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The method of reduction of transfer matrix for modulated systems

Grzegorz Wiatrowski*, Adam Krzemieniewski

Solid State Physics Department, University of Łódź, Pomorska 149/153, 90-236 Łódź, Poland

Abstract

We present a new method of calculation of partition function for the layered systems with the arbitrary spin-modulated structure in the linear cluster approximation. The thermodynamic description of the system in question is based on the Bogolyubov variational principle (inequality). The transfer matrix technique is used to determine the partition function, finally the free energy of the system, in terms of its largest eigenvalue. However, the compositional modulation introduces different types of transfer matrices related to different pure components of the system as well as the interface regions between them. The reduction of transfer matrices related to high-spin components obtained by a partial summation of the partition function gives us a simplified expression for the free energy in characteristic form already known for a low-spin component.

In particular, we study two periodic magnetic superstructures ABAB with a strong perpendicular anisotropy, spin SA = ½ and the large spin value SB = 1 or SB = 3/2. In each case, the method presented leads to a simple renormalized expression for the free energy of anisotropic homogeneous structure with only spins S = ½. Next, as a numerical result interesting discontinuous thermal transition between new stable ordered phases is obtained.

1. Introduction

In recent years, a great effort has been made to tailor the appropriate magnetic properties of artificially layered systems. Compositionally modulated films are produced by alternately evaporating layers of two different pure materials upon a substrate. This usually results in a sinusoidal varying composition profile along the film normal [1]. However, modern techniques allow to obtain the superstructures with even submonolayer composition [2]. This provides a possibility of obtaining the properties different from those of particular components, especially, when the uniaxial anisotropy of perpendicular type occurs in such systems [3].

It is well known that homogeneous bulk systems with a high integer spin value and its high half-integer counterpart exhibit a rich variety of ferromagnetic properties when the uniaxial anisotropy is strong enough [4]. The discontinuous transitions between different ordered phases can occur as a

*Corresponding author: *e-mail address*: wiatr@uni.lodz.pl

result of sequential switching off the spin z-component at the ground state of the system with strong negative (perpendicular) anisotropy [5]. Each of the integer and half-integer spin systems represent their own type of thermal behaviour, but bulk materials with $S = 1$ do not exhibit the above mentioned discontinuous transition due to the lack of possible phases. Recently, it has been shown, by contrast, that the bilayer structure composed of spin-½ and spin-1 films can exhibit such a transition because of a spin-polarisation effect [6]. Below, we extend our previous analysis to the more general case of superlattice and multilayer structures.

In the presented model we concentrate on the system ABAB which consists of two alternating ferromagnetic layers of A and B-atoms with spin-A and spin-B where $S_A = ½$ and $S_B \geq 1$, respectively. The ferromagnetic interlayer coupling is treated exactly in the frame of the Ising model in the perpendicular linear cluster (PELC) approach contrary to the recently applied parallel variant [3,6,7]. The transfer matrix method and the Bogolyubov variational principle determine the upper bound for the free energy for which the derived expression is of a common form for the arbitrary large spin-B value. That method of linear cluster has been well known for homogeneous systems since the pioneering papers by Kramers and Wannier [8] and occurs to be particularly useful in the Monte-Carlo simulations [9,10].

Our aim is to determine the thermal behaviour of layered magnetizations in compositionally modulated superstructures. In particular, we would like to establish whether both layered magnetizations vary continuously with temperature or a discontinuous transition between different ferromagnetic stable phases occurs provided a strong negative uniaxial anisotropy exists in high spin-B layers. The transfer matrix technique is applied to determine the partition function, finally the free energy of the system, in terms of its largest eigenvalue. The compositional modulation introduces different types of transfer matrices (even non-symmetric ones) related to different pure components of the system as well as the interface regions between them. The idea of reduction of transfer matrices related to the high-spin components gives us a simplified expression for the free energy in the characteristic form already known for a low-spin component of the system in question.

This paper presents the results of our analysis in the following way: the outline of the model is formulated in section 2, the numerical results, figures and conclusions are given in section 3. The explicit form of all coefficients in both expressions for reduced transfer matrix, free energy and layered magnetizations are collected in the Appendix for $S_B = 1$ and $S_B = 3/2$, respectively.

2. Outline of the model

We will consider below the s.c. periodic superlattice structure ABAB in the frame of Ising model (Fig. 1). The Hamiltonian for such spin-alternating layered system can be written in the form:

$$H = -\sum_{X,Y=A,B}\sum_{ij} J_{ij}^{XY} S_i^X S_j^Y - D\sum_i \left(S_i^B\right)^2 - \sum_{X=A,B}\sum_i h_i^X S_i^X \,, \tag{1}$$

where S_j^X is the spin operator at the site $\boldsymbol{j}$ of the plane X (= A, B) which takes on the values (A) ±½ and (B) -s, -s+1,..., s-1, s, respectively. Above D is the uniaxial anisotropy and h_j^X is the local magnetic field acting on the site $\boldsymbol{j}$ of plane X. In the present variational approach this local field plays a role of the variational parameter and will be established from the known Bogolyubov upper bound for the real free energy [11]

$$\Phi \le F\left(H_0\right) \equiv F_0 + \left\langle H - H_0 \right\rangle_0 , \tag{2}$$

where F_0 is a trial free energy obtained below from the transfer matrix method in the PELC approximation. Then, the Hamiltonian H_0 is considered as a sum H^{PELC} of energy operators of linear clusters assumed to be taken along the stack direction of the superlattice and immersed into the local magnetic fields of both types h_i^X ($X = A$, B):

$$H^{PELC} = -\sum_i \sum_{X,Y=A,B}\left[J_{ii}^{XY} S_i^X S_i^Y + D\left(S_i^B\right)^2 + \sum_X h_i^X S_i^X \right]. \tag{3}$$

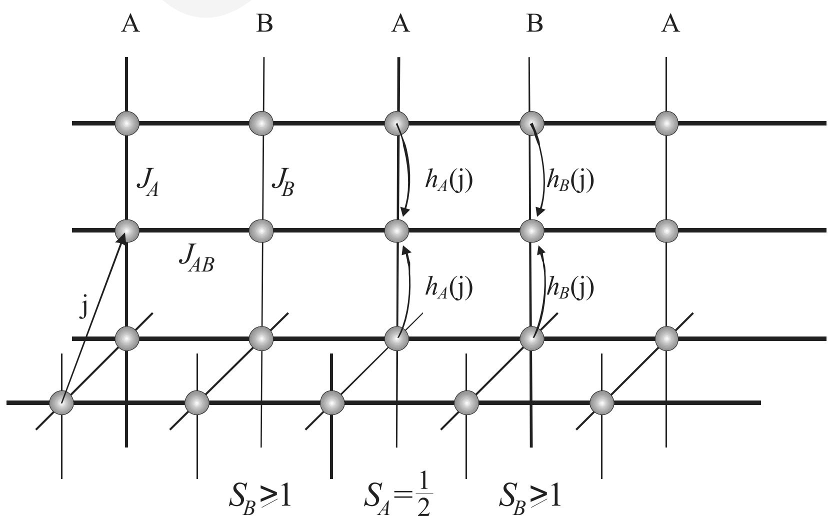

Fig. 1

The reduced transfer matrix $\hat{P}_{ABA}$ is defined as a product of usually considered transfer matrices $\hat{P}_{AB}$ and $\hat{P}_{BA}$ between the successive interacting nearest neighbours. In the case of the spin-modulated system ABAB each of transfer matrices, $\hat{P}_{AB}$ and $\hat{P}_{BA}$, is obviously non-symmetric, even non-quadratic, because of different spin-values assumed in advance in A and B counterparts of the system:

$$\left\langle S_i^A \middle| \hat{P}_{AB} \middle| S_i^B \right\rangle = \exp\left[\beta\left(J_{ii}^{AB} S_i^A S_i^B + \tfrac{1}{2} D\left(S_i^B\right)^2 + \tfrac{1}{2}\left(h_i^A S_i^A + h_i^B S_i^B\right)\right)\right]. \quad (4)$$

with $\beta = 1/k_B T$, where k_B is the Boltzmann constant and T stands for the temperature [8]. However, after simple calculations, $\hat{P}_{ABA}$ can be found as a square matrix independent of the values of spin S^B

$$\hat{P}_{ABA} = \hat{P}_{AB} \times \hat{P}_{BA} = \hat{P}_{AB} \times \hat{P}_{AB}^{\mathrm{T}} = \begin{bmatrix} A_1 & B \\ B & A_2 \end{bmatrix}, \quad (5)$$

where the superscript T denotes the transposed matrix. The coefficients A_i and B for the two values $S^B = 1$ and $S^B = 3/2$, are explicitly given in the Appendix.

To sum up, the partition function Z_{PELC} for the spin-modulated system in the PELC approximation obtained applying the standard transfer matrix representation (4)

$$Z_{PELC} = \ldots \sum_{S_i^A} \sum_{S_i^B} \sum_{S_i^{A'}} \cdots \prod_{\ldots A,B,A'\ldots} \left\langle S_i^A \middle| \hat{P}_{AB} \middle| S_i^B \right\rangle \left\langle S_i^B \middle| \hat{P}_{BA'} \middle| S_i^{A'} \right\rangle \quad (6)$$

reduces to the simplified form containing only the reduced transfer matrices $\hat{P}_{ABA}$ in our method. Thus, we have

$$Z_{PELC} = \ldots \sum_{S_i^A} \sum_{S_i^{A'}} \cdots \prod_{\ldots A,A'\ldots} \left\langle S_i^A \middle| \hat{P}_{ABA'} \middle| S_i^{A'} \right\rangle. \quad (7)$$

Finally, the trial free energy of the system in the thermodynamic limit is described by the largest eigenvalue λ_+^{ABA} of the reduced transfer matrix $\hat{P}_{ABA}$ given by Eq. (5):

$$F_0 = -k_B T \, \log\left[Z_{PELC}\right] = -k_B T \, \log\left[\lambda_+^{ABA}\right], \quad (8)$$

with the eigenvalue given in a general form known for the systems with the lowest spins $S = ½$

$$\lambda_{\pm}^{ABA} = A_+ \pm \sqrt{A_-^2 + B^2}\,,\ \left(A_{\pm} = \left(A_1 \pm A_2\right)/2\right). \quad (9)$$

The minimization of the upper bound free energy $F(H_0)$ in (2) leads to the mean field solution for the variational parameters in each of the layers of the structure considered (see also [3])

$$h_i^X = \sum_j J_{ij}^{XX} \left\langle S_j^X \right\rangle_0, \ (X = A, B). \quad (10)$$

The average layered magnetizations m_A and m_B are obtained from trial free energy (8) according to the thermodynamic definition and after simple algebra can be written in the form

$$m_A \equiv \left\langle S_i^A \right\rangle_0 = \tfrac{1}{2} \frac{A_-}{\sqrt{A_-^2 + B^2}}\,, \tag{11a}$$

and

$$m_B \equiv \left\langle S_i^B \right\rangle_0 = \frac{k_B T}{\lambda_+^{ABA}} \left(\frac{\partial A_+}{\partial h_i^B} + 2m_A \frac{\partial A_-}{\partial h_i^B} + \frac{\partial B}{\partial h_i^B} \frac{B}{\sqrt{A_-^2 + B^2}} \right), \tag{11b}$$

with the coefficients as determined in expressions (5) and (9), respectively.

3. Numerical results and conclusions

The most important task when discussing the magnetic properties of superstructures with high spin components is to determine all possible solutions for layered magnetizations, it means all stable as well as unstable ordered phases. In that case, the function of free energy should be evaluated and the unique stable phase must be found at any temperature like that one which minimizes this functional. The minimization procedure is continued up to the critical region, however, it happens that the proper solution for magnetizations may change discontinuously between different ordered phases provided the perpendicular anisotropy is large enough [6,7].

On the basis of the reduced transfer matrix outlined in Section 2, the thermal variation of layered magnetizations for two spin-modulated superlattice structures is investigated in detail. In Figs. 2 and 3, we present all possible solutions indicating the stable behaviour (solid line) of magnetization for superlattices ABAB with the most characteristic values of anisotropy constant D while large-spin $S^B = 1$ and $S^B = 3/2$, respectively.

A new effect of the first order phase transitions between the ordered phases is reported in Fig. 2 for the compositionally spin-modulated structure with the large spin equal one. The effect is qualitatively similar to that usually occurring in homogeneous bulk spin-3/2 systems and does not exist in the homogeneous spin-1 structure [4].

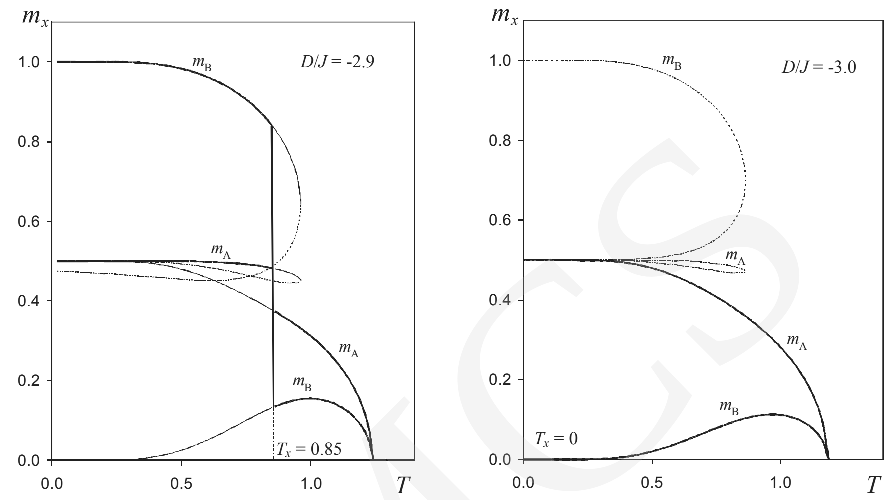

Fig. 2

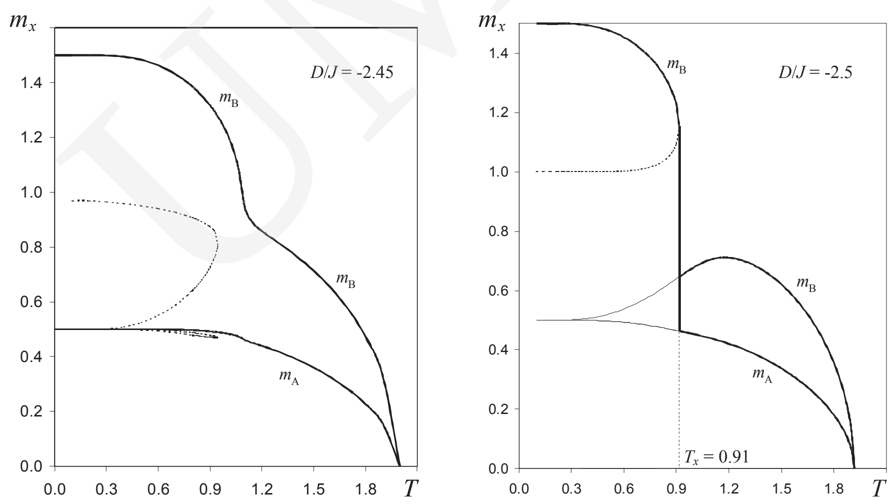

Fig. 3

The above considered modulated layered structures reveal different properties from those of the respective mixed-spin systems based on the same types of atoms arranged in the form of two interpenetrating sublattices. In this case the local properties of one constituent are strongly delocalized into the counterpart region via the spin-polarization effect. That phenomenon can lead to the continuous thermal behaviour in sublattice with spin-1 even for very large negative values of uniaxial anisotropy, while on the other hand, spin-1/2 subsystem may undergo the first order transition if only the intra-B-layer exchange coupling is strong enough.

It should be stressed that algorithm presented above is completely general, however, performed here only for the lowest spin-B values and the simplest periodic ABAB superlattice structure. It can be easily extended for an arbitrary case of any multilayer superstructure with very high spin values.

Appendix

The explicit form of coefficients in (5) and (7) for spin $S_B = 1$ is given by

$$A_+ = (A_1 + A_2)/2 = ED(1)\left[EJ(1)C(2) + EJ(-1)C(-2) + C(0)\right], \tag{A1}$$

$$A_- = (A_1 - A_2)/2 = ED(1)\left[EJ(1)S(2) + EJ(-1)S(-2) + S(0)\right], \tag{A2}$$

and

$$B = 1 + 2ED(1)\cosh\left(\beta h^B\right), \tag{A3}$$

while for spin $S_B = 3/2$, we obtain

$$\begin{aligned} A_+ = (A_1 + A_2)/2 = ED(9/4)\left[EJ(3/2)C(3) + EJ(-3/2)C(-3)\right] + \\ ED(1/4)\left[EJ(1/2)C(1) + EJ(-1/2)C(-1)\right] \end{aligned}, \tag{A4}$$

$$\begin{aligned} A_- = (A_1 - A_2)/2 = ED(9/4)\left[EJ(3/2)S(3) + EJ(-3/2)S(-3)\right] + \\ ED(1/4)\left[EJ(1/2)S(1) + EJ(-1/2)S(-1)\right] \end{aligned}, \tag{A5}$$

and

$$B = 2ED(9/4)\cosh\left(3\beta h^B/2\right) + 2ED(1/4)\cosh\left(\beta h^B/2\right). \tag{A6}$$

For simplicity we have introduced the following notation:

$$C(x) = \cosh\left(\beta\left(h^A + xh^B\right)/2\right), \tag{A7}$$

$$S(x) = \sinh\left(\beta\left(h^A + xh^B\right)/2\right), \tag{A8}$$

$$ED(x) = \exp\left(x\beta D\right), \tag{A9}$$

$$EJ(x) = \exp\left(x\beta J^{AB}\right). \tag{A10}$$

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