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Journal of Magnetism and Magnetic Materials 272–276 (2004) 304–305
journal of magnetism and magnetic materials
www.elsevier.com/locate/jmmm

First principles fully relativistic study on low energy magnetic excitations of thin films

L. Udvardi[a,b,*], L. Szunyogh[a,b], K. Palotás[b], P. Weinberger[b]

[a] *Department of Theoretical Physics, Budapest University of Technology and Economics, Budafoki út 8, H-1111, Budapest 1521, Hungary*
[b] *Center for Computational Materials Science, Technical University Vienna, Gumpendorfer Str. 1a, Vienna A-1060, Austria*

Abstract

The long wavelength behaviour of the magnon spectrum for Co monolayer on Cu(0 0 1) is investigated from first-principle. An asymmetry due to a Dzyaloshinsky–Moriya type interaction has been found resulting in a linear term in the magnon dispersion relation in a direction perpendicular to the magnetization.

PACS: 75.10.Jm; 75.30.Ds; 75.30.Gw; 75.70.Ak

Keywords: Relativistic; Magnon; Spin–wave; Anisotropy

Magnetic thin films have been in the focus of the experimental and theoretical studies for several years due to their technological importance in magnetic storage technology. The relativistic effects such as the spin–orbit coupling in thin films are more pronounced than in bulk materials.

In order to describe the spin–wave excitations of ferromagnets the itinerant electronic system is often mapped onto an effective classical Heisenberg model,

$$H = \frac{1}{2}\sum_{i \neq j} J_{ij}\boldsymbol{\sigma}_i\boldsymbol{\sigma}_j, \tag{1}$$

where $\boldsymbol{\sigma}_i$ is a classical unit vector parallel to the magnetization at site i and J_{ij} is the exchange interaction energy between sites i and j. The exchange couplings can be calculated from first principle by using the method of infinitesimal rotation [1] or by means of the frozen magnon approximation [2,3]. The simple Heisenberg hamiltonian can not account for the gap in the magnon spectrum at zero wave number or for other relativistic effects.

We have recently developed a novel, relativistic first-principles method based on the adiabatic approach and on the magnetic force theorem in order to study low-energy spin–wave excitations of itinerant ferromagnets [4]. A spin–wave Hamiltonian has been constructed starting from the Landau–Lifshitz equation and using a harmonic approximation for the free–energy. Although our method is not based on any generalization of the Heisenberg model it is useful to compare their results to those provided by a model hamiltonian. The most general spin hamiltonian has the following form:

$$H = \frac{1}{2}\sum_{i \neq j} J_{ij}\boldsymbol{\sigma}_i\boldsymbol{\sigma}_j + \frac{1}{2}\sum_{i \neq j} \boldsymbol{D}_{ij}\boldsymbol{\sigma}_i \times \boldsymbol{\sigma}_j + \frac{1}{2}\sum_{i \neq j} \boldsymbol{\sigma}_i^{+} A_{ij}\boldsymbol{\sigma}_j + \sum_i K_i(\boldsymbol{\sigma}_i), \tag{2}$$

The additional terms to the Heisenberg hamiltonian are the Dzyaloshinsky–Moriya interaction (DMI), the pseudo-dipolar interaction and the on–site anisotropy, respectively. The on–site anisotropy including the second-order uniaxial anisotropy and the fourth-order in–plane anisotropy is responsible for the gap in the magnon spectrum.

*Corresponding author. Department of Theoretical Physics, Budapest University of Technology and Economics, Budafoki út 8, H-1111, Budapest 1521, Hungary. Tel.: +36-1-463-4109; fax: +36-1-463-3567.

E-mail address: udvardi@bolyai.phy.bme.hu (L. Udvardi).

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doi:10.1016/j.jmmm.2003.12.404

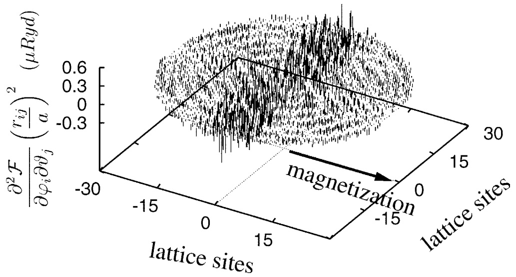

Fig. 1. The mixed partial derivatives of the free energy for Co_1/Cu(0 0 1).

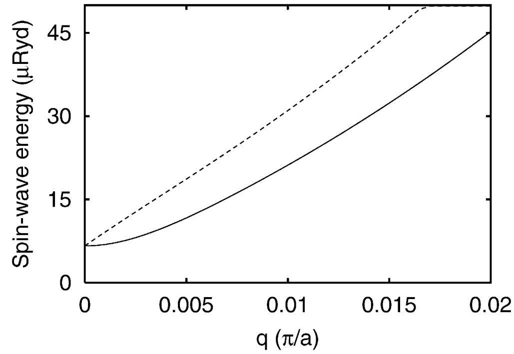

Fig. 2. Spin–wave spectrum for Co_1/Cu(0 0 1) in the vicinity of the Γ point. The solid and dashed lines represent the directions parallel and perpendicular to the magnetization, respectively.

In the following we are concerned on the second term in Eq. (2). Fully relativistic screened KKR calculations on a Co monolayer on Cu(0 0 1) substrate resulted in in–plane easy axis. In the case of in–plane magnetized thin films the inversion symmetry of the system is lifted and DMI can appear. The only special direction is the direction of the magnetization and the coupling constants can be written as: $\boldsymbol{D}_{ij} = D_{ij}\boldsymbol{n}$, where $\boldsymbol{n}$ is a unit vector parallel to the magnetization. In the method of Ref. [4] DMI appears via the mixed partial derivatives of the free energy with respect of the polar and azimuthal angles. The asymptotic behaviour of the exchange couplings for itinerant systems has RKKY character and $D_{ij} \propto 1/R_{ij}^3$. In order to eliminate the decay of the couplings the mixed partial derivatives of the free energy for Co_1/Cu(001) in Fig. 1 is multiplied by R_j^3. According to Eq. (2) there are no interactions between the spins parallel to the magnetization as it is clearly shown by Fig. 1. Consequently, the spin–wave spectrum in directions parallel and perpendicular to the magnetization will be different. The calculated magnon spectrum for Co_1/Cu(0 0 1) in the vicinity of the Γ point is depicted on Fig. 2. The magnons have parabolic dispersion in the long wave–length limit: $\varepsilon(\boldsymbol{q}) = \Delta + D(q_x^2 + q_y^2)$, where Δ is the gap and D is the spin stiffness. However, the presence of the DMI introduces a new linear term which is the consequence of the antisymmetric behaviour of the cross product. Obviously, this linear term appears only in the directions perpendicular to the easy axis as it is shown by Fig. 2. The dispersion relation can be written as $\varepsilon(\boldsymbol{q}) = \Delta + D(q_x^2 + q_y^2) + Aq_y$. $\Delta = 14.4\,\mu\text{Ryd}$, $D = 518\,\text{meV\AA}^2$, $A = 5.5\,\text{meV\,\AA}$ for Co_1/Cu(0 0 1). All values are estimated by applying the regularization procedure proposed by Ref. [5].

The study was supported by the Research and Technological Cooperation Project between Austria and Hungary (Contract No. A-23/01) and the Hungarian National Scientific Research Foundation (OTKA T037856, T038191).

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