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Anisotropic susceptibilities of thin ferromagnetic films within many-body Green function theory: single-ion anisotropy versus exchange anisotropy

P Fröbrich[1,2,3] **and P J Kuntz**[1]

[1] Hahn-Meitner-Institut Berlin, Glienicker Straße 100, D-14109 Berlin, Germany
[2] Institut für Theoretische Physik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin, Germany

E-mail: pfo@hmi.de (P Fröbrich)

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Abstract

Using many-body Green function theory for thin ferromagnetic Heisenberg films, we compare the static susceptibilities (transverse and parallel) calculated for uniaxial single-ion anisotropy and exchange anisotropy, respectively. Although there are qualitative differences in the results of these calculations with respect to the temperature dependence of the easy and hard axis magnetizations and susceptibilities, the calculated values of these observables are quantitatively so similar that it is unlikely that experimental measurements could decide on which type of anisotropy is acting in a real ferromagnetic film.

1. Introduction

Recently, Jensen *et al* [1] have reported measurements of the parallel and transverse susceptibilities of a bilayer cobalt film having an *in-plane* uniaxial anisotropy. They analysed their results with the help of a many-body Green function theory assuming an *exchange* anisotropy and a value for the spin of $S = 1/2$. In a recent paper [2], we generalized their theoretical model, extending it to multilayers and arbitrary spin. In both papers, an exchange anisotropy was assumed because it is easier to treat than the *single-ion* anisotropy, which requires a different decoupling procedure of the Green function hierarchy. Despite this complication, it would be useful to have at our disposal results analogous to those in [2] but with the single-ion anisotropy replacing the exchange anisotropy. A comparison of the two cases would allow an evaluation of the robustness of the theoretical conclusions as well as possibly identifying any qualitative differences which might enable an experiment to discern which type of anisotropy is acting in a real film.

[3] Author to whom any correspondence should be addressed.

Accordingly, in this paper we investigate the parallel and transverse susceptibilities for arbitrary spin in multilayer systems, but we assume a *single-ion* anisotropy instead of an *exchange* anisotropy. In keeping with the earlier work [1, 2], we use the Green function formalism and neglect the dipole–dipole interaction, since it is nearly isotropic for the in-plane case. Whereas an RPA decoupling is reasonable for the terms coming from the exchange interaction and the exchange anisotropy, it leads to incorrect expressions for the single-ion anisotropy terms. For the latter we therefore use the method proposed by Anderson and Callen [3] at the level of lowest order in the Green function hierarchy. This is certainly an adequate approximation for small anisotropies, as we have shown in [4] for the case of an out-of-plane single-ion anisotropy of a monolayer by comparing with 'exact' quantum Monte Carlo calculations. We refer the reader to the literature for a discussion of the roles of the single-ion- [5–7] and exchange- [8] anisotropies with respect to *reorientation* of the magnetization of a ferromagnetic film with an *out-of-plane* anisotropy as a function of temperature and film thickness.

The paper is organized as follows. In section 2 we explain the model and establish the Green function formalism. Section 3 displays the numerical results and presents a discussion of the similarities and differences between the single-ion and exchange anisotropies. In section 4 we summarize the results and present our conclusions.

2. The model and the Green function formalism

The general formalism parallels our previous work, differing in the terms containing the single-ion anisotropy and in the way in which the decoupling of the Green function hierarchy is implemented. The Hamiltonian consists of an isotropic Heisenberg exchange interaction with strength J_{kl} between nearest neighbour lattice sites, a second-order *in-plane* single-ion lattice anisotropy with strength $K_{2,k}$, and an external magnetic field $\mathbf{B} = (B^x, B^y, B^z)$:

$$\mathcal{H} = -\tfrac{1}{2}\sum_{\langle kl\rangle} J_{kl}(S_k^- S_l^+ + S_k^z S_l^z) - \sum_k K_{2,k}(S_k^z)^2 - \sum_k \left(\tfrac{1}{2}B^- S_k^+ + \tfrac{1}{2}B^+ S_k^- + B^z S_k^z\right). \tag{1}$$

Here the notation $S_k^{\pm} = S_k^x \pm \mathrm{i}S_k^y$ and $B^{\pm} = B^x \pm \mathrm{i}B^y$ is introduced, where k and l are lattice site indices and $\langle kl\rangle$ indicates summation over nearest neighbours only. We restrict ourselves to a simple cubic lattice with the in-plane lattice directions taken as the x- and z-axes and a lattice constant of unity. For generality, we retain the y-component of the field, B^y, which will be set to zero later on.

In order to treat the problem for general spin S, we need the following Green functions in the energy representation:

$$G_{ij,\eta}^{\alpha,mn}(\omega) = \langle\langle S_i^{\alpha}; (S_j^z)^m (S_j^-)^n\rangle\rangle_{\omega,\eta}, \tag{2}$$

where $\alpha = (+, -, z)$ takes care of all directions in space, $\eta = \pm 1$ refers to the anticommutator or commutator Green functions, respectively, and $n \geqslant 1$, $m \geqslant 0$ are positive integers, necessary for dealing with higher spin values S.

The exact equations of motion are

$$\omega G_{ij,\eta}^{\alpha,mn}(\omega) = A_{ij,\eta}^{\alpha,mn} + \langle\langle [S_i^{\alpha}, \mathcal{H}]_-; (S_j^z)^m (S_j^-)^n\rangle\rangle_{\omega,\eta} \tag{3}$$

with the inhomogeneities

$$A_{ij,\eta}^{\alpha,mn} = \langle [S_i^{\alpha}, (S_j^z)^m (S_j^-)^n]_{\eta}\rangle, \tag{4}$$

where $\langle\cdots\rangle = \mathrm{Tr}(\cdots \mathrm{e}^{-\beta\mathcal{H}})/\mathrm{Tr}(\mathrm{e}^{-\beta\mathcal{H}})$. The equations are given explicitly by

$$\begin{aligned}\omega G_{ij,\eta}^{\pm,mn} &= A_{ij,\eta}^{\pm,mn} \mp \sum_k J_{ik}(\langle\langle S_i^z S_k^{\pm}; (S_j^z)^m (S_j^-)^n\rangle\rangle - \langle\langle S_k^z S_i^{\pm}; (S_j^z)^m (S_j^-)^n\rangle\rangle) \\ &\quad \pm K_{2,i}\langle\langle (S_i^{\pm} S_i^z + S_i^z S_i^{\pm}); (S_j^z)^m (S_j^-)^n\rangle\rangle \\ &\quad \mp B^{\pm} G_{ij,\eta}^{z,mn} \pm B^z G_{ij,\eta}^{\pm,mn} \\ \omega G_{ij,\eta}^{z,mn} &= A_{ij(\eta)}^{z,mn} + \tfrac{1}{2}\sum_k J_{ik}\langle\langle (S_i^- S_k^+ - S_k^- S_i^+); (S_j^z)^m (S_j^-)^n\rangle\rangle \\ &\quad - \tfrac{1}{2}B^- G_{ij,\eta}^{+,mn} + \tfrac{1}{2}B^+ G_{ij,\eta}^{-,mn}.\end{aligned} \tag{5}$$

After solving these equations, the components of the magnetization can be determined from the Green functions via the spectral theorem. A solution is possible only after obtaining a closed system of equations by decoupling the higher-order Green functions on the right-hand sides. Retaining only the lowest-order Green functions, we terminate the hierarchy for the exchange-interaction terms using the generalized Tyablikov- (or RPA-) decoupling:

$$\langle\langle S_i^{\alpha} S_k^{\beta}; (S_j^z)^m (S_j^-)^n\rangle\rangle_{\eta} \simeq \langle S_i^{\alpha}\rangle G_{kj,\eta}^{\beta,mn} + \langle S_k^{\beta}\rangle G_{ij,\eta}^{\alpha,mn}. \tag{6}$$

The terms from the single-ion anisotropy have to be decoupled differently, because an RPA decoupling leads to unphysical results; e.g. for spin $S = 1/2$, the terms due to the single-ion anisotropy do not vanish in the RPA, as they should do, because in this case $\sum_i K_{2,i}\langle (S_i^z)^2\rangle$ is a constant and should not influence the equations of motion. In the appendix of [7], we investigated different decoupling schemes proposed in the literature, e.g. those of Lines [9] or that of Anderson and Callen [3], which should be reasonable for single-ion anisotropies that are small compared to the exchange interaction. We found the Anderson–Callen decoupling to be the most suitable. It consists in implementing the suggestion of Callen [10] to improve the RPA by including the diagonal terms arising from the single-ion anisotropy in the decoupling. This leads to

$$\langle\langle (S_i^{\pm} S_i^z + S_i^z S_i^{\pm}); (S_j^z)^m (S_j^-)^n\rangle\rangle_{\eta} \simeq 2\langle S_i^z\rangle\left(1 - \frac{1}{2S^2}[S(S+1) - \langle S_i^z S_i^z\rangle]\right) G_{ij,\eta}^{\pm,mn}. \tag{7}$$

This term vanishes for $S = 1/2$ as it should.

For a ferromagnetic film with N layers, one obtains, after a Fourier transform to momentum space, $3N$ equations of motion for a $3N$-dimensional Green function vector $\mathbf{G}^{mn}$:

$$(\omega\mathbf{1} - \mathbf{\Gamma})\mathbf{G}^{mn} = \mathbf{A}^{mn}, \tag{8}$$

where $\mathbf{1}$ is the $3N \times 3N$ unit matrix. The Green function vectors and inhomogeneity vectors each consist of N three-dimensional subvectors which are characterized by the layer indices i and j:

$$\mathbf{G}_{ij}^{mn}(\mathbf{k},\omega) = \begin{pmatrix} G_{ij}^{+,mn}(\mathbf{k},\omega) \\ G_{ij}^{-,mn}(\mathbf{k},\omega) \\ G_{ij}^{z,mn}(\mathbf{k},\omega) \end{pmatrix}, \qquad \mathbf{A}_{ij}^{mn} = \begin{pmatrix} A_{ij}^{+,mn} \\ A_{ij}^{-,mn} \\ A_{ij}^{z,mn} \end{pmatrix}. \tag{9}$$

The equations of motion are then expressed in terms of these layer vectors, and 3×3 submatrices $\mathbf{\Gamma}_{ij}$ of the $3N \times 3N$ matrix $\mathbf{\Gamma}$:

$$\left[\omega\mathbf{1} - \begin{pmatrix} \mathbf{\Gamma}_{11} & \mathbf{\Gamma}_{12} & \dots & \mathbf{\Gamma}_{1N} \\ \mathbf{\Gamma}_{21} & \mathbf{\Gamma}_{22} & \dots & \mathbf{\Gamma}_{2N} \\ \dots & \dots & \dots & \dots \\ \mathbf{\Gamma}_{N1} & \mathbf{\Gamma}_{N2} & \dots & \mathbf{\Gamma}_{NN} \end{pmatrix}\right]\begin{bmatrix} \mathbf{G}_{1j} \\ \mathbf{G}_{2j} \\ \dots \\ \mathbf{G}_{Nj} \end{bmatrix} = \begin{bmatrix} \mathbf{A}_{1j}\delta_{1j} \\ \mathbf{A}_{2j}\delta_{2j} \\ \dots \\ \mathbf{A}_{Nj}\delta_{Nj} \end{bmatrix}, \qquad j = 1, \dots, N. \tag{10}$$

After the decoupling procedures (6) and (7), the $\mathbf{\Gamma}$-matrix reduces to a band matrix with zeros in the $\mathbf{\Gamma}_{ij}$ submatrices, when $j > i + 1$ and $j < i - 1$. The diagonal submatrices $\mathbf{\Gamma}_{ii}$ are of size 3×3 and have the form

$$\mathbf{\Gamma}_{ii} = \begin{pmatrix} H_i^z & 0 & -H_i^+ \\ 0 & -H_i^z & H_i^- \\ -\frac{1}{2}H_i^- & \frac{1}{2}H_i^+ & 0 \end{pmatrix}, \tag{11}$$

where

$$H_i^z = Z_i + \langle S_i^z\rangle J_{ii}(q-\gamma_{\mathbf{k}}),$$
$$Z_i = B_i^z + J_{i,i+1}\langle S_{i+1}^z\rangle + J_{i,i-1}\langle S_{i-1}^z\rangle + K_{2,i}2\langle S_i^z\rangle\left(1-\frac{1}{2S^2}[S(S+1)-\langle S_i^z S_i^z\rangle]\right), \tag{12}$$
$$H_i^{\pm} = B_i^{\pm} + \langle S_i^{\pm}\rangle J_{ii}(q-\gamma_{\mathbf{k}}) + J_{i,i+1}\langle S_{i+1}^{\pm}\rangle + J_{i,i-1}\langle S_{i-1}^{\pm}\rangle.$$

For a square lattice with the lattice constant taken to be unity, $\gamma_{\mathbf{k}} = 2(\cos k_x + \cos k_y)$, and $q = 4$ is the number of intra-layer nearest neighbours.

The 3×3 off-diagonal submatrices $\mathbf{\Gamma}_{ij}$ for $j = i \pm 1$ are of the form

$$\mathbf{\Gamma}_{ij} = \begin{pmatrix} -J_{ij}\langle S_i^z\rangle & 0 & J_{ij}\langle S_i^+\rangle \\ 0 & J_{ij}\langle S_i^z\rangle & -J_{ij}\langle S_i^-\rangle \\ \frac{1}{2}J_{ij}\langle S_i^-\rangle & -\frac{1}{2}J_{ij}\langle S_i^+\rangle & 0 \end{pmatrix}. \tag{13}$$

To calculate the components of the magnetization of the monolayer, one can use the spectral theorem with the commutator Green functions as in [7] for the case of spin $S = 1$ and an out-of-plane single-ion anisotropy. In order to obtain sufficient equations, it is necessary to include equations coming from the condition that the commutator Green functions be regular at $\omega = 0$ (the *regularity conditions*).

The treatment of multilayers is only practicable with the eigenvector method developed in [6]. The essential features are as follows. One starts with a transformation, which diagonalizes the $\mathbf{\Gamma}$-matrix of equation (8):

$$\mathbf{L\Gamma R} = \mathbf{\Omega}, \tag{14}$$

where $\mathbf{\Omega}$ is a diagonal matrix with eigenvalues ω_τ ($\tau = 1,\ldots,3N$). For the problem above it turns out that there is one eigenvalue equal to zero for each layer, which has to be handled appropriately. The transformation matrix $\mathbf{R}$ and its inverse $\mathbf{R}^{-1} = \mathbf{L}$ are obtained from the right eigenvectors of $\mathbf{\Gamma}$ as columns and from the left eigenvectors as rows, respectively. These matrices are normalized to unity: $\mathbf{RL} = \mathbf{LR} = \mathbf{1}$.

Multiplying the equation of motion (8) from the left by $\mathbf{L}$ and inserting $\mathbf{1} = \mathbf{RL}$, one finds

$$(\omega\mathbf{1} - \mathbf{\Omega})\mathbf{L}\mathbf{G}_\eta^{mn} = \mathbf{L}\mathbf{A}_\eta^{mn}. \tag{15}$$

Defining $\mathcal{G}_\eta^{mn} = \mathbf{L}\mathbf{G}_\eta^{mn}$ and $\mathcal{A}_\eta^{mn} = \mathbf{L}\mathbf{A}_\eta^{mn}$, one obtains

$$(\omega\mathbf{1} - \mathbf{\Omega})\mathcal{G}_\eta^{mn} = \mathcal{A}_\eta^{mn}. \tag{16}$$

$\mathcal{G}_\eta^{mn}$ is a vector of new Green functions, each component τ of which has but a single pole,

$$\mathcal{G}_\eta^{mn,\tau} = \frac{\mathcal{A}_\eta^{mn,\tau}}{\omega - \omega_\tau}. \tag{17}$$

This is the important point because it allows application of the spectral theorem, e.g. [11], to each component separately. We obtain for the component τ of correlation vector $\mathcal{C}^{mn} = \mathbf{L}\mathbf{C}^{mn}$ (where $\mathbf{C}^{mn} = \langle (S^z)^m (S^-)^n S^\alpha\rangle$ with $(\alpha = +, -, z)$)

$$\mathcal{C}^{mn,\tau} = \frac{\mathcal{A}_\eta^{mn,\tau}}{\mathrm{e}^{\beta\omega_\tau} + \eta} + \frac{1}{2}(1-\eta)\frac{1}{2}\lim_{\omega\to 0}\omega\frac{\mathcal{A}_{\eta=+1}^{mn,\tau}}{\omega - \omega_\tau}. \tag{18}$$

We emphasize that when $\eta = -1$, which we use in the following, the second term of this equation, which is due to the anticommutator Green function, has to be taken into account. This term occurs for $\omega_\tau = 0$ and can be simplified by using the relation between anticommutator and commutator:

$$\mathcal{A}_{\eta=+1}^{mn,0} = \mathcal{A}_{\eta=-1}^{mn,0} + 2\mathcal{C}^{mn,0} = \mathbf{L}_0(A_{\eta=-1}^{mn} + 2\mathbf{C}^{mn}), \tag{19}$$

where the index $\tau = 0$ refers to the eigenvector with $\omega_\tau = 0$.

The term $\mathbf{L}_0 A^{mn}_{\eta=-1} = 0$ vanishes due to the fact that the commutator Green function has to be regular at the origin:

$$\lim_{\omega\to 0} \omega G^{\alpha,mn}_{\eta=-1} = 0, \tag{20}$$

which leads to the regularity conditions

$$H^x A^{+,mn}_{\eta=-1} + H^x A^{-,mn}_{\eta=-1} + 2H^z A^{z,mn}_{\eta=-1} = 0. \tag{21}$$

For details, see [6].

This is equivalent to

$$\mathbf{L}_0 A^{mn}_{\eta=-1} = 0, \tag{22}$$

because the left eigenvector of the $\mathbf{\Gamma}$-matrix with eigenvector zero has the structure

$$\mathbf{L}_0 \propto (H^x, H^x, 2H^z), \tag{23}$$

as can be seen analytically. For more details concerning the use of the regularity conditions, see [2, 6].

The equations for the correlations are obtained by multiplying equation (18) from the left with $\mathbf{R}$ and using equation (22); i.e.

$$\mathbf{C} = \mathbf{R}\mathcal{E}\mathbf{L}\mathbf{A} + \mathbf{R}_0\mathbf{L}_0\mathbf{C}, \tag{24}$$

where $\mathcal{E}$ is a diagonal matrix with matrix elements $\mathcal{E}_{ij} = \delta_{ij}(\mathrm{e}^{\beta\omega_i} - 1)^{-1}$ for eigenvalues $\omega_i \neq 0$, and 0 for eigenvalues $\omega_i = 0$.

This set of equations has to be solved self-consistently together with the regularity conditions (21). This determines the magnetizations and the moments of the magnetizations $\langle (S^z)^n \rangle$ for $n = 1, \ldots, 2S+1$, where S is the total spin. For details see appendix A of [8], where an analogous set of similar equations is given more explicitly for the case of the out-of-plane situation.

The susceptibilities with respect to the easy (χ_{zz}) and hard (χ_{xx}) axes are calculated as differential quotients:

$$\begin{aligned} \chi_{zz} &= (\langle S^z(B^z)\rangle - \langle S^z(0)\rangle)/B^z \\ \chi_{xx} &= (\langle S^x(B^x)\rangle - \langle S^x(0)\rangle)/B^x, \end{aligned} \tag{25}$$

where the use of $B^{z(x)} = 0.01/S$ turns out to be small enough; see also [2].

3. Numerical results

In this section we compare numerical results obtained with the single-ion anisotropy with those from the exchange anisotropy, for which the relevant equations were derived in [2]. As the single-ion anisotropy is not active for $S = 1/2$ we show results for $S \geqslant 1$. In an attempt to obtain universal curves in [2] (i.e. independent of the spin quantum number S), we scaled the parameters ($B^{x(z)}$, J, D) in the Hamiltonian as $\tilde{B}^{x(z)}/S = B^{x(z)}$, $\tilde{J}/S(S+1) = J$, and $\tilde{D}/S(S+1) = D$ (D being the strength of the exchange anisotropy). In the present paper, we also scale the strength of the single-ion anisotropy: $\tilde{K}_2/(S-1/2) = K_2$. This is shown in [6] to be the proper scaling because it leads to the correct limit, $\lim_{T\to 0}(K_2(T)/K_2(0)) = 1$, when calculating the temperature-dependent anisotropy by minimizing the free energy with respect to the equilibrium orientation angle of the magnetization.

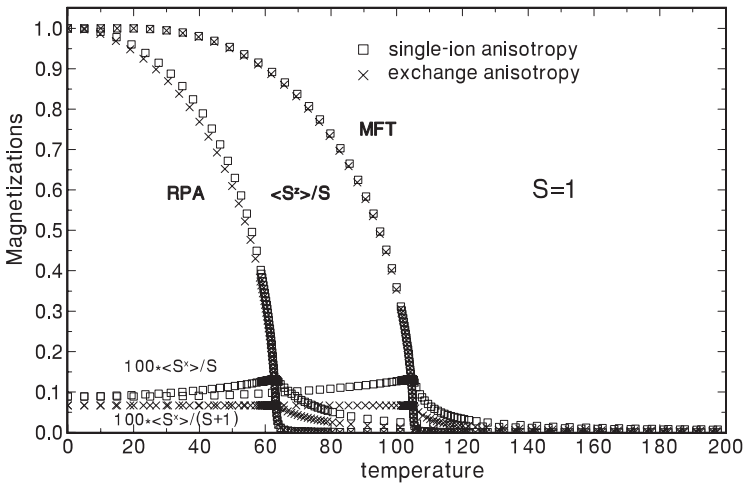

Figure 1. The magnetization $\langle S^z\rangle/S$ of a ferromagnetic spin $S = 1$ Heisenberg monolayer for a square lattice shown as function of the temperature. A comparison is made between Green function (indicated by RPA) calculations with exchange anisotropy $D = 5$ (crosses), and the single-ion anisotropy ($K_2 = 5.625$) (open squares), in the Anderson–Callen approximation. We also show the quantities $100 * \langle S^x\rangle/(S+1)$ for the exchange anisotropy and $100 * \langle S^x\rangle/S$ for the single-ion anisotropy; the factor 100 is introduced to make the curves visible. The corresponding results for mean field theory (MFT) calculations are also displayed.

3.1. The monolayer with arbitrary spin

In order to compare results obtained with the single-ion anisotropy with those of the exchange anisotropy, we set the strength of the single-ion anisotropy to $K_2 = 5.625$ for a square lattice monolayer with spin $S = 1$, so that the easy axis magnetization $\langle S^z\rangle/S$ lies as close as possible to the magnetization obtained with the exchange anisotropy ($D = 5$) used previously [2]. The exchange interaction parameter is $J = 100$, and there is a small magnetic field in the x-direction, $B^x = 0.01/S$, which stabilizes the calculation. The comparison is shown in figure 1.

It is surprising that the results for the easy axis magnetization $\langle S^z\rangle$ are very similar over the whole temperature range, although the physical origin for the anisotropies is very different. An analogous result was observed for the out-of plane situation discussed in [8]. For the exchange anisotropy the hard axis magnetization is a constant below the Curie temperature, whereas for the single-ion anisotropy it rises slightly up to the Curie temperature. In [2] it was shown analytically that the hard axis magnetization for the exchange anisotropy is universal for a scaling $\langle S^x\rangle/(S+1)$. For the single-ion anisotropy, a scaling $\langle S^x\rangle/S$ is found to be more appropriate. Comparison with the corresponding mean field (MFT) calculations, obtained by putting $\gamma_{\mathbf{k}} = 0$ in equation (12), shows the well-known shift to larger Curie temperatures (by a factor of about two for the monolayer with the present choice of the parameters) due to the missing magnon excitations.

In figures 2 and 3 we show the easy and hard axis magnetizations for a monolayer with different spin values S. Whereas in figure 2 one observes a nearly perfect scaling for the RPA calculations with the exchange anisotropy ($S = 1/2, 1, 3/2, 2, 3, 4, 6, 13/2$, from [2]) and a universal Curie temperature $T_C(S)$ for RPA and MFT, this is not the case for the corresponding results with the single-ion anisotropy shown for $S = 1, 3/2, 4, 5$ in figure 3, although the violation of scaling is not dramatic.

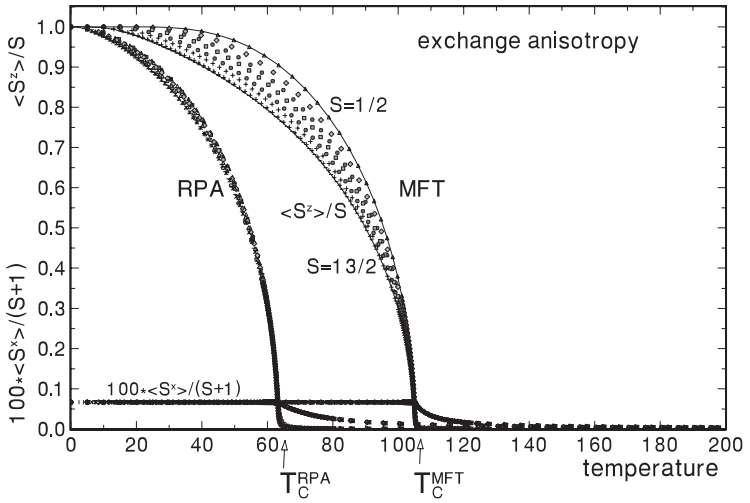

Figure 2. The magnetizations $\langle S^z\rangle/S$ of spin $S = 1/2, 1, 3/2, 2, 3, 4, 6, 13/2$ Heisenberg monolayers for a square lattice are shown as functions of the temperature, from [2]. A comparison is made between Green function (RPA) calculations and the results of mean field theory (MFT), using the exchange anisotropy strength, $D = 5$. Also shown is the hard axis magnetization, which scales to a universal curve $100 * \langle S^x\rangle/(S+1)$, where the factor 100 is introduced to make the curves visible.

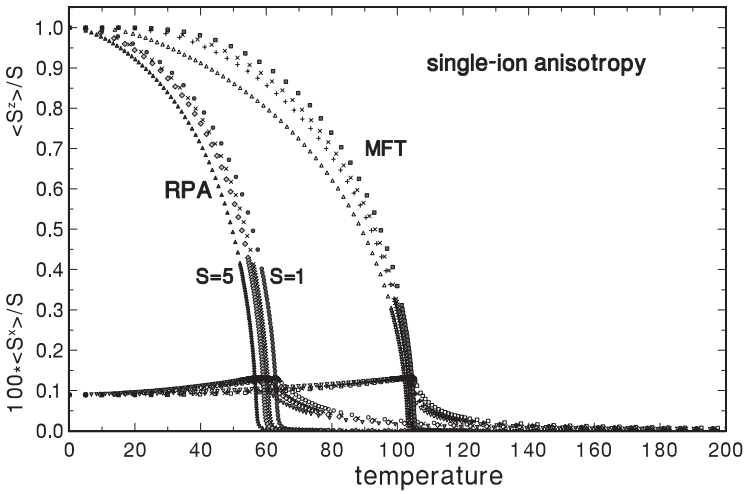

Figure 3. The magnetization $\langle S^z\rangle/S$ of ferromagnetic spin $S = 1, 2, 3/2, 5$ Heisenberg monolayers for a square lattice as a function of the temperature. For Green function (RPA) calculations using the single-ion anisotropy strength of $K_2 = 5.625$ and the corresponding results of mean field theory (MFT). Also shown are the quantities $100 * \langle S^x\rangle/S$; the factor 100 is introduced to make the curves visible.

Turning to the inverse easy and hard axes susceptibilities χ_{zz}^{-1} and χ_{xx}^{-1}, we find very similar results for the exchange anisotropy and the single-ion anisotropy. In particular, in the paramagnetic region ($T > T_{\text{Curie}}$), the inverse susceptibilities as a function of temperature are curved owing to the presence of spin waves, whereas the corresponding MFT calculations show a Curie–Weiss (linear in temperature) behaviour. There is slightly less universal behaviour for

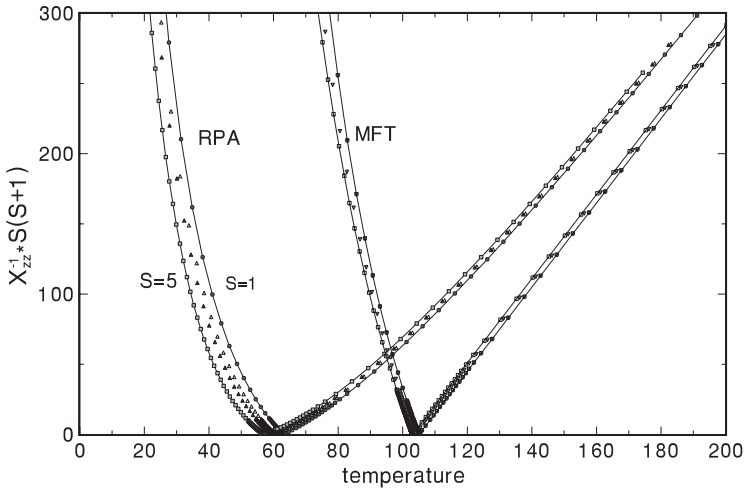

Figure 4. 'Universal' inverse easy axis susceptibilities $\chi_{zz}^{-1} * S(S+1)$ of an in-plane anisotropic ferromagnetic square lattice Heisenberg monolayer as functions of the temperature for single-ion anisotropy and spins $S = 5, 2, 3/2, 1$. A comparison is made between Green function (RPA) and mean field theory (MFT) calculations.

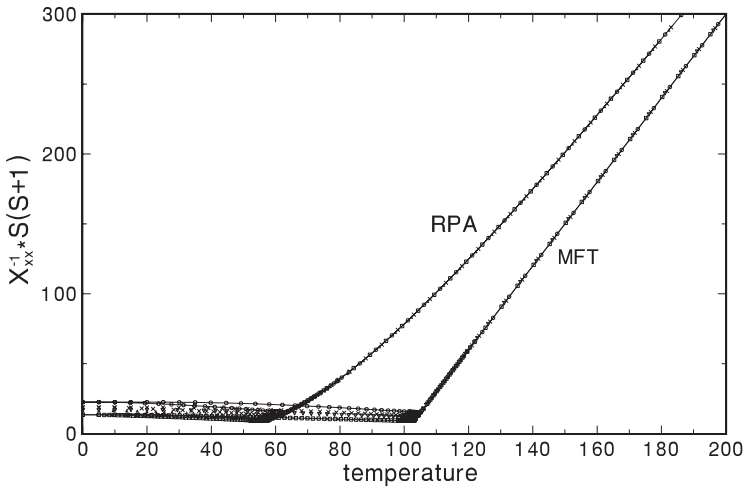

Figure 5. 'Universal' inverse hard axis susceptibilities $\chi_{xx}^{-1} * S(S+1)$ of an in-plane anisotropic ferromagnetic square lattice Heisenberg monolayer as functions of the temperature for single-ion anisotropy and spins $S = 5, 2, 3/2, 1$. A comparison is made between Green function (RPA) and mean field theory (MFT) calculations.

the single-ion anisotropy (figures 4 and 5) than for the exchange anisotropy (figures 2 and 3 of [2]). This is connected with the fact that the exchange anisotropy exhibits universal values for the Curie temperatures $T_{\mathrm{C}}^{\mathrm{RPA}}(S)$ and $T_{\mathrm{C}}^{\mathrm{MFT}}(S)$, which is not strictly the case for the single-ion anisotropy, (figure 3). We were also able to show analytically in [2] that $\chi_{xx}^{-1} * S(S+1)$ is universal for $T < T_{\mathrm{C}}$ for the exchange anisotropy; this is not the case for the single-ion anisotropy. The only difference is in the curves for the imperfectly scaled Green function results for χ_{zz}^{-1}: for the exchange anisotropy, the curve with the lowest spin value lies to the left of the curves with the higher spin values, whereas the converse is true for the exchange anisotropy.

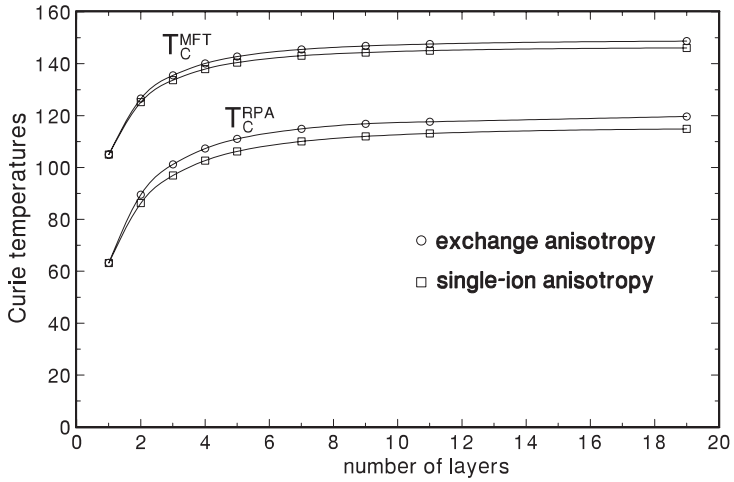

Figure 6. Curie temperatures of ferromagnetic spin $S = 1$ multilayers shown as functions of the film thickness for RPA and MFT with exchange (open circles) and single-ion (open squares) anisotropies.

This is not a very pronounced effect and does not lead to a significant difference between the results for the various anisotropies.

3.2. Multilayers at fixed spin $S = 1$

In treating multilayers with the exchange anisotropy in [2], we considered only the case of $S = 1/2$. The single-ion anisotropy term in the Hamiltonian is a constant for $S = 1/2$; therefore it is not active when calculating the magnetization, so we have to use a larger spin here. In the following, we use spin $S = 1$ as an example, but we also have results for $S > 1$ which scale with respect to the spin in the same way as in the monolayer case.

In figure 6 we compare the Curie temperatures for $S = 1$ multilayers for exchange and single-ion anisotropies in Green function theory and MFT, using for each layer the same parameters as for the monolayer. Remember that the parameters are fixed such that the Curie temperatures for both types of anisotropies coincide for the monolayer. The Curie temperatures for the multilayers $N = 2, \ldots, 19$ (for $N = 19$ one is already close to the bulk limit) are only slightly lower for the single-ion anisotropy than those for the exchange anisotropy.

In figures 7 and 8 we compare easy and hard axis inverse susceptibilities for the multilayer case calculated with single-ion and exchange anisotropy. In order to avoid cluttering the figures we restrict ourselves to a multilayer with $N = 9$ layers and spin $S = 1$. For $N > 9$ the corresponding curves would shift only slightly in accordance with the saturation of T_C with increasing film thickness (see figure 6). We display only the RPA results for the multilayer ($N = 9$) and compare with the RPA monolayer ($N = 1$) result. Again there is no significant difference in the results for both anisotropies. We do not plot the corresponding mean field results which are shifted to higher temperatures, and show in the paramagnetic region only a linear in T Curie–Weiss behaviour, whereas the RPA results have curved shapes owing to the influence of spin waves, which are completely absent in MFT.

4. Summary and conclusions

We have employed a many-body Green function formalism to calculate in-plane anisotropic static susceptibilities of ferromagnetic Heisenberg films using the single-ion anisotropy and

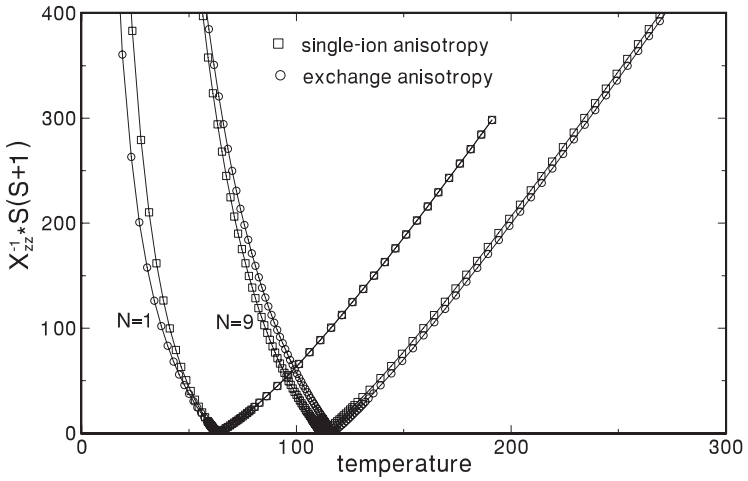

Figure 7. The inverse easy axis susceptibilities χ_{zz}^{-1} of ferromagnetic films in RPA for spin $S = 1$ for a monolayer ($N = 1$) and a multilayer ($N = 9$) as functions of the temperature for single-ion and exchange anisotropies.

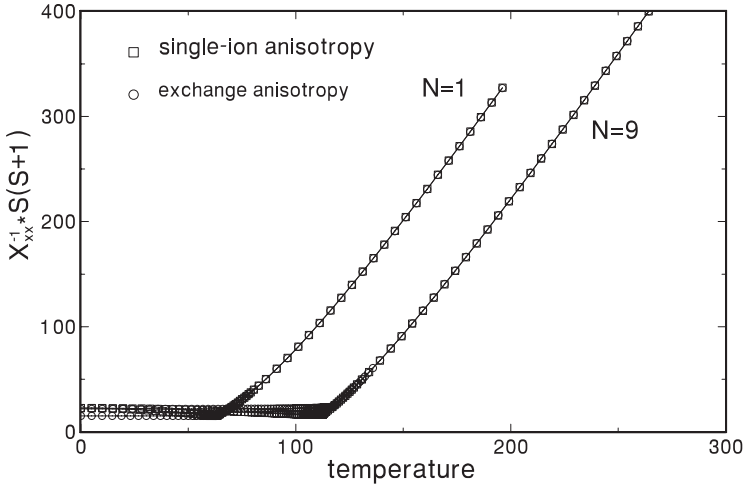

Figure 8. The inverse hard axis susceptibilities χ_{xx}^{-1} of ferromagnetic films in RPA for spin $S = 1$ for a monolayer ($N = 1$) and a multilayer ($N = 9$) as functions of the temperature for single-ion and exchange anisotropies.

have compared the results with previous calculations [2] for an exchange anisotropy. Although both kinds of anisotropy are of very different physical origin, it is possible, by fitting the strengths of the anisotropies properly, to obtain nearly identical values for the easy axis magnetizations over the complete temperature range for an $S = 1$ monolayer. Using the parameters obtained in this way for monolayers with higher spin values and for multilayers, we looked for differences in the results of calculations with both kinds of anisotropy.

By using scaled variables we find a fairly universal behaviour (independent of the spin quantum number S) of easy and hard axis magnetizations and inverse susceptibilities. Universality holds better for the exchange anisotropy; for example, we find a universal Curie

temperature $T_C(S)$ for RPA and MFT. The scaling is not as perfect for the single-ion anisotropy, but there are *no* dramatic deviations which might enable an experiment to distinguish between the two types of anisotropy. The general statement made in [2] that it is sufficient to do a calculation for a particular S and then to apply scaling to obtain the results for other spin values remains valid to a large extent for the single-ion anisotropy. It also remains true *in principle* that the measurement of the hard axis susceptibility together with the Curie temperature allows one to obtain information about the parameters of the model, the exchange interaction and the anisotropy strengths. One should, however, keep in mind that the quantitative results of the present calculations correspond to a square lattice. They could change significantly for other lattice types. Further changes could result from the use of layer-dependent exchange interactions and anisotropies. Such calculations are possible, because the numerical program is written in such a way that layer-dependent coupling constants can be used.

As a general result, we state that our investigations up to now have *not* led to any significant *quantitative* differences for the calculated observables (easy and hard axis magnetizations and susceptibilities) when using on the one hand the single-ion anisotropy and on the other hand the exchange anisotropy. Therefore, it is not possible on the basis of our results to propose an experiment that could decide which kind of anisotropy is acting in a real ferromagnetic film.

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