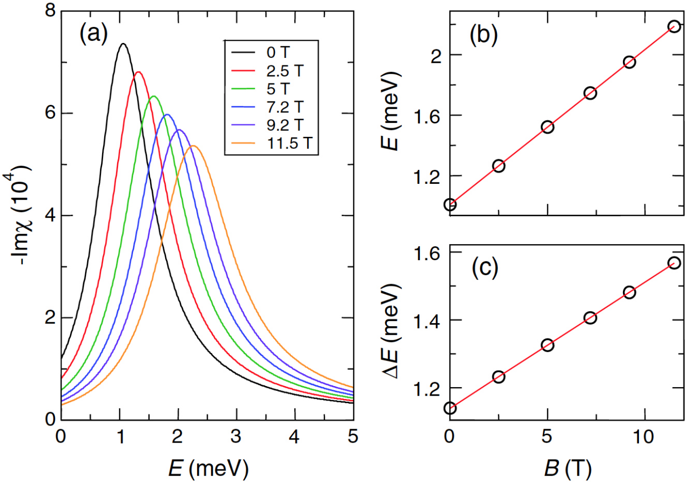
Fe adatom on Cu(111) surface



$\bar{g} \approx 2$

PRL **106**, 037205 (2011).

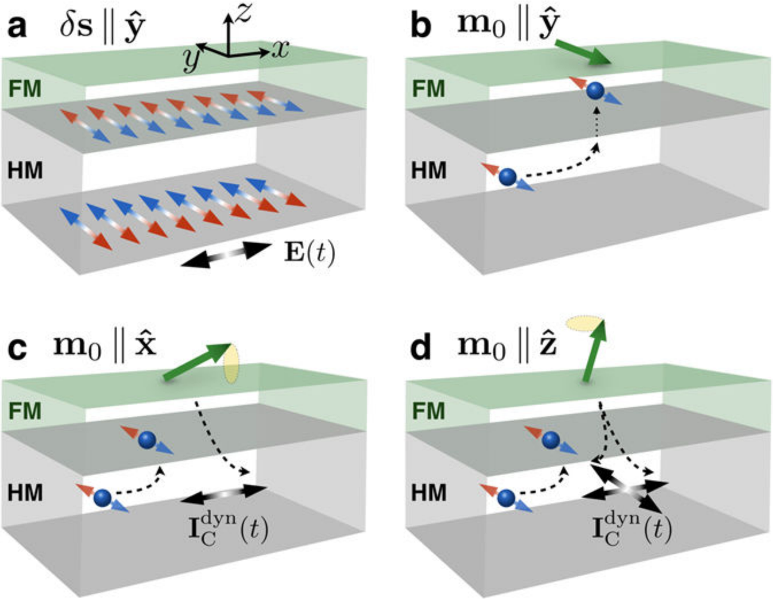
Fe adatom on Cu(111) surface - Calculations



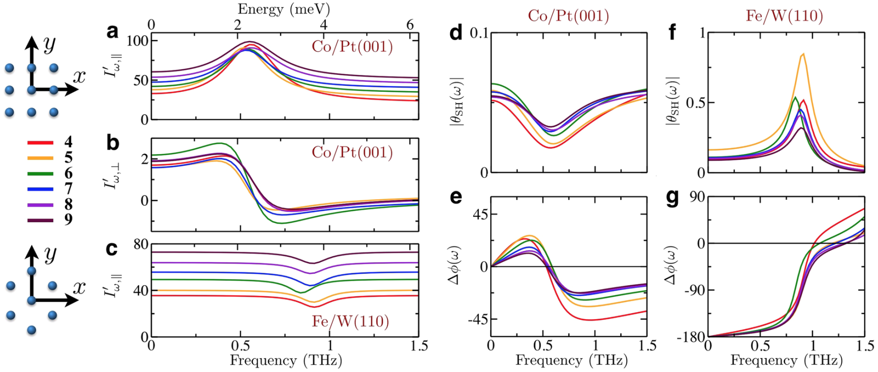
$g = 1.8$; magnetic anisotropy ~ 1 meV.

PRL **106**, 037205 (2011).

Dynamical (THz) Spin Hall Effects



Dynamical (THz) Spin Hall Effects



Scientific Reports **7**, 3686 (2017).

Ongoing project: adatoms on topological insulators

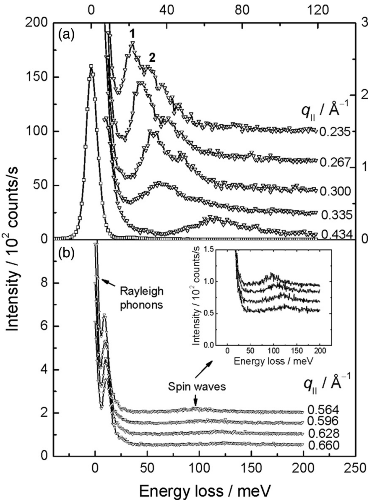
Do spin excitations couple to "topological states"?

- How does the coupling affects the spin excitations?
- How does the coupling affect the "topological character" of the edge states?
- Is it possible to modulate the edge spin current via the coupling?
- Do adatoms couple to each other through the edge states?
- ...

Concluding remarks

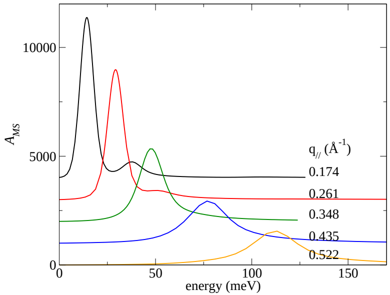
- We have a method for calculating spin excitation spectra that requires nothing more than tight-binding parameters provided by a DFT-based calculation.
- All damping mechanisms are intrinsic to our approach, except those coming from magnon-magnon scattering.
- We can address results from many different experimental techniques with essentially the same formalism.
- Dynamical Spin Hall Effects are the latest addition to our capabilities.

Spin wave spectra of ultrathin films - 8Co/Cu(001)



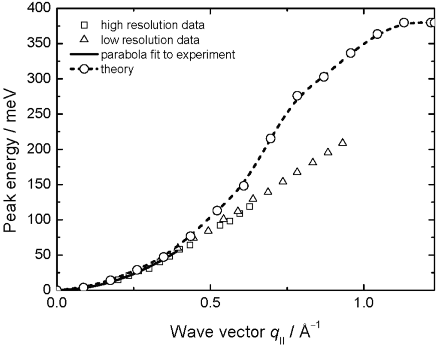
First experimental observation of optical spin wave modes on ultrathin metallic films.

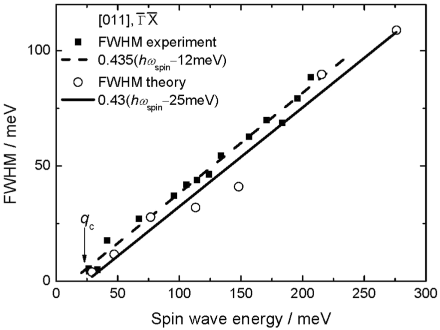
Theory



PRB **86**, 165436 (2012)

Spin waves on 8Co/Cu(001) - dispersion and linewidths





PRB **86**, 165436 (2012)