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Quantum Model for Ferromagnetic Thin Films with an Alternating Crystal Field

J. Kecer

Department of Physics, Technical University
Park Komenského 2, 040 01 Košice, Slovak Republic

and S. Tuleja

High School Humenné, Komenského 2, 060 01 Humenné, Slovak Republic

Within the framework of many-body Green's function theory there are studied the properties of the quantum Blume–Capel model for ferromagnetic films with an alternating single-ion anisotropy on the odd atomic layers and on the even ones. We analyse various possible phase diagrams for the surface exchange couplings and the single-ion anisotropy parameters.

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1. Model and method

The ferromagnetic Blume–Capel–Ising (BCI) model has been studied within the mean field approximation [1], the effective field theory [2], the two-spin cluster approximation in the cluster expansion method [3, 4], Monte Carlo simulations [5], a thermodynamically self-consistent theory based on an Ornstein–Zernike approximation [6], the exact solution based on the Bethe lattice by means of the exact recursion relations [7]. Most of the studies mentioned above displays also the existence of a tricritical point at which the phase transition changes from second order to first order when the value of K_2 becomes negative. Our work represents the first atempt to consider a quantum version of BCI model. Within quantum Blume–Capel (QBC) model we will study the influence of the enhancement of the surface exchange coupling and the alternative single-ion anisotropy $K_2(1)$ on the odd atomic layers and $K_2(2)$ on the even ones on the critical behaviour of thin ferromagnetic films.

The Hamiltonian of the considered system consists a Heisenberg exchange interaction with strength $J_{ij} > 0$ between nearest neighbour lattice sites, an exchange anisotropy with strength $D > 0$, and a second-order single-ion anisotropy with strength $K_2 > 0$:

$$H = -\frac{1}{2}\sum_{\langle i,j\rangle} J_{ij}(S_i^- S_j^+ + S_i^z S_j^z) - \frac{1}{2}D\sum_{\langle i,j\rangle} S_i^z S_j^z + K_2\sum_i (S_i^z)^2. \quad (1)$$

Here the notation $S_k^\pm = S_k^x \pm \mathrm{i}S_k^y$ $(k = i, j)$ is introduced, where i and j are lattice site indices and $\langle ij\rangle$ indicates summation over nearest neighbour spins in the atomic layers and in the adjacent layers for sc lattice with (001) surfaces, K_2 takes the different values: $K_2(1)$ on the odd layers and $K_2(2)$ on the even ones and the exchange parameter takes the value J_S at the surfaces and J inside of the film.

In order to treat the problem for general spin S, we need the following Green functions $G_{ij}^l(\omega) = \langle\langle S_i^+; (S_j^z)^l S_j^-\rangle\rangle_\omega$, where $l \geq 0$ is integer, necessary for dealing with higher spin values S. The equations of motion for calculation of $G_{ij}^l(\omega)$ are $\omega G_{ij}^{(l)}(\omega) = A_{ij}^{(l)}\delta_{ij} + \langle\langle [S_i^+; H]; (S_j^z)^l S_j^-\rangle\rangle_\omega$ with the inhomogeneities $A_{ij}^{(l)} = \langle [S_i^+, (S_j^z)^l S_j^-]\rangle$, where $\langle\cdots\rangle = \mathrm{Tr}(\cdots \mathrm{e}^{-\beta H})/\mathrm{Tre}^{-\beta H}$ denotes the thermodynamic expectation value, the brackets $[\cdots]$ denote the commutator, $\beta = 1/k_\mathrm{B}T$ and δ_{ij} is the Kronecker symbol. The higher Green functions due to the exchange interaction term are decoupled by Tyablikov–Bogolyubov (or RPA) approximation [8]. For the terms stemming from the single-ion anisotropy we have chosen the Anderson–Callen decoupling procedure [9] gives good results [10, 11] for the magnetization if the anisotropy parameter K_2 is much smaller than the parameter of the exchange coupling. Using the eigenvector method (EVM) described, for example, in [12–14] we obtain after a two-dimensional Fourier transform to momentum space, the L coupled equations of motion for Green's functions $G_{\nu\mu}^{(l)}(\boldsymbol{q}, \omega)$ of layer labeled by μ. By using the spectral theorem, for the spontaneous magnetization per site in each atomic layer of the film with spin S we obtain

$$\langle S_\mu^z\rangle_S = \frac{(S - \Phi_{\mu\mu})(1 + \Phi_{\mu\mu})^{2S+1} + (1 + S + \Phi_{\mu\mu})\Phi_{F\mu\mu}^{2S+1}}{(1 + \Phi_{\mu\mu})^{2S+1} - \Phi_{\mu\mu}^{2S+1}} \quad (2)$$

where $\Phi_{\mu\mu} = \frac{1}{\pi^2}\int_0^\pi\int_0^\pi \mathrm{d}q_x \mathrm{d}q_y \sum_{\nu=1}^L \sum_{\kappa=1}^L R_{\mu\nu}\mathcal{E}_{\nu\kappa}\delta_{\nu\kappa}L_{\kappa\mu}$. $\boldsymbol{R}$ is matrix whose columns are the right eigenvectors of matrix $\boldsymbol{P}_L$ of L coupled equations of motion, its inverse $\boldsymbol{L} = \boldsymbol{R}^{-1}$ contains the left eigenvectors as rows, $\mathcal{E}_{\nu\kappa}\delta_{\nu\kappa} = (\mathrm{e}^{\beta\omega_\nu} - 1)^{-1}$ are matrix elements of a diagonal matrix $L \times L$ and ω_ν are the eigevalues of matrix $\boldsymbol{P}_L$. The reduction Curie temperature $k_\mathrm{B}T_\mathrm{C}^f/J$ of the film we get, for example for spin $S = 1$, from the set of L equations: $k_\mathrm{B}T_\mathrm{C}^f/J = 2/3\widetilde{\Phi}_2$, $\langle S_2^z\rangle = \widetilde{\Phi}_1/\widetilde{\Phi}_2, \cdots, \langle S_L^z\rangle = \widetilde{\Phi}_1/\widetilde{\Phi}_L$ where the overtilde designates a scaled quantity in terms of $\langle S_1^z\rangle$.

2. Results

First we consider in Fig. 1 the phase diagrams in $(K_2(1)/J, k_\mathrm{B}T_\mathrm{C}^f/J)$ plane when $K_2(2)/J = 0.1$ (Fig. 1A) and in $(K_2(2)/J, k_\mathrm{B}T_\mathrm{C}^f/J)$ plane when $K_2(1)/J = 0.01$ (Fig. 1B). In both cases we observe cross-over points at which Curie temperature of thin film does not depend on film thickness: $K_2^\mathrm{C}(1)/J$ and $K_2^\mathrm{C}(2)/J$. The tricritical points (denoted by C) are marked by filled circles.

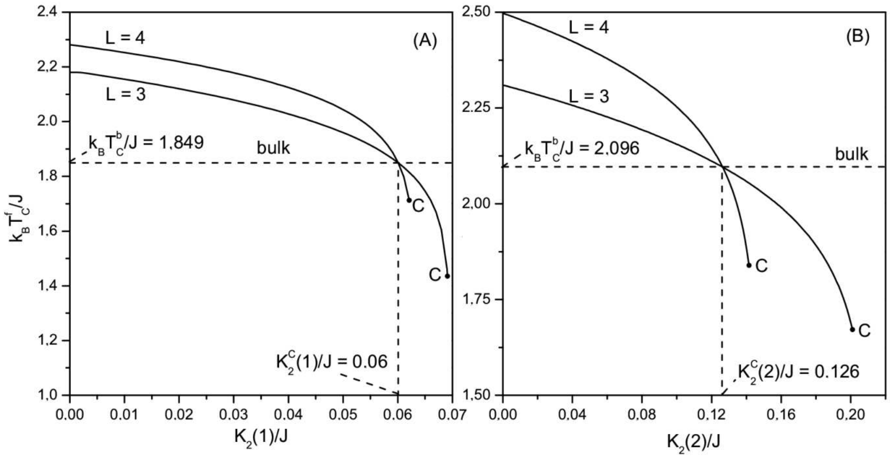

Fig. 1. Film Curie temperature $k_{\rm B}T_{\rm C}^f/J$ as a function: (A) of the anisotropy parameter $K_2(1)/J$ when $K_2(2)/J = 0.1$; (B) of anisotropy parameter $K_2(2)/J$ when $K_2(1)/J = 0.01$ for films with with spin $S = 1$, with thicknesses $L = 3$ and 4 in the case when $\Delta_S = J_S/J = 1, D/J = 0.01$. The dashed line labeled by "bulk" corresponds to the bulk Curie temperature.

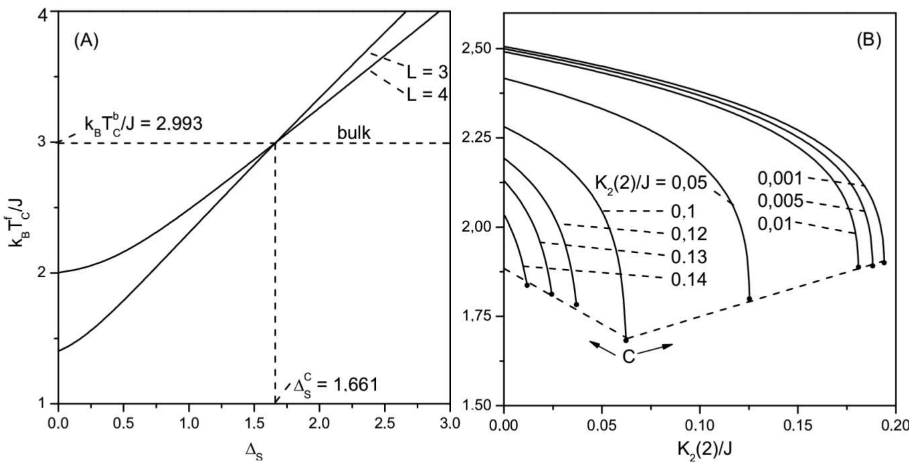

Fig. 2. Film Curie temperature $k_{\rm B}T_{\rm C}^f/J$: (A) as a function of parameter Δ_S for films with spin $S = 1$, with thicknesses $L = 3$ and 4 when $D/J = 0.01$, $K_2(1)/J = 0.005$, $K_2(2)/J = 0.01$; (B) as a function of anisotropy parameter $K_2(1)/J$ for different $K_2(2)/J$ when $S = 1$ for film with thickness $L = 4$, $\Delta_S = 14$, $D/J = 0.01$.

In Fig. 2A there is plotted the phase diagram in $(\Delta_S, k_{\rm B}T_{\rm C}^f/J)$ plane. The critical parameter $\Delta_S^{\rm C} = J_S^{\rm C}/J$ represents other cross-over point. The cross-over points can be observed only in the cases: anisotropic exchange couplings when the surface exchange coupling differs from the bulk one; when the single-ion anisotropy is different in the odd and in the even atomic layers of the films, etc. In Fig. 2B there are plotted the tricritical points in the phase diagrams in the $(K_2(1), k_B T_C^f/J)$ plane for different values of the single-ion anisotropy parameters $K_2(2)/J$.

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