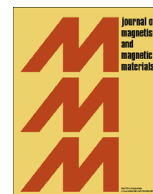




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Comparison of the effect of the exchange and single-ion anisotropy on the magnetic properties of thin ferromagnetic films

Vladimir Ilkovič¹

Bogoliubov Laboratory of Theoretical Physics, JINR, 141980 Dubna, Moscow region, Russia

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ABSTRACT

Using the many-body Green function theory, we calculate the magnetic reorientation temperature and the anisotropic parallel susceptibility of ferromagnetic Heisenberg thin films with the exchange and single-ion anisotropy. Particularly, we compare the effect of these anisotropies on the above mentioned observables. On the basis of our results, one cannot generally claim that these anisotropies are equivalent in the whole range of their parameters.

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1. Introduction

Among the different experimental methods the measurement of the magnetic susceptibility is a very powerful method for the analysis of thin film systems. The parallel and transverse susceptibilities of ferromagnetic ultrathin cobalt films with in-plane exchange anisotropy were measured in [1]. The isotropic exchange interaction and the exchange anisotropy were determined by comparison with a theoretical analysis of the susceptibilities. In [2], the Green function theory was employed to calculate susceptibilities of ferromagnetic thin films with the exchange and single-ion anisotropy, respectively. We note, only one value of the strength of the exchange and single-ion anisotropy, respectively, was used in the calculation. The calculated values of these observables were, in this case, quantitatively so similar that it was unlikely that experimental measurements could decide on which type of anisotropy was acting in a real ferromagnetic film. This may appear somewhat surprising, since these anisotropies originate from very different physical mechanisms. The aim of our work is the investigation within the Green function theory of the magnetic reorientation temperature and the parallel susceptibility in the ferromagnetic thin films with the exchange and single-ion anisotropy in a wide range of their parameters.

2. Theory and fundamental equations

We consider a ferromagnetic thin film consisting of a superposition of L atomic planes (layers) of a square lattice (L is the thickness of the film). We start with following Hamiltonian:

$$H = -\frac{1}{2} \sum_{\langle jk \rangle} J_{jk} (S_j^x S_k^x + S_j^z S_k^z) - \frac{1}{2} D \sum_{\langle jk \rangle} S_j^z S_k^z - K_2 \sum_j (S_j^z)^2 - g\mu_B H^x \sum_j S_j^x - g\mu_B H^z \sum_j S_j^z. \quad (1)$$

Here the notation $S_{j(k)}^\pm = S_{j(k)}^x \pm iS_{j(k)}^y$ is introduced and $\langle jk \rangle$ indicates summation over the nearest neighboring lattice sites. The Hamiltonian consists of Heisenberg exchange interaction with strength $J > 0$ between the nearest neighboring lattice sites, an uniaxial in-plane exchange anisotropy in the z -direction with strength $D > 0$, a second-order in-plane single-ion anisotropy with strength $K_2 > 0$, an external transverse H^x and longitudinal H^z magnetic fields.

The applied Green function method in this work is based on transformation of the fixed coordinate system (x, y, z) into a local coordinate system (X, Y, Z) . The Z -axis is set to be parallel to the z -component of the magnetization. Note that the new coordinate system is rotated by θ_μ in layer μ , where θ_μ is the angle between the z -axis and the magnetization in the layer μ . This theory was described in detail elsewhere [3] and [4]. A remarkable result of this theory is that the effective field aligned parallel to the Z -axis can be written as a sum of the external magnetic field and a single-ion effective anisotropy field:

E-mail address: vilko@theor.jinr.ru¹ Permanent address: Institute of Experimental Physics, Slovak Academy of Sciences, Watsonova 47, 040 01 Košice, Slovak Republic.

$$g\mu_B H_{ef} = g\mu_B H^x \sin \theta_\mu + g\mu_B H^z \cos \theta_\mu + 2K_2 \langle S^z \rangle Q^{(5)} \left[\cos^2 \theta_\mu - \frac{1}{2} \sin^2 \theta_\mu \right], \quad (2)$$

where $Q^{(5)} = 1 - [S(S+1) - \langle (S^z)^2 \rangle] / 2S^2$. The rotation angle θ_μ is determined from the condition that the commutator of S^z with the Hamiltonian vanishes in the rotated frame. In [3] and [4], the expression for the equilibrium angle θ_μ was derived:

$$-g\mu_B H^x + 2K_2 \langle S^z \rangle Q^{(5)} \sin \theta_\mu = 0 \quad (3)$$

Combining expression (2) with condition (3), we can write the components of the effective field in the fixed coordinate system as

$$g\mu_B H_{ef}^x = g\mu_B H^x - K_2 \langle S^z \rangle Q^{(5)} \sin^3 \theta_\mu, \\ g\mu_B H_{ef}^z = g\mu_B H^z + 2K_2 \langle S^z \rangle Q^{(5)} \left(1 - \frac{1}{2} \sin^2 \theta_\mu \right) \cos \theta_\mu. \quad (4)$$

The orientation angle θ_μ of the magnetization is determined by the components of the effective field $\tan \theta_\mu = g\mu_B H_{ef}^x / g\mu_B H_{ef}^z$.

In order to treat the magnetic properties of ferromagnetic thin films with spin $S = 1$, we need the following Green function in energy space $\tilde{G}_{jk}^{(m)}(\omega) = \langle \langle S_j^+; (S_k^z)^m S_k^- \rangle \rangle_\omega$ defined in the local reference frame:

$$\tilde{G}_{jk}^{(m)}(\omega) = \langle \langle S_j^+; (S_k^z)^m S_k^- \rangle \rangle_\omega, S_{j(k)}^\pm = S_{j(k)}^x \pm iS_{j(k)}^y, \quad (5)$$

where $m = 0, 1$. The equation of motion for the Green function $\tilde{G}_{jk}^{(m)}(\omega)$ is

$$\omega \tilde{G}_{jk}^{(m)}(\omega) = U_{jk}^{(m)} \delta_{jk} + \langle \langle [S_j^+, H]; (S_k^z)^m S_k^- \rangle \rangle_\omega, \quad (6)$$

with the inhomogeneity

$$U_{jj}^{(m)} = \langle [S_j^+, (S_j^z)^m S_j^-] \rangle \\ = 2 \langle (S_j^z - 1)^m S_j^z \rangle + \langle [(S_j^z - 1)^m - (S_j^z)^m] [2 - S_j^z - (S_j^z)^2] \rangle. \quad (7)$$

For a ferromagnetic film because of the translation symmetry, the Green function $\tilde{G}_{jk}^{(m)}(\omega)$ and the inhomogeneity $U_{jj}^{(m)}$ will depend only on the position μ of layers involved, so that $\tilde{G}_{jk}^{(m)}(\omega) = \tilde{G}_{\mu\nu}^{(m)}(\omega)$ and $U_{jj}^{(m)} = U_{\mu\mu}^{(m)}$. The higher-order Green functions in the set of equations of motion have to be decoupled to obtain a closed set of equations of motion. We combine the usual random phase approximation for the Green function that appearing in the nonlocal exchange term and a generalized Anderson–Callen approximation, developed in [3], in the local anisotropy term.

After a two-dimensional Fourier transform to momentum space one obtains the resulting equations of motion for the Green function $G_{\mu\nu}^{(m)}(\Omega, \mathbf{q}) = J \tilde{G}_{\mu\nu}^{(m)}(\Omega, \mathbf{q})$ (where $\Omega = \omega/J$), which can be written for the film with thickness $L = 3$ ($\mu(\nu) = 1, 2, 3$) in the matrix form

$$\Delta(\Omega) \mathbf{G}_\mu^{(m)}(\Omega, \mathbf{q}) = \mathbf{U}_\mu^{(m)} \quad (8)$$

with

$$\mathbf{G}_\mu^{(m)}(\Omega, \mathbf{q}) = \begin{pmatrix} G_{1,\mu}^{(m)}(\Omega, \mathbf{q}) \\ G_{2,\mu}^{(m)}(\Omega, \mathbf{q}) \\ G_{3,\mu}^{(m)}(\Omega, \mathbf{q}) \end{pmatrix}, \mathbf{U}_\mu^{(m)} = \begin{pmatrix} U_{1,\mu}^{(m)} \delta_{1,\mu} \\ U_{2,\mu}^{(m)} \delta_{2,\mu} \\ U_{3,\mu}^{(m)} \delta_{3,\mu} \end{pmatrix}, \quad (9)$$

$$\Delta(\Omega) = \begin{pmatrix} \Omega - A_1 & B_1 & 0 \\ B_2 & \Omega - A_2 & B_2 \\ 0 & B_3 & \Omega - A_3 \end{pmatrix}, \quad (10)$$

We assume that both surfaces of the thin layers are

symmetrical, i.e. valid $A_3 = A_1, B_3 = B_1$ and A_μ, B_μ (for $\mu = 1, 2$) are given as follows:

$$A_1 = \langle S_1^z \rangle [4 - \gamma_q + 4d] + h^x \sin \theta_1 + h^z \cos \theta_1 \\ + k_2 \langle S_1^z \rangle Q_1^{(1)} (\cos^2 \theta_1 - \frac{1}{2} \sin^2 \theta_1) + \langle S_2^z \rangle (1 + d) \quad (11)$$

$$A_2 = \langle S_2^z \rangle [4 - \gamma_q + 4d] + h^x \sin \theta_2 + h^z \cos \theta_2 \\ + k_2 \langle S_2^z \rangle \tilde{Q}_2^{(1)} (\cos^2 \theta_2 - \frac{1}{2} \sin^2 \theta_2) + 2 \langle S_1^z \rangle (1 + d), \quad (12)$$

$$B_\mu = \langle S_\mu^z \rangle, \quad (13)$$

and

$$\gamma_q = 2[\cos(q_x) + \cos(q_y)], h^x = g\mu_B H^x/J, h^z = g\mu_B H^z/J, \langle S_3^z \rangle = \langle S_1^z \rangle, \\ k_2 = K_2/J, d = D/J.$$

The spin-wave spectrum Ω_i is obtained by solving the secular equation: $\det \Delta(\Omega) = 0$. From (8) one obtains

$$\mathbf{G}_{\mu\mu}^{(m)}(\Omega, \mathbf{q}) = U_{\mu\mu}^{(m)} \sum_{i=1}^3 \frac{R_{\mu\mu}(\Omega_i, \mathbf{q})}{\Omega - \Omega_i} \quad (14)$$

where $R_{\mu\mu}(\Omega_i, \mathbf{q}) = \Delta_{\mu\mu}(\Omega_i) / \prod_{j \neq i} (\Omega_i - \Omega_j)$ and $\Delta_{\mu\mu}(\Omega_i)$ is obtained from determinant $\Delta(\Omega_i)$ by omitting the first row and first column ($\mu = 1$) or second row and second column ($\mu = 2$). After using the spectral theorem we finally obtain the correlation function for the layers $\mu = 1$ and $\mu = 2$:

$$\langle \langle (S_\mu^z)^m S_\mu^- S_\mu^+ \rangle \rangle = U_{\mu\mu}^{(m)} \Phi_\mu \quad (15)$$

where

$$\Phi_\mu = \frac{1}{\pi^2} \int_0^\pi \int_0^\pi dq_x dq_y \sum_{i=1}^3 \frac{\Delta_{\mu\mu}(\Omega_i)}{\prod_{j \neq i} (\Omega_i - \Omega_j)} \frac{1}{e^{\Omega_i/kT} - 1}, \quad (16)$$

$$\langle \langle (S_\mu^z)^m S_\mu^- S_\mu^+ \rangle \rangle = 2 \langle \langle (S_\mu^z)^m \rangle \rangle - \langle \langle (S_\mu^z)^{m+1} \rangle \rangle - \langle \langle (S_\mu^z)^{m+2} \rangle \rangle \quad (17)$$

We obtain from (8), (15) and (17) with $m = 0$ and $m = 1$ the equations for magnetization $\langle S_\mu^z \rangle$ and second moment $\langle \langle (S_\mu^z)^2 \rangle \rangle$:

$$\langle S_\mu^z \rangle = \frac{1 + 2\Phi_\mu}{1 + 3\Phi_\mu + 3\Phi_\mu^2}, \langle \langle (S_\mu^z)^2 \rangle \rangle = \frac{1 + 2\Phi_\mu + 2\Phi_\mu^2}{1 + 3\Phi_\mu + 3\Phi_\mu^2}. \quad (18)$$

Eq. (18) have to be solved numerically in order to obtain $\langle S_\mu^z \rangle$ and $\langle \langle (S_\mu^z)^2 \rangle \rangle$. Since $\langle S_\mu^z \rangle$ depends on the magnetizations of the other layers via Ω_i , we have to solve self-consistently the set of Eq. (18) written for all layers, to obtain magnetizations of all layer magnetizations at the temperature T . The components of the magnetization in the fixed system (x, y, z) can be calculated from the following equations:

$$\langle S_\mu^z \rangle = \langle S_\mu^z \rangle \cos \theta_\mu, \langle S_\mu^x \rangle = \langle S_\mu^z \rangle \sin \theta_\mu \quad (19)$$

The susceptibility χ_μ^{zz} along the easy axis will be determined numerically as differential quotient

$$\chi_\mu^{zz} = (\langle S_\mu^z(h^z) \rangle - \langle S_\mu^z(0) \rangle) / h^z. \quad (20)$$

3. Results

The reorientation temperature $T_{R\mu}$ of the layer μ is defined as the temperature where the longitudinal magnetization $M_\mu^z \equiv \langle S_\mu^z \rangle$ vanishes; the transverse magnetization $M_\mu^x \equiv \langle S_\mu^x \rangle$ is not zero and the equilibrium orientation angle $\theta_\mu = 90^\circ$. By performing numerical integrations in (18) and using (19) we can estimate the

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