Multilayer transition in a spin-1 Blume–Capel model with RKKY interaction and quantum transverse anisotropy

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Using mean-field theory, we have studied the effect of quantum transverse anisotropies with RKKY interaction on the multi-layer transition and magnetic properties of the spin-1 Blume–Capel model of a system formed by two magnetic multi-layer materials, of different thicknesses, separated by a non-magnetic spacer of thickness M. It is found that the multilayer magnetic order–disorder transition temperature depends strongly on the value of the transverse anisotropy. The multilayer transition temperature decreases when increasing the transverse anisotropy. Furthermore, there exists a critical quantum transverse anisotropy Δ_{xL} beyond which the separate transitions occur in the two magnetic layers. The critical transverse anisotropy Δ_{xL} decreases (increases) on increasing the non-magnetic spacer of thickness M (on increasing the crystal field), and Δ_{xL} undergoes oscillations as a function of the Fermi level.

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1. Introduction

In the last few years, with the development of the artificial fabrication and its application to the growth of thin films, a renewed interest has been aroused in ferro-electric thin films both experimentally[1−4] and theoretically,[5−11] because of their significance in the fields of micro-electronic and opto-electronics. A good candidate to describe the H-bonded ferro-electric systems is generally believed to be the transverse Ising model within the framework of the pseudo-spin theory. The transverse Ising model was first introduced by de Gennes[12] to describe the phase transition of order–disorder type ferro-electrics. However, the magnetic properties of multi-layer have attracted much attention due to novel properties leading to a range of applications including the possibility of spintronics-based devices. Furthermore, there existed the different types of multi-layer, such as Pd/Co, Fe/Si, and Fe/Cr, have been studied intensively in the context of magnetic and transport parameters. In case of metallic multi-layers, a giant magneto-resistance (GMR) effect[13] and oscillatory exchange coupling[14] are observed after applying a magnetic field which depends on the number and thickness of the multi-layers. In multi-layer GMR two or more ferro-magnetic layers are separated by a very thin non-ferromagnetic spacer (e.g. Fe/Cr/Fe). At certain thicknesses the Ruderman–Kittel–Kasuya–Yosida (RKKY) coupling[15,16] between adjacent ferromagnetic layers with a crystal field becomes antiferro-magnetic, making it energetically preferable for the magnetizations of adjacent layers to align antiparallel.[17−24] Moreover, the layering transitions in Ising thin film have been studied using a real spacer renormalization group and the mean field theory.[25,26] Recently, many theoretical works have studied the effect of the transverse field without the RKKY interaction and the non-magnetic thickness.[27−30] Furthermore, the singe-ion anisotropy term has been investigated by various theoretical methods: molecular field approximation,[31,32] high-density expansion method,[33] finite cluster approximation,[34] and effective field theory with differential pair operator technique,[35,36] linear chain approximation,[37] constant coupling[38] and the renormalization group technique.[39] However, the effect of the crystal field with RKKY interaction on the multi-layer transition without the quantum transverse anisotropy has been studied in detail.[40] Our aim in this work is to study, using mean-field theory, the effect of the quantum transverse anisotropy on the multi-layer transition with RKKY interaction and magnetic properties of a spin-1 Blume–Capel model of a system formed by

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two magnetic multi-layer materials, of different thicknesses, separated by a non-magnetic spacer of thickness M. The paper is organized as follows: In Section 2, we present the model and methods. Results and discussion are given in Section 3 and Section 4 is reserved for conclusion.

2. Model and method

Sandwiches and super-lattices of magnetic/nonmagnetic/magnetic materials have attracted several theoretical and experimental studies because of their technological applications. In this material the coupling exchange undergoes an oscillation period known as the RKKY interaction.[15] In the other side, the transverse anisotropy is due in general to the dislocation in Mn_{12} acetate crystals.[41] Indeed, its existence is proved experimentally by the magnetization measuremental in single-molecule magnets such as $[Mn_{12}O_{12}(O_2CCH_2CH_2Cl)16(H_2O)_4]\cdot CH_2ClCH_2CO_2H]$ known as $Mn_{12}-PrCl$.[42] To combine both effects of quantum transverse anisotropy and RKKY coupling on the magnetic properties of theses materials, we consider a spin-1 ferromagnetic simple-cubic lattice system formed by two magnetic blocs A and B separated by a non-magnetic layer of thickness M. The blocs A and B are formed by $N1$ and $N2$ magnetic layers respectively (see Fig. 1).

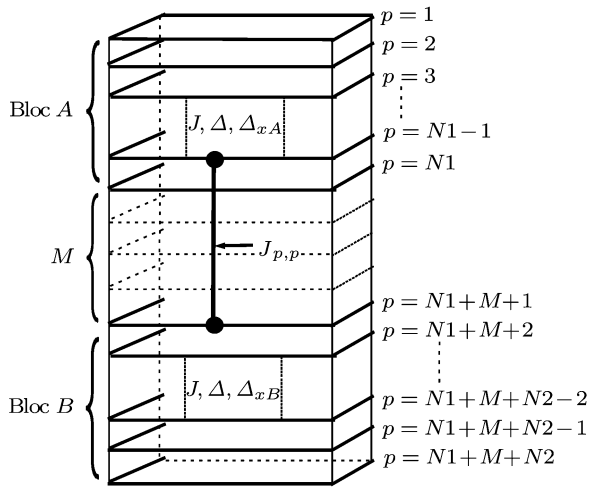


Fig. 1. A schematic illustration of the model.

The system is infinite and symmetric in the x and y directions and of finite thickness in the z direction. The Hamiltonian of this system is given by

$$H = -J\sum_{<i,j>} S_{iz}S_{jz} - \sum_{<p,p'>} J_{p,p'} \sum_{<i,j>'} S_{iz}S_{jz} - \Delta\sum_i S_{iz}^2 - \sum_i \Delta_{xi}S_{ix}^2, \quad (1)$$

where J is the bilinear exchange interaction, the first sum runs over all pairs of nearest-neighbour sites of the system. $\sum_{<p,p'>}$ means the summation over all pairs of layers p ($p \in$ bloc A) and p' ($p' \in$ bloc B), $\sum_{<i,j>'}$ means the summation over axially (with the axis being perpendicular to the non-magnetic layers) connected pairs of sites i and j in layers p and p', respectively, see Fig. 1, and $\sum_i$ means the summation over all site of blocs A and B. $J_{p,p'}$ is the 'RKKY-like' coupling, across the non-magnetic layers, between the layers p and p', given by

$$J_{p,p'} = \frac{aJ_0}{(p-p')^2}\cos(k_{\rm F}(p-p')), \quad (2)$$

where $k_{\rm F}$ is the Fermi level, a is the lattice constant, J_0 is a magnetic coupling constant,[15] Δ is the longitudinal crystal field, and Δ_{xi} is the quantum transverse anisotropy, which takes the value Δ_{xA} on the bloc A and Δ_{xB} on the bloc B. For simplicity we assume $a = 1$ and $J_0 = 1$. $\boldsymbol{S}_{ix}$ and $\boldsymbol{S}_{iz}$ are the spin-1 Pauli matrices given by

$$\boldsymbol{S}_{ix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix},$$

$$\boldsymbol{S}_{iz} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

Using the mean field approximation based on the variation principle for free energy[43]

$$F^{\rm exact} \le F = {\rm Tr}(\boldsymbol{\rho}_0 H) + \left(\frac{1}{\beta}\right){\rm Tr}(\boldsymbol{\rho}_0 \log(\boldsymbol{\rho}_0 H)), \quad (3)$$

where $F^{\rm exact}$ and F are the exact and approximate free energies, respectively, and ρ_0 is any trial density matrix. The equality sign holds if $\rho_0 = {\rm e}^{-\beta H}/{\rm Tr}\ {\rm e}^{-\beta H}$. Tr, means the trace performed over all spin configurations, and $\beta = \frac{1}{k_{\rm B}T}$, $k_{\rm B}$ is the Boltzmann constant, and T is the absolute temperature. We minimize the right-hand side of Eq. (3) for the most general density matrix that is factored into single density matrices. Hence, $\boldsymbol{\rho}_0 = {\rm e}^{-\beta H_0}/{\rm Tr}\ {\rm e}^{-\beta H_0}$, where H_0 is the mean field Hamiltonian given by:

$$H_0 = -\sum_i h_{i\rm eff}\boldsymbol{S}_{iz} - \sum_i h_{i\rm eff}^{\rm RKKY}\boldsymbol{S}_{iz}$$

$$- \sum_i \Delta_i \boldsymbol{S}_{iz}^2 - \sum_i \Delta_{xi} \boldsymbol{S}_{ix}^2, \tag{4}$$

which can be written as

$$H_0 = \sum_i H_{0i}, \tag{5}$$

where $h_{i\text{eff}}$ and $h_{i\text{eff}}^{\text{RKKY}}$ are the effective field and effective field of RKKY interaction, respectively, which could minimize the mean field free energy F.

The longitudinal (transversal) magnetization and quadrupolar moment of a site i are given in the mean field approximation, respectively, by

$$m_{i\alpha} = \frac{\text{Tr } S_{i\alpha} \mathrm{e}^{-\beta H_0}}{\text{Tr } \mathrm{e}^{-\beta H_0}}, \tag{6}$$

$$q_{i\alpha} = \frac{\text{Tr } S_{i\alpha}^2 \mathrm{e}^{-\beta H_0}}{\text{Tr } \mathrm{e}^{-\beta H_0}} \tag{7}$$

by calculating the three eigenvalues λ_k ($k = 1,\ 2,\ 3$) of H_{0i} and their corresponding eigenvectors $|\psi_k\rangle = \alpha_k |+\rangle + \beta_k |-\rangle + \gamma_k |0\rangle$ (e.g. these eigenvalues and eigenvectors are calculated numerically), one can perform the traces of Eqs. (6) and (7). Since the system is invariant by translation in both x and y directions of the lattice, it is clear that for each site i of a layer p ($p = 1, 2, \ldots, N1 + M + N2$); $\lambda_{ki} = \lambda_k(p)$; $|\psi_{ki}\rangle = |\psi_k(p)\rangle$; $m_{i\alpha} = m_\alpha(p)$ and $q_{i\alpha} = q_\alpha(p)$ with $\alpha = z, x$. Hence, $m_\alpha(p)$ and $q_\alpha(p)$ denote, respectively, the longitudinal (transversal) magnetization and quadrupolar moment of the layer p; the latter plays the role of density in the lattice–gas interpretation. Their expressions are given, respectively, by

$$m_z(p) = \frac{\sum_{k=1}^{3} (\alpha_k^2(p) - \beta_k^2(p)) \exp(-\beta\lambda_k(p))}{\sum_{k=1}^{3} \exp(-\beta\lambda_k(p))}, \tag{8}$$

$$m_x(p) = 0, \tag{9}$$

$$q_z(p) = \frac{\sum_{k=1}^{3} (\alpha_k^2(p) + \beta_k^2(p)) \exp(-\beta\lambda_k(p))}{\sum_{k=1}^{3} \exp(-\beta\lambda_k(p))}, \tag{10}$$

$$q_x(p) = \frac{\sum_{k=1}^{3} ((\alpha_k(p) + \beta_k(p))^2/2 + \gamma_k^2(p)) \exp(-\beta\lambda_k(p))}{\sum_{k=1}^{3} \exp(-\beta\lambda_k(p))}. \tag{11}$$

The reduced longitudinal ($\alpha = z$) and transversal ($\alpha = x$) magnetization ($m_{\alpha,A}$ and $m_{\alpha,B}$) and quadrupolar moment ($q_{\alpha,A}$ and $q_{\alpha,B}$) of blocs A and B respectively are given by

$$m_{\alpha,A} = \frac{1}{N1} \sum_{p=1}^{N1} m_\alpha(p),$$

$$q_{\alpha,A} = \frac{1}{N1} \sum_{p=1}^{N1} q_\alpha(p), \tag{12}$$

$$m_{\alpha,B} = \frac{1}{N2} \sum_{p=N1+M+1}^{N1+M+N2} m_\alpha(p),$$

$$q_{\alpha,B} = \frac{1}{N2} \sum_{p=N1+M+1}^{N1+M+N2} q_\alpha(p). \tag{13}$$

Hence, the total magnetizations and the total quadrupolar moments of the system are given respectively by

$$m_{\alpha,T} = \frac{1}{N1+N2} \Bigg[\sum_{p=1}^{N1} m_\alpha(p) + \sum_{p=N1+M+1}^{N1+M+N2} m_\alpha(p) \Bigg], \tag{14}$$

$$q_{\alpha,T} = \frac{1}{N1+N2} \Bigg[\sum_{p=1}^{N1} q_\alpha(p) + \sum_{p=N1+M+1}^{N1+M+N2} q_\alpha(p) \Bigg] \tag{15}$$

with $\alpha = z, x$.

However, the mean-field reduced free energy of such a system can be written as follows:

$$F = -k_{\text{B}}T \sum_{p=1}^{N1+M+N2} \log \left[\sum_{k=1}^{3} \mathrm{e}^{-\frac{\lambda_k(p)}{T}} \right] + \frac{1}{2} \sum_{p=1}^{N1+M+N2} \left[m_p m_{p-1} + 4m_p^2 + m_p m_{p+1} \right] + \frac{1}{2} \sum_{p=1}^{N1+M+N2} \left[\sum_{p''=N1+M+1}^{N1+M+N2} J_{p,p'''} m_p m_{p''} + \sum_{p'=1}^{N1} J_{p,p''} m_p m_{p''} \right]. \tag{16}$$

3. Results and discussions

We are now able to study the magnetic properties in the multi-layer (i.e. transition temperature) of the ferromagnetic Ising model in a quantum transverse anisotropy (Δ_x) with RKKY interaction. In order to examine the effect of the thickness of the magnetic multi-layer N ($N = N1 + N2$) and the quantum transverse anisotropy (Δ_x) on the transition temperature of the model (1), we have studied, using mean field theory, the behaviour of the transition temperature as a function of the thickness of the magnetic multi-layer$N$ (i.e. for $N = N1 + N2$, there exist several possible choices of $N1$ and $N2$, for example, when $N = 6$, there exist three possible choices, such as the case 1 ($N1 = 1$ and $N2 = 5$, $N1 = 2$ and $N2 = 4$ and $N1 = 3$ and $N2 = 3$). These three different possibilities can lead to three different transition temperatures. However, in Fig. 2(a) we considered the case of $N1 = N2$ for different values of the transverse anisotropy (Δ_x), for $\Delta/J = 1$, $k_{\rm F} = 0.1$ and $M = 6$. Then, it is necessary to calculate the critical temperatures from the behaviour of the corresponding magnetization, because, in the case of multilayer transition we can not use the linearization method since, in principle, the magnetizations are not simultaneously closed to zero. It is found that the multilayer transition temperature increases with increasing the thickness of the magnetic multi-layer $N1$ and/or $N2$ (Fig. 2(a)); reaching the bulk critical temperature $T_{\rm c}^{\rm b}$, for sufficiently large values of $N1$ and/or $N2$, these bulk critical temperature decreases with increasing the quantum transverse anisotropy. Indeed, for $\Delta_x/J = 0.1$, $T_{\rm c}^{\rm b}/J = 4.248$, for $\Delta_x/J = 5$, $T_{\rm c}^{\rm b}/J = 3.049$ (i.e. in the case$\Delta_x = \Delta_{xA} = \Delta_{xB}$, the two blocs A and B transit simultaneously at the same temperature $T_{\rm c} = T_{{\rm c}_A} = T_{{\rm c}_B}$). Moreover, Fig. 2(b) shows that the multi-layer transition temperature decreases when increasing the quantum transverse anisotropy ($\Delta_x = \Delta_{xA} = \Delta_{xB}$), for different values of the thickness of the system N ($N = N1 + N2$ with $N1 = N2$), for $\Delta/J = 1$, $k_{\rm F} = 0.1$ and $M = 6$. Furthermore, for $\Delta_{xA} > \Delta_{xB}$(for example $\Delta_{xA}/J = 7$ and $\Delta_{xB}/J = 0.1$), the two blocs A and B exhibit at different transition temperatures $T_{{\rm c}_A}$ and $T_{{\rm c}_B}$ (Fig. 3(a)). Moreover, for sufficiently large values of the quantum transverse anisotropy Δ_{xA} (Δ_{xB} fixed), the multi-layers bloc A and bloc B exhibit an order–disorder transition at different critical temperatures $T_{{\rm c}_A}$ and $T_{{\rm c}_B}$, respectively. For $\Delta_{xA} > \Delta_{xB}$(for example: $\Delta_{xA}/J = 7$ and $\Delta_{xB}/J = 0$), $T_{{\rm c}_A} < T_{{\rm c}_B}$, while for small value of the quantum transverse field Δ_{xA}, the RKKY interaction becomes strongly dominant in comparison with the thermal fluctuation and then the magnetism in the bloc A is reinforced by the magnetism of bloc B via RKKY interaction, and then the two blocs exhibit an order–disorder transition at the same temperature ($T_{{\rm c}_A} = T_{{\rm c}_B}$).

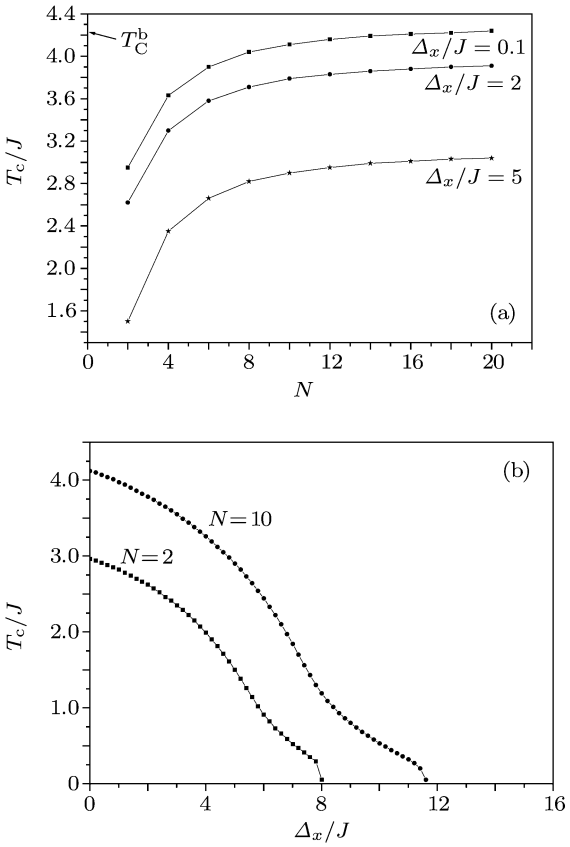


Fig. 2. The dependence of the transition temperature as a function: (a) of the thickness of the system ($N = N1+N2$) for different values of (Δ_x); (b) of the quantum transverse anisotropy (Δ_x) for different values of N. For $\Delta/J = 1$, $k_{\rm F} = 0.1$ and $M = 6$.

It is clear that the quantum transverse anisotropy (Δ_{xA}) applied in the bloc A decreases the longitudinal magnetization in this bloc A and without the effect on the longitudinal magnetization in the bloc B. This result is illustrated in Figs. 3(b) and 3(c), for fixed values of $N1$, $N2$, M and $k_{\rm F}$ (i.e. $N1 = N2$). On the other hand, in absence (present) of the crystal field, for $T \prec (T_{{\rm c}_A}$ or $T_{{\rm c}_B})$, the quadrupolar moment (q_{zA} or q_{zB}) decreases and (q_{xA} or q_{xB}) increases with increasing the temperature, passing through cups at $T_{{\rm c}_A}$ ($T_{{\rm c}_B}$) and reaching their asymptotic value at high temperature ($T \succ T_{{\rm c}_A}$ ($T_{{\rm c}_B}$)). It is clear that we change the Δ_{xA} ($\Delta_{xB}/J = 0$) the variation of the quadrupolar moment of the bloc A (q_{zA}) is similar so that it decreases from the saturation value at $T = 0$ (q_{zA})

to an asymptotic value while decreasing when we increase Δ_{xA}, but the quadrupolar moment of the bloc B (q_{xB}) is independent of Δ_{xA}.

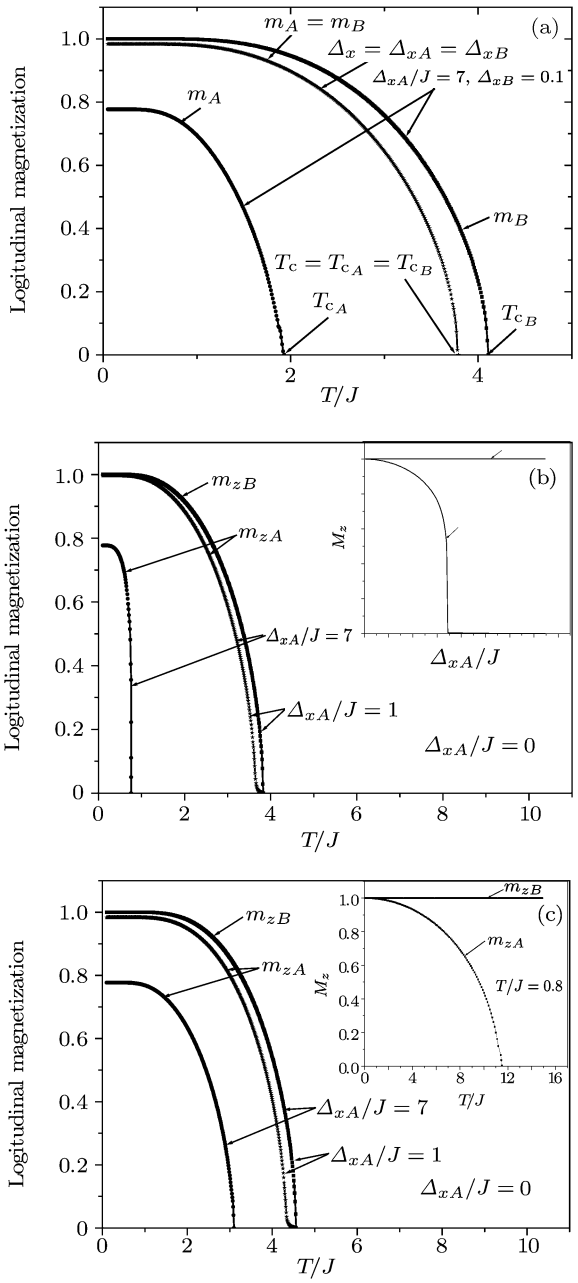


Fig. 3. The dependence of the longitudinal magnetization as a function of the temperature for $N1 = N2 = 5$, $k_F = 0.1$ and $M = 6$; (a) $\Delta/J = 1$, (b) $\Delta/J = 0$ and (c)$\Delta/J = 3$.

Moreover, for the transverse quadrupolar moment of the bloc A (q_{xA}), the variation is similar when we change Δ_{xA}. It is clear that the q_{xA} increases with the increasing of Δ_{xA}, but q_{xB} of the bloc B is independent of the quantum transverse anisotropy Δ_{xA} (Fig. 4(a) and 4(b)). We note that the larger the transverse anisotropy (the larger the transverse quadrupolar moment), the smaller the longitudinal magnetization and quadrupolar moment, which means that the transverse anisotropy inhibits the magnetic ordering in the z direction and plays a role in the crystal defects (dislocation). This is qualitatively in good agreement with experimental results[41] and theoretical calculations obtained in previous works.[29]

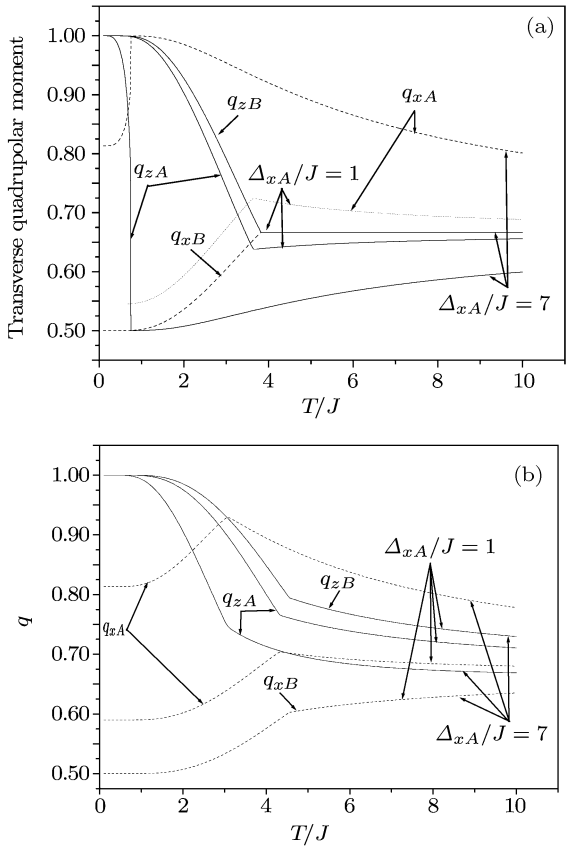


Fig. 4. The dependence of the quadrupolar moment (solid lines) and transverse quadrupolar moment (dashed lines) as a function of temperature for $N1 = N2 = 5$, $k_F = 0.1$, $\Delta_{xB}/J = 0$ and $M = 6$; (a)$\Delta/J = 0$, and (b)$\Delta/J = 3$.

However, using the mean field approximation the phase diagrams presented in Fig. 5, exhibit three different phases, namely: (1) the two magnetic blocs A and B are ordered, (2) the magnetic bloc A is disordered and the magnetic bloc B is ordered, and (3) the two magnetic blocs A and B are disordered. It is clear that the multi-layer transition, where A and B exhibit an order–disorder transition separately, occurs above a certain value of the quantum transverse anisotropy (Δ_{xL}). We note that Δ_{xL} depends strongly on the crystal fields Δ, and the RKKY interaction (e.g. the Fermi level k_F and the non-magnetic spacer of thickness M). Moreover, Δ_{xL} increases with increasing the crystal field Δ. Indeed, for Δ/J=0, $\Delta_{xL}/J = 0.435$,

and for $\Delta/J = 3$, $\Delta_{xL}/J = 1.353$ (Fig. 5).

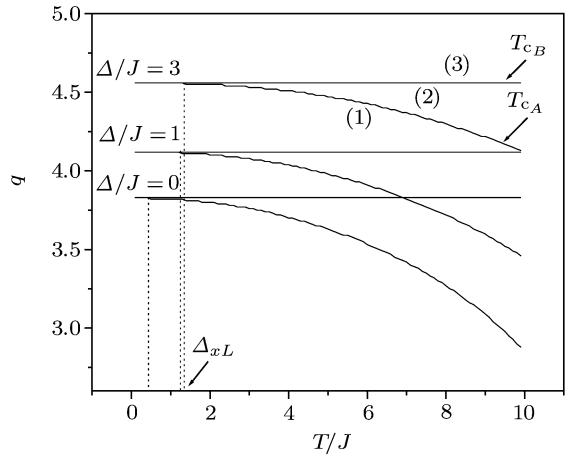


Fig. 5. The dependence of the transition temperature as a function of the quantum transverse anisotropy for several values of the crystal field. For $N1 = N2 = 5$, $k_{\rm F} = 0.1$, $\Delta_{xB}/J = 0$ and $M = 6$.

In contrast, the critical temperature of the bloc B is independent of Δ_{xA} because of the large value of its non-magnetic spacer of thickness ($M = 6$). On the other hand, in absence (present) of the longitudinal crystal field, Δ_{xL} decreases when increasing the non-magnetic spacer of thickness (M) (Fig. 6).

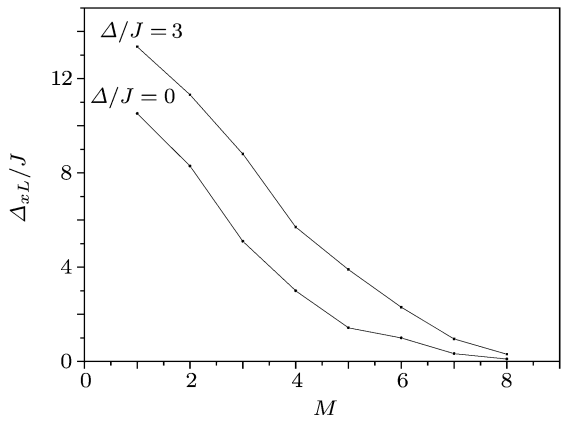


Fig. 6. The dependence of the critical quantum transverse anisotropy as a function of the thickness of non-magnetic spacer for several values of the crystal field. For $N1 = N2 = 5$, $k_{\rm F} = 0.1$, $\Delta_{xB}/J = 0$.

However, at certain thickness of the non-magnetic spacer of thickness M the critical quantum transverse anisotropy Δ_{xL} disappears completely, i.e, the two magnetic blocs A and B exhibit an order–disorder transition separately. Besides, Δ_{xL} depends strongly on the values of the Fermi level, indeed it oscillates as a function of $k_{\rm F}$ (Fig. 7).

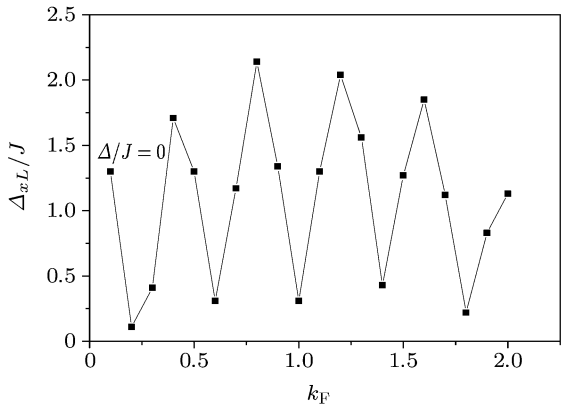


Fig. 7. The dependence of the critical quantum transverse anisotropy as a function of the Fermi level for $N1 = N2 = 5$, $M = 6$, $\Delta_{xB}/J = 0$ and $\Delta/J = 0$.

4. Conclusion

We have studied, using mean-field theory, the effect of the quantum transverse anisotropy with RKKY interaction on the multi-layer transition of a spin-1 Blume–Capel model formed by two magnetic blocs (A and B) separated by non-magnetic spacer of finite thickness M. We have shown that the magnetic order in the two blocs depends strongly on the quantum transverse anisotropy (Δ_{xA} and Δ_{xB}) and RKKY interaction. In particular, we have shown the existence of a critical quantum transverse anisotropy Δ_{xL} above which the multi-layer blocs undergo a transition separately at different temperature. Besides, we have shown that (Δ_{xL}) increases (decreases) with increasing the magnetic crystal field (increasing the non-magnetic spacer of thickness). Moreover, Δ_{xL} undergoes oscillations as a function of the Fermi level for fixed value of the non-magnetic thickness M. Finally, in this paper, we have shown that the quantum transverse anisotropy plays an opposite role in RKKY coupling.

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