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Critical properties of Ising multilayer systems: cluster approximation

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Abstract. The theoretical framework for investigating the critical behaviour of an Ising multilayer system consisting of alternating spin-1/2 and spin-S ($S \geqq \frac{1}{2}$) magnetic layers is given within the cluster approximation introduced into the differential operator technique. It has the statistical accuracy corresponding to the Bethe–Peierls approximation. The critical temperatures T_C of some multilayer systems are studied numerically. We find some characteristic features, including the behaviour of a critical transverse field in the transverse spin-1/2 ferromagnetic multilayer system and the different behaviour of the T_C curve in an alternating spin-1/2 and spin-S ($S > \frac{1}{2}$) Ising multilayer system, depending on whether S is an integer or a half-integer.

1. Introduction

In recent years, the research on thin magnetic films with multilayer structures has received much interest both from the theoretical and experimental point of view. These new materials give the potential for many technological advances in information storage [1]. The study of a magnetic multilayer has been motivated by the concept that the magnetic properties may be significantly different from those of their constituents. In fact, many new phenomena have been observed in these magnetic systems [1]. Furthermore, there has been considerable interest in the theoretical and experimental study of thin ferroelectric films [2]. From the theoretical point of view, ferroelectric films have been described with an Ising model in a transverse field. An infinite ferroelectric superlattice with alternating two different slabs has been examined within such a model [3].

The effective-field theory (EFT) with correlation based on Ising spin identities [4, 5] has been widely used for Ising spin systems. Although mathematically simple, this approach has proved to be superior to the standard mean-field approximation and has been successfully applied to a variety of thin (ferromagnetic or ferroelectric) film problems [6–9] as well as infinite superlattice problems [10–12]. The EFT just corresponds to the Zernike approximation [13] when it is applied to spin-1/2 Ising problems. It has often been called the single-site cluster approximation. Over two decades, attempts have been made to extend the effective-field method within the framework of the single-site cluster theory to the two-site cluster approximation, such as the correlated EFT [14] and the two-site EFT [15] based on both Ising spin identities and the differential operator technique. In these approaches, the intra-cluster spin correlation is taken into account, so that the obtained value of critical temperature is improved. As far as we know, however, the concept of the effective-field corresponding to the so-called Bethe–Peierls approximation of a spin-1/2 Ising problem [16] has not been

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introduced into the effective-field method based on Ising spin identities (namely the differential operator technique). Such a trial has been done very recently by the present author [17] and also the Bethe–Peierls approximation of a spin-1/2 Ising problem has been extended to a higher spin ($S > \frac{1}{2}$) Ising problem.

The aim of this work is to study the critical property (transition temperature or critical transverse field) of an Ising multilayer system within the new framework of the cluster approximation introduced into the differential operator technique. The system consists of alternating two ferromagnetic monolayers (A and B) with different bulk (two-dimensional) properties coupled with an interlayer coupling, such as ferrimagnetic $Fe_2O_4/CoFe_2O_4$ multilayers [18] (or ferroelectric $BaTiO_3/SrTiO_3$ multilayers [19]). The two magnetic constituents A and B are considered to have different spins. Spin S_A in the monolayer A is fixed at $S_A = \frac{1}{2}$ and spin S_B of the monolayer B is taken as an arbitrary spin value ($S_B \geqq \frac{1}{2}$). Furthermore, when $S_B > \frac{1}{2}$, we would like to study the influence of single-ion anisotropy D in the monolayer B on the transition temperature, as has been done in [10]. Theoretically, it is important to treat these problems within a simple framework.

The outline of this work is as follows. In section 2, we present the general formulation of a multilayer Ising spin system within the framework of the cluster (Bethe–Peierls-like) approximation. The general formulation of the transition temperature in the system is derived in section 3. In section 4, we study the phase diagrams of an Ising multilayer system with $S_A = S_B = \frac{1}{2}$ in a transverse field as a special case of the general formulation. The results obtained numerically prove that the formulation is equivalent to that of the Bethe–Peierls approximation for spin-1/2 Ising problems. It is shown that the critical transverse field at which the transition temperature reduces to zero exhibits a characteristic behaviour. In section 5, the effects of single-ion anisotropy on the transition temperature in the multilayer system with $S_A = \frac{1}{2}$ and $S_B \geqq \frac{1}{2}$ are investigated numerically, selecting the two values of S_B as $S_B = 1$ and $S_B = \frac{3}{2}$ and taking some typical values of exchange interactions. We also find some characteristic behaviour of the T_C curve induced by the negative single-ion anisotropy on monolayer B for the system with $S_B = 1$ (or an integer spin).

2. Formulation

We consider a ferromagnetic multilayer system, consisting of two alternating magnetic monolayers (A and B) with different spins ($S_A = \frac{1}{2}$ and $S_B \geqq \frac{1}{2}$). For simplicity, we restrict our attention to the case of an infinite simple cubic Ising-type structure where each monolayer is defined on the x–y plane. The Hamiltonian of the system is given by

$$H = -J_A \sum_{(ij)} \mu_i^z \mu_j^z - J_B \sum_{(mn)} S_m^z S_n^z - J_{AB} \sum_{(im)} \mu_i^z S_m^z - D \sum_m (S_m^z)^2 \tag{1a}$$

or

$$H = -J_A \sum_{(ij)} \mu_i^z \mu_j^z - J_B \sum_{(mn)} S_m^z S_n^z - J_{AB} \sum_{(im)} \mu_i^z S_m^z - \Omega\left(\sum_i \mu_i^x + \sum_m S_m^x \right) \tag{1b}$$

where the first two summations are carried out only over nearest-neighbour pairs of spins in A and B layers. μ_i^z and S_m^α ($\alpha = z$ and x) are spin operators on monolayers A and B, respectively. D in (1a) is the single-ion anisotropy constant which should be taken into account when $S_B > \frac{1}{2}$. Ω in (1b) is a transverse field. J_α ($\alpha = A$ or B) is the exchange interaction constant in the monolayer α. J_{AB} is the interlayer exchange constant.

The problem is now the evaluation of the expectation values $\sigma_0 = \langle \mu_i^z \rangle$ and $m_0 = \langle S_m^z \rangle$ when the site i or m is selected as the central site of the spin cluster. It can be done by the use of both exact Ising spin identities [20, 21] and the differential operator technique [4, 5], when we treat the multilayer system with (1*a*). They are given by

$$\sigma_0 = \langle \mu_i^z \rangle = \langle \exp(\theta_i \nabla) \rangle f(x)|_{x=0} \tag{2}$$

with

$$\theta_i = J_A \sum_\delta \mu_{i+\delta}^z + J_{AB} \sum_{\delta'} S_{i+\delta'}^z \tag{3}$$

and

$$m_0 = \langle S_m^z \rangle = \langle \exp(\Theta_m \nabla) \rangle F(x)|_{x=0} \tag{4}$$

with

$$\Theta_m = J_B \sum_\delta S_{m+\delta}^z + J_{AB} \sum_{\delta'} \mu_{m+\delta'}^z \tag{5}$$

where δ and δ' denote the nearest neighbours of sites i and m and $\nabla = \partial/\partial x$ is a differential operator. The function $f(x)$ is given by, when we consider the multilayer system described by the Hamiltonian (1*a*),

$$f(x) = \tfrac{1}{2} \tanh(\tfrac{1}{2}\beta x) \tag{6}$$

with $\beta = 1/k_B T$. The explicit form of function $F(x)$ then depends on the value of S_B, and is given in appendix A. In the following, the formulation will be discussed for the multilayer system described by the Hamiltonian (1*a*), but it can be easily extended to the multilayer system in a transverse field presented by the Hamiltonian (1*b*), when the functions $f(x)$ and $F(x)$ are replaced by those in a transverse field [5, 22].

In order to rewrite (2) and (4) in the treatable forms, let us introduce the exact Ising spin identity

$$\exp(c\mu_i^z) = \cosh(c/2) + 2\mu_i^z \sinh(c/2) \tag{7}$$

for $S_A = \frac{1}{2}$ and the approximated identity

$$\exp(cS_m^z) = \cosh(\eta_0 c) + (S_m^z/\eta_0) \sinh(\eta_0 c) \tag{8}$$

with

$$(\eta_0)^2 = \langle (S_m^z)^2 \rangle = \langle \exp(\Theta_m \nabla) \rangle G(x)|_{x=0} \tag{9}$$

for $S_B \geqq \frac{1}{2}$, where the function $G(x)$ also depends on the value of S_B and the explicit form is given in appendix A. When $S_B = \frac{1}{2}$, (8) reduces exactly to (7) because $\eta_0 = \frac{1}{2}$. Using these relations, (2) and (4) can be written in the forms

$$\sigma_0 = \left\langle \prod_\delta [\cosh(a/2) + 2\mu_{i+\delta}^z \sinh(a/2)] \prod_{\delta'} [\cosh(\eta_1 c) + (S_{i+\delta'}^z/\eta_1) \sinh(\eta_1 c)] \right\rangle f(x)|_{x=0} \tag{10}$$

with

$$(\eta_1)^2 = \langle (S_{i+\delta'}^z)^2 \rangle \tag{11}$$

and

$$m_0 = \left\langle \prod_\delta [\cosh(\eta_2 b) + (S_{m+\delta}^z/\eta_2) \sinh(\eta_2 b)] \prod_{\delta'} [\cosh(c/2) + 2\mu_{m+\delta'}^z \sinh(c/2)] \right\rangle F(x)|_{x=0} \tag{12}$$

with

$$(\eta_2)^2 = \langle (S_{m+\delta'}^z)^2 \rangle \tag{13}$$

where $a = J_A\nabla$, $b = J_B\nabla$ and $c = J_{AB}\nabla$. The parameter η_0 defined by (9) is also given by

$$(\eta_0)^2 = \left\langle \prod_{\delta}[\cosh(\eta_2 b) + (S^z_{m+\delta}/\eta_2)\sinh(\eta_2 b)] \times \prod_{\delta'}[\cosh(c/2) + 2\mu^z_{m+\delta'}\sinh(c/2)] \right\rangle G(x)|_{x=0}. \tag{14}$$

In order to obtain the statistical accuracy corresponding to the Bethe–Peierls approximation, let us now define the effective spin operators for the perimeter spins of central spins μ^z_i and S^z_m, namely $\mu^z_{i+\delta}$, $S^z_{i+\delta'}$, $\mu^z_{m+\delta}$ and $S^z_{m+\delta'}$, defined in (10) and (12), as

$$\begin{aligned}
\mu^z_{i+\delta} &= a_1 + 2a_2\mu^z_i \equiv A\\
S^z_{i+\delta'} &= b_1 + 2b_2\mu^z_i \equiv A'\\
S^z_{m+\delta} &= b_3 + b_4 S^z_m = B\\
\mu^z_{m+\delta'} &= a_3 + a_4 S^z_m = B'
\end{aligned} \tag{15}$$

with

$$\begin{aligned}
a_1 &= \cosh(a/2) f(x + 3h_{AA} + 2h_{BA})|_{x=0}\\
a_2 &= \sinh(a/2) f(x + 3h_{AA} + 2h_{BA})|_{x=0}\\
b_1 &= \cosh(c/2) F(x + 4h_{BB} + h_{AB})|_{x=0}\\
b_2 &= \sinh(c/2) F(x + 4h_{BB} + h_{AB})|_{x=0}\\
b_3 &= \cosh(\eta_0 b) F(x + 3h_{AA} + 2h_{BA})|_{x=0}\\
b_4 &= (1\eta_0)\cosh(\eta_0 b) F(x + 3h_{AA} + 2h_{BA})|_{x=0}\\
a_3 &= \cosh(\eta_0 c) f(x + 4h_{AA} + h_{BA})|_{x=0}\\
a_4 &= (1/\eta_0)\sinh(\eta_0 c) f(x + 4h_{AA} + h_{BA})|_{x=0}
\end{aligned} \tag{16}$$

where $h_{\alpha\beta}$ represents the unknown effective field per spin acting from an atom on the monolayer α to an atom on the monolayer β. Performing the thermal average of (15), we obtain

$$\begin{aligned}
\sigma_1 &= \langle\mu^z_{i+\delta}\rangle = a_1 + 2a_2\sigma_0\\
m_1 &= \langle S^z_{i+\delta'}\rangle = b_1 + 2b_2\sigma_0\\
m_2 &= \langle S^z_{m+\delta}\rangle = b_3 + 2b_4 m_0\\
\sigma_2 &= \langle\mu^z_{m+\delta'}\rangle = a_3 + 2a_4 m_0.
\end{aligned} \tag{17}$$

Here, the physical background of (15) and (17) comes from the following approximation: for instance,

$$\langle\mu^z_{i+\delta}\rangle = \langle\exp(\theta_{i+\delta}\nabla)\rangle f(x)|_{x=0} \tag{18}$$

with

$$\theta_{i+\delta} = J_A\mu^z_i + J_A\Sigma\mu^z_{i+\delta+\delta'} + J_{AB}\Sigma S^z_{i+\delta+\delta'} \risingdotseq J_A\mu^z_i + 3h_{AA} + 2h_{AB}. \tag{19}$$

By performing the same procedure as (17), the parameters defined by (11) and (13) are given by

$$\begin{aligned}
(\eta_1)^2 &= d_1 + 2d_2\sigma_0\\
(\eta_2)^2 &= d_3 + d_4 m_0
\end{aligned} \tag{20}$$

with

$$\begin{aligned}
d_1 &= \cosh(c/2) G(x + 4h_{BB} + h_{AB})|_{x=0}\\
d_2 &= \sinh(c/2) G(x + 4h_{BB} + h_{AB})|_{x=0}\\
d_3 &= \cosh(\eta_0 b) G(x + 3h_{BB} + 2h_{AB})|_{x=0}\\
d_4 &= (1/\eta_0)\sinh(\eta_0 b) G(x + 3h_{BB} + 2h_{AB})|_{x=0}.
\end{aligned} \tag{21}$$

Substituting (15) into (10), (12) and (14), we obtain

$$\sigma_0 = \langle [\cosh(a/2) + 2A\sinh(a/2)]^4 [\cosh(\eta_1 c) + (A'/\eta_1)\sinh(\eta_1 c)]^2 \rangle f(x)|_{x=0} \quad (22)$$

$$m_0 = \langle [\cosh(\eta_2 b) + (B/\eta_2)\sinh(\eta_2 b)]^4 [\cosh(c/2) + 2B'\sinh(c/2)]^2 \rangle F(x)|_{x=0} \quad (23)$$

$$(\eta_0)^2 = \langle [\cosh(\eta_2 b) + (B/\eta_2)\sinh(\eta_2 b)]^4 [\cosh(c/2) + 2B'\sinh(c/2)]^2 \rangle G(x)|_{x=0}. \quad (24)$$

Within the present cluster theory, the four unknown parameters $h_{\alpha\beta}$ are included through the coefficients defined by (15). They can be determined from the four conditions, namely

$$\sigma_1 = \sigma_2 \qquad m_1 = m_2 \quad (25)$$

and

$$\sigma_0 = \sigma_1 (\text{or } \sigma_2) \qquad m_0 = m_1 (\text{or } m_2). \quad (26)$$

3. Transition temperature

Let us discuss how the transition temperature of a multilayer system can be obtained from the formulation in section 2. In the vicinity of the transition temperature T_C, we can assume that the four parameters $h_{\alpha\beta}$ are very small. The coefficients a_1, b_1, b_3 and a_3 in (15), (16) and (17) are proportional to the parameters $h_{\alpha\beta}$, but other coefficients can be taken as constants independent of the four parameters $h_{\alpha\beta}$: for instance, $a_2 = f(J_A/2)$.

Expanding the right hand sides of (22)–(24) and taking the terms linear in the parameters $h_{\alpha\beta}$ as well as σ_0 and m_0, (22) can be written as

$$\sigma = U_1(3 + 2\gamma) + U_2(4\varepsilon + \delta) \quad (27)$$

with

$$U_1 = \frac{8O_1}{1 - 4\Gamma_1} \qquad U_2 = \frac{2O_2}{1 - 4\Gamma_1} \quad (28)$$

and the equation (23) is given by

$$m = U_3(4 + \gamma) + U_4(3\varepsilon + 2\delta) \quad (29)$$

with

$$U_3 = \frac{4P_1}{1 - 4\Gamma_2} \qquad U_4 = \frac{4P_2}{1 - 4\Gamma_2} \quad (30)$$

where σ, m, γ, ε and δ are defined by

$$\sigma = (\sigma_0/\beta h_{AA}) \qquad m = (m_0/\beta h_{AA}) \qquad \gamma = (h_{BA}/h_{AA}) \qquad \varepsilon = (h_{BB}/h_{AA}) \\ \text{and } \delta = (h_{AB}/h_{AA}). \quad (31)$$

The coefficients O_1, O_2, P_1, P_2, Γ_1 and Γ_2 are defined in appendix B. From (24), the parameter η_0 (or $q_0 = (\eta_0)^2$) can be determined by solving the equation numerically

$$q_0 = Q_1 + 2q_0[3Q_2(b_2)^2 + 8Q_3 a_4 b_4 + 2Q_4(a_4)^2] \\ +(q_0)^2[Q_5(b_4)^4 + 16Q_6 a_4(b_4)^3 + 24Q_7(a_4)^2(b_4)^2] + 4(q_0)^3 Q_8 a_4(b_4)^4 \quad (32)$$

where the coefficients Q_i ($i = 1$–8) are defined in appendix B.

At this point, one should notice that, when expanding the right hand sides of (22)–(24), the averaged value of a moment higher than S_m^z may appear, such as $\langle (S_m^z)^n \rangle$ with an integer n larger than $n = 1$. It can be easily calculated from

$$\langle \exp(xS_m^z) \rangle = \cosh(\eta_0 x) + \frac{\langle S_m^z \rangle}{\eta_0} \sinh(\eta_0 x) \quad (33)$$

by differentiating both sides of it; for example

$$\langle (S_m^z)^3 \rangle = [(\nabla)^3 \langle \exp(x S_m^z) \rangle]_{x=0} = q_0 \langle S_m^z \rangle.$$

On the other hand, from (17), $\sigma_0 = \sigma_1$ and $m_0 = m_1$, we can obtain the relations

$$\sigma = U_5(3 + 2\gamma) \tag{34}$$

and

$$m = U_6(3\varepsilon + 2\delta) \tag{35}$$

with

$$U_5 = \frac{R_1}{1 - 2a_2} \text{ and } U_6 = \frac{R_2}{1 - b_4} \tag{36}$$

where R_1 and R_2 are defined by

$$R_1 = \frac{1}{\beta}[\nabla f(x)]_{x=r} \text{ and } R_2 = \frac{1}{\beta}[\nabla F(x)]_{x=s} \tag{37}$$

where $r = J_A/2$ and $s = J_B\eta_0$. Furthermore, from the relations $m_1 = m_2$ and $\sigma_1 = \sigma_2$, we can obtain the two equations

$$\sigma = \frac{U_7}{d_0} - \frac{U_8}{d_0}\gamma + \frac{U_9}{d_0}\varepsilon - \frac{U_{10}}{d_0}\delta \tag{38}$$

and

$$m = \frac{U_{11}}{d_0} - \frac{U_{12}}{d_0}\gamma + \frac{U_{13}}{d_0}\varepsilon - \frac{U_{14}}{d_0}\delta \tag{39}$$

with

$$d_0 = a_2 b_4 - a_4 b_2 \tag{40}$$

where the coefficients U_i ($i = 7$–14) are defined in appendix B.

By the use of these six relations for σ and m, we can obtain the matrix equation

$$M \begin{pmatrix} 1 \\ \gamma \\ \varepsilon \\ \delta \end{pmatrix} = 0 \tag{41}$$

with

$$M = \begin{pmatrix} 3(U_1 - U_5) & 2(U_1 - U_5) & 4U_2 & U_2 \\ 4U_3 & U_3 & 3(U_4 - U_6) & 2(U_4 - U_6) \\ (3d_0U_1 - U_7) & (2d_0U_1 + U_8) & (4d_0U_2 - U_9) & (d_0U_2 + U_{10}) \\ (4d_0U_3 - U_{11}) & (d_0U_3 + U_{12}) & (3d_0U_4 - U_{13}) & (2d_0U_4 + U_{14}) \end{pmatrix}. \tag{42}$$

The transition temperature of an Ising multilayer system described by (1a) or (1b) can be determined from the condition

$$\det M = 0. \tag{43}$$

4. Spin-1/2 multilayer system in a transverse field

The formulation given in sections 2 and 3 at first sight seems to be rather different from the standard method of the Bethe–Peierls approximation applied to a spin-1/2 Ising system. In this section, let us discuss numerically that the results of the spin-1/2 Ising multilayer system in a transverse field obtained from the formulation are completely equivalent to these of the Bethe–Peierls approximation.

The starting point for the examination of the multilayer system described by (1b) where S_m^α ($\alpha = z$ and x) are the spin-1/2 operators is to use the approximated relation introduced in [23]. Then, the function $f(x)$ in (2) should be replaced by

$$f(x) = \frac{1}{y}\tanh\left(\frac{\beta}{2}y\right) \tag{44}$$

with

$$y = (x^2 + \Omega^2)^{1/2}. \tag{45}$$

Furthermore, the function $F(x)$ defined in (4) is also given by (44) and the parameters η_0, η_1 and η_2 defined by (9), (11) and (13) must be $\eta_0 = \eta_1 = \eta_2 = \frac{1}{2}$. Then, the approximated identity (8) with $\eta_0 = \frac{1}{2}$ becomes equivalent to the identity (7). Substituting these relations into (42) and (43) and solving them numerically, we can obtain the transition temperature T_C of the Ising multilayer system in a transverse field consisting of alternating spin-1/2 ferromagnetic monolayers with different properties.

First, let us show the numerical result of the multilayer system with $\Omega = 0.0$, introducing the following ratios

$$A = J_A/J \qquad B = J_B/J \text{ and } C = J_{AB}/J. \tag{46}$$

As shown in figure 1, the transition temperature of the system with a fixed value of B may change continuously with variation of C and the T_C curves reduce to the same point at $C = 0.0$ which is given by $4k_BT_C/J = 2.8854$. At $C = 0.0$, the multilayer system is decomposed into two independent spin-1/2 monolayers and hence the T_C must be equivalent to the T_C result of the two-dimensional Ising system ($z = 4$), if our formulation is equivalent to that of the spin-1/2 Bethe–Peierls approximation (or $4k_BT_C/J = 2/[\log\{(z/(z-2)\}]$, where z is a coordination number). The T_C result at $C = 0.0$ is clearly nothing but the Bethe–Peierls one. Furthermore, when $A = B = C = 1.0$, the multilayer system reduces to the spin-1/2 simple cubic Ising system and hence the T_C must be $4k_BT_C/J_A = 4.9327$ for $z = 6$, when the present formulation is equivalent to the Bethe–Peierls approximation. It is also satisfied in figure 1, when putting $A = B = C = 1.0$. Thus, the formulation given in section 3 reproduces correctly the T_C values of the Bethe–Peierls approximation in the limits.

Figure 2 shows the phase diagram (T_C versus Ω plot) of the spin-1/2 multilayer system, selecting $A = 1.0$ and $B = 0.5$ and changing the value of C from $C = 1.0$ to $C = 0.0$. Each curve decreases monotonically with the increase of Ω and reduces to zero at the critical value Ω_C. In particular, when $C = 0.0$, the critical value Ω_C is given by $2\Omega_C/J_A = 2.3934$ which value is independent of the value of B, as is understood from figure 1 (or see figure 3). The critical value can be compared with that of the EFT ($2\Omega_C/J = 2.752$ for $z = 4$).

In figure 3, the critical value Ω_C of the multilayer system with $A = 1.0$ is plotted as a function of C, changing the value of B from $B = 1.0$ to $B = 0.0$. As discussed in figure 2, the critical value Ω_C for the system with $C = 0.0$ is given by $2\Omega_C/J_A = 2.3934$ in figure 3. The critical value Ω_C for the system with $A = B = C = 1.0$ is then given by $2\Omega_C/J_A = 4.4813$, which should be compared with that of the EFT ($2\Omega_C/J = 4.706$ for $z = 6$) [17, 22]. In particular, one should notice that the features of the Ω_C versus C plots are rather similar to those of figure 1, although, in detail, some small differences can be observed.

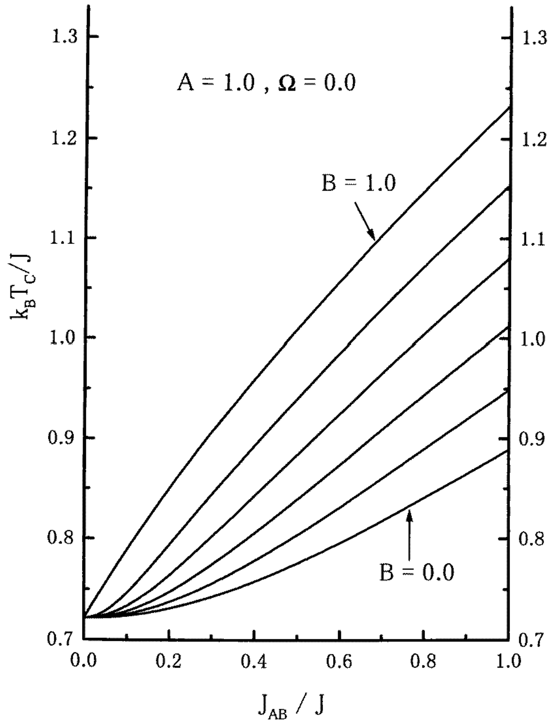

Figure 1. The phase diagram (T_C versus J_{AB}/J plot) of the spin-1/2 Ising multilayer system with $J_A/J = A = 1$ and zero transverse field ($\Omega = 0.0$), when the value of $B(\equiv J_B/J)$ is changed from $B = 1.0$ to $B = 0.0$ with the variation of 0.2.

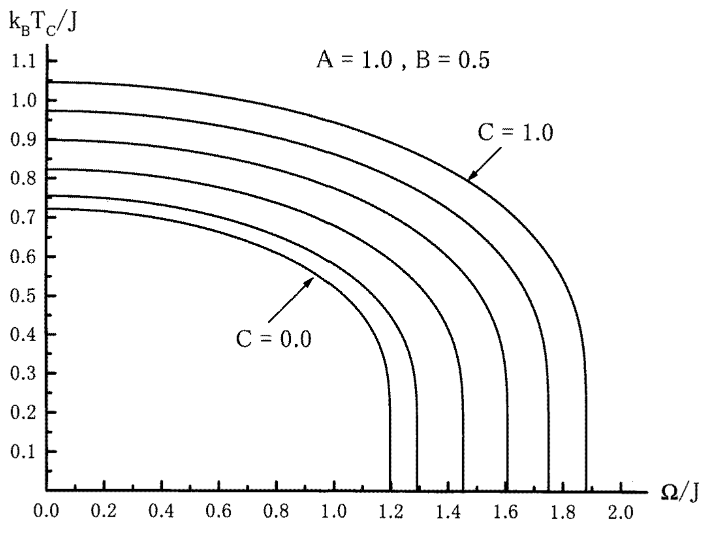

Figure 2. The phase diagram (T_C versus Ω plot) of the spin-1/2 Ising multilayer system with $A = 1.0$ and $B = 0.5$, when the value of $C(\equiv J_{AB}/J)$ is changed from $C = 1.0$ to $C = 0.0$ with the variation of 0.2.

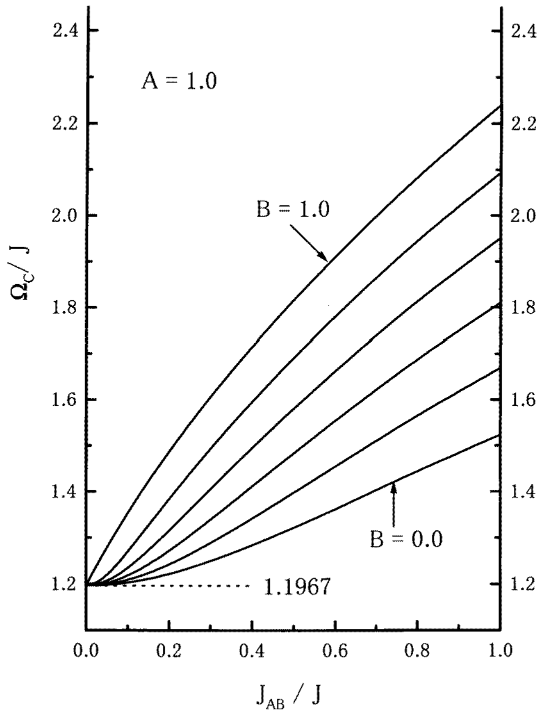

Figure 3. The critical value Ω_C of Ω at which the T_C curve of figure 2 reduces to zero is plotted as a function of J_{AB}/J for the spin-1/2 Ising multilayer system with $A = 1.0$, when the value of $B(\equiv J_B/J)$ is changed from $B = 1.0$ to $B = 0.0$ with the variation of 0.2.

5. Some numerical results

In this section, let us show some typical results of the T_C curve in the Ising multilayer system with a spin value S_B ($S_B > \frac{1}{2}$) described by the Hamiltonian (1a) by solving (42) and (43) numerically. In particular, it is important to compare the present results with those obtained from the framework of the EFT in [10] and [11] for the same Ising multilayer system.

Figure 4 shows the T_C versus D plots in two Ising multilayer systems with fixed values of $S_B = 3/2$ and $C = 0.1$, selecting the values of A and B as $A = 1.0$, $B = 0.5$ in figure 4(a) and $A = 0.5$, $B = 1.0$ in figure 4(b). In the figure, the curves labelled EFT are the results obtained from the framework of the EFT in [10] and the curves labelled BP are the present results. The features of figure 4 clearly express that the present formulation improves the T_C value of the multilayer system in a reasonable direction. In particular, one should notice that the T_C curves labelled EFT and BP in figure 4 go to the same values in the limit of $D/J \to -\infty$. In the limit, the spin state of B monolayers is given by the $S_m^z = \pm\frac{1}{2}$ state, the multilayer system of figure 4(a) is equivalent to that of figure 4(b) and hence the T_C values of the two systems must be identical.

In figure 5, the T_C versus D plots of the multilayer systems with $S_B = 1$ and $C = 0.1$ are depicted by selecting the same values of A and B as these of figure 4. The curves labelled EFT and BP in figure 5(a) exhibit behaviour similar to that of figure 4(a), while the curves of figure 5(b) are clearly different from those of figure 4(b) and 5(a). Both figures show clearly that the present formulation improves the T_C value in a reasonable direction. In particular,

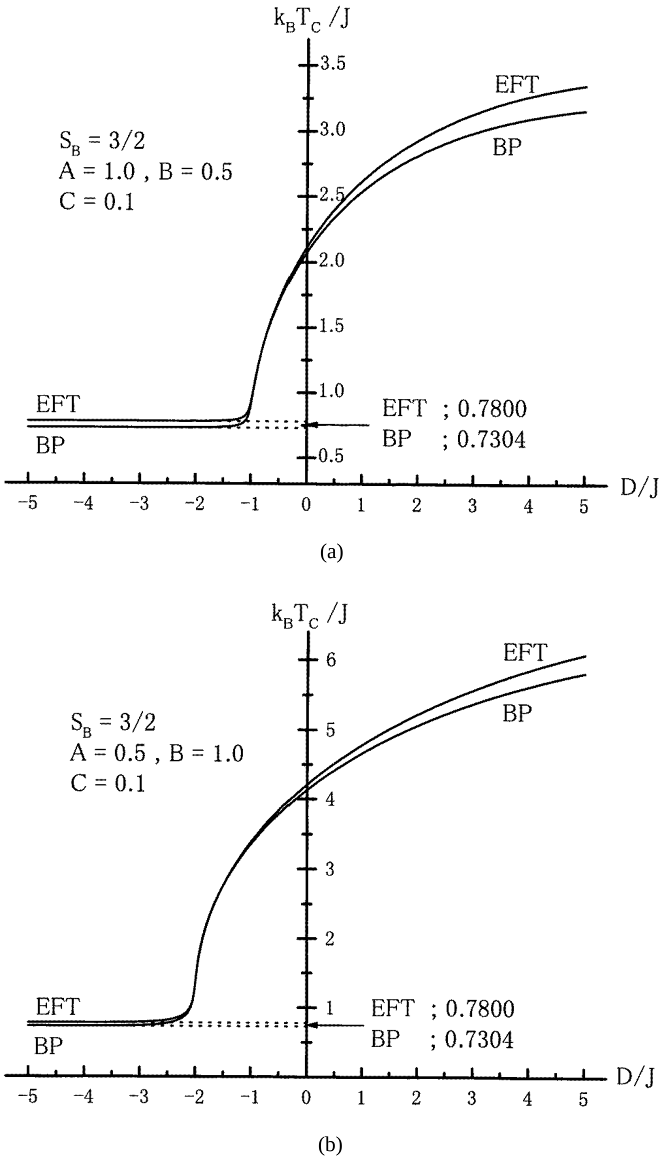

Figure 4. The T_C curve of the Ising multilayer system with a fixed value of C ($C = 0.1$) consisting of alternating spin-1/2 monolayer and spin-3/2 monolayer is depicted as a function of single-ion anisotropy D on spin-3/2 atoms, taking the two theoretical frameworks and selecting the two cases, namely the system with $A = 1.0$ and $B = 0.5$ in (a) and the system with $A = 0.5$ and $B = 1.0$ in (b). The curves labelled EFT and BP express the results obtained from the effective-field theory with correlation (EFT) [10] and the present framework, respectively.

the horizontal lines in figure 5 observed for large negative values of D give the T_C values of the two-dimensional spin-1/2 Ising system, namely $4k_BT_C/J = 3.090$ for the EFT and $4k_BT_C/J = 2.885$ for the Bethe–Peierls approximation. The reason comes from the fact that the spin state of B monolayers at $T = 0$ K may change from the $S_m^z = \pm 1$ state to the $S_m^z = 0$

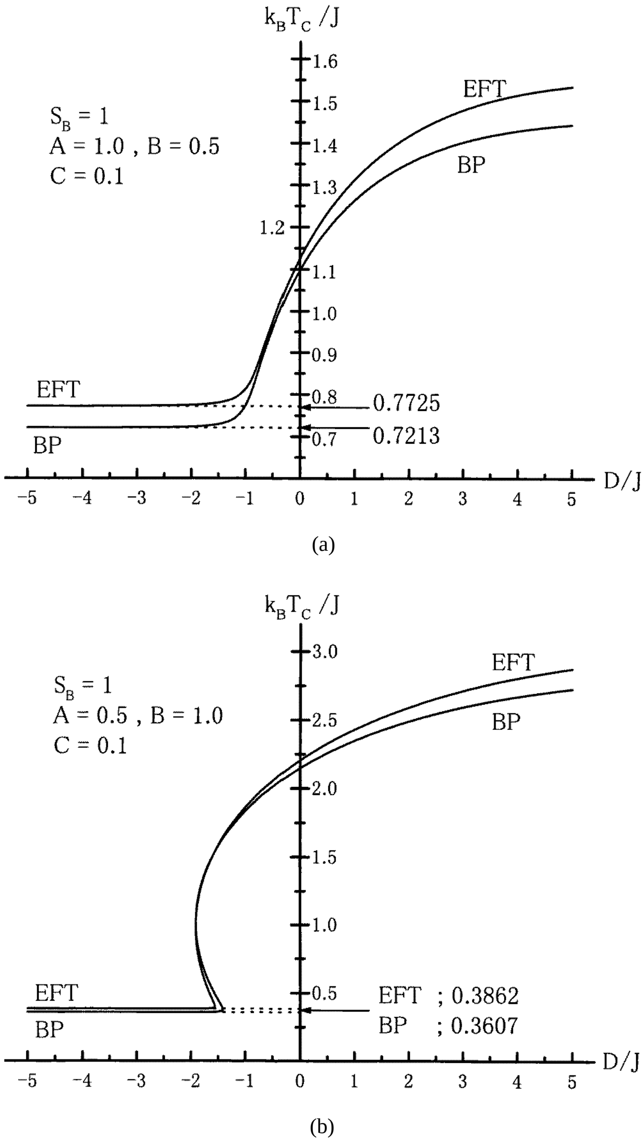

Figure 5. The T_C curve of the Ising multilayer system with a fixed value of C ($C = 0.1$) consisting of alternating spin-$1/2$ monolayers and spin-1 monolayers is depicted as a function of single-ion anisotropy D on spin-1 atoms, taking the two theoretical frameworks and selecting the two cases, namely the system with $A = 1.0$ and $B = 0.5$ in (a) and the system with $A = 0.5$ and $B = 1.0$ in (b). The curves labelled EFT and BP express the results obtained from the effective-field theory with correlation (EFT) [10, 11] and the present framework, respectively.

state at the critical value D_C of D; it is given by

$$\frac{D_C}{J_A} = -\left[2\left(\frac{J_B}{J_A}\right) + \frac{J_{AB}}{J_A}\right]. \tag{47}$$

When $D < D_C$, the ground state of the B monolayer is given by the $S_m^z = 0$ state and hence the transition temperature of the multilayer system becomes equivalent to that of the spin-$1/2$ square lattice with $z = 4$, as shown in figures 5(a) and 5(b).

As has been discussed in [10], however, one should notice that the results of figure 5 might not give the correct phase diagrams of the multilayer system with $S_B = 1$. In fact, a spin-1 Ising system with a negative D (or the Blume–Capel model) exhibits a tricritical point in the phase diagram at which the phase transition changes from second order to first order. Within the formulation of the EFT, we have discussed in [10] that such a tricritical behaviour may be observed even in the Ising multilayer system with an integer value of S_B ($S_B = 1$): the double-valued phenomenon observed for the negative region of D in figure 5(b) implies that tricritical behaviour may exist in the multilayer system with $S_B = 1$. Thus, as discussed in [10], two critical points where the second-order transition line is separated into the first-order transition may appear in the T_C curves of figure 5, although such a discussion has been neglected in [11].

6. Conclusions

In this work, we have discussed the cluster theory of a simple cubic Ising multilayer system consisting of two alternating magnetic monolayers A and B within the framework of the differential operator technique. As shown in sections 4 and 5, the cluster theory presents the same accuracy of the transition temperature as that obtained from the Bethe–Peierls approximation of the spin-$1/2$ Ising model, when the spin value S_B of B monolayers is taken as $S_B = \frac{1}{2}$ or can be seen as if it is in the $S_m^z = \pm\frac{1}{2}$ state. When we use the approximated relation (8) for $S_B > \frac{1}{2}$, the statistical accuracy becomes a very little worse than that of the Bethe–Peierls approximation, as noted in [17]. But, one should notice that the present formulation is rather different from the standard treatment of the Bethe–Peierls approximation.

The formulation of T_C derived in section 3 can be applied to a certain Ising multilayer system described by the Hamiltonian ($1a$) or ($1b$). For instance, it can be also applied to study the phase diagram of an Ising multilayer system with $S_A = \frac{1}{2}$ and $S_B > \frac{1}{2}$ in a transverse field, while we have examined the place diagram of the transverse Ising multilayer system with $S_A = S_B = \frac{1}{2}$ in section 4.

On the basis of the formulation of section 3, we have, in section 5, examined the behaviour of T_C with the variation of D for the Ising multilayer system with the Hamiltonian ($1a$). The formulation can be applied reasonably to a bilayer system with a half-integer spin S_B, as shown in figure 4. But, the results of figure 5(b) clearly indicate that tricritical behaviour may exist in the Ising multilayer system with an integer spin S_B, as discussed in [10]. For clarification, we need to investigate the temperature dependence of the total magnetization in the system, like [10].

Finally, one should notice that the present formulation for calculating the T_C of the ferromagnetic multilayer system can be also applied straightforwardly to the ferrimagnetic multilayer system with a negative value of J_{AB}. Of course, the present approach is based on the effective field concept introduced in section 2, so that we could not derive accurate critical indices.

Appendix A

The functions $F(x)$ and $G(x)$ defined in (4) and (9) for the system with the Hamiltonian ($1a$) are given by

$$F(x) = \frac{2\sinh(\beta x)}{2\cosh(\beta x) + \exp(-D\beta)} \tag{A.1}$$

and

$$G(x) = \frac{2\cosh(\beta x)}{2\cosh(\beta x) + \exp(-D\beta)} \tag{A.2}$$

for $S_B = 1$,

$$F(x) = \frac{1}{2}\frac{3\sinh(1.5x\beta) + \exp(-2D\beta)\sinh(0.5x\beta)}{\cosh(1.5x\beta) + \exp(-2D\beta)\cosh(0.5x\beta)} \tag{A.3}$$

and

$$G(x) = \frac{1}{4}\frac{9\cosh(1.5x\beta) + \exp(-2D\beta)\cosh(0.5x\beta)}{\cosh(1.5x\beta) + \exp(-2D\beta)\cosh(0.5x\beta)} \tag{A.4}$$

for $S_B = 3/2$, where these functions for $S_B > 3/2$ can be easily derived and can be also obtained from [5]. When one treats the multilayer system with $S_B > \frac{1}{2}$ in a transverse field (or the system described by (1*b*)), the functions $F(x)$ and $G(x)$ are defined in [20].

Appendix B

The coefficients O_1, O_2, P_1, P_2, Γ_1 and Γ_2 defined in (28) and (30) are given by

$$O_1 = R_1[K_1 + 12K_2(a_2)^2 + 12K_4a_2b_2 + K_5(b_2)^2 + 16K_6(a_2)^3b_2 + 12K_7(a_2)^2(b_2)^2] \tag{B.1}$$

$$O_2 = R_3[K_2 + 24K_4(a_2)^2 + 8K_5a_2b_2 + 16K_6(a_2)^4 + 32K_7b_2(a_2)^3] \tag{B.2}$$

$$P_1 = R_4[L_2 + \{6L_4(b_4)^2 + 8L_5a_4b_4\}q_0 + \{L_6(b_4)^4 + 8L_7a_4(b_4)3\}(q_0)^2] \tag{B.3}$$

$$\begin{aligned} P_2 = R_2[L_1 &+ \{3L_3(b_4)^2 + 12L_4a_4b_4 + 4L_5(a_4)^2\}q_0 \\ &+\{4L_6a_4(b_4)^3 + 12L_7(a_4)^2(b_4)^2\}(q_0)^2] \end{aligned} \tag{B.4}$$

$$\begin{aligned} \Gamma_1 = 4K_1a_2 &+ K_2b_2 + 16K_3(a_2)^3 + 24K_4b_2(a_2)^2 + 4K_5a_2(b_2)^2 + 16K_6b_2(a_2)^4 \\ &+16K_7(a_2)^3(b_2)^2 \end{aligned} \tag{B.5}$$

$$\begin{aligned} \Gamma_2 = L_1b_4 &+ L_2a_4 + \{L_3(b_4)^3 + 6L_4a_4(b_4)^2 + 4L_5(a_4)^2b_4\}q_0 \\ &+\{L_6a_4(b_4)^4 + 4L_7(a_4)^2(b_4)^3\}(q_0)^2] \end{aligned} \tag{B.6}$$

with

$$R_3 = \frac{1}{\beta}[\nabla F(x)]_{x=r} \tag{B.7}$$

$$R_4 = \frac{1}{\beta}[\nabla f(x)]_{x=s} \tag{B.8}$$

where $r = J_{AB}/2$ and $s = J_{AB}\eta_0$. The coefficients K_i and L_i (i = 1–7) are defined by

$$\begin{aligned} K_1 &= \sinh(a/2)\cosh 3(a/2)\cosh^2(\eta_1 c)f(x)|_{x=0} \\ K_2 &= (1/\eta_1)\sinh(\eta_1 c)\cosh(\eta_1 c)\cosh^4(a/2)f(x)|_{x=0} \\ K_3 &= \sinh^3(a/2)\cosh(a/2)\cosh^2(\eta_1 c)f(x)|_{x=0} \\ K_4 &= (1/\eta_1)\sinh(\eta_1 c)\cosh(\eta_1 c)\sinh^2(a/2)\cosh^2(a/2)f(x)|_{x=0} \\ K_5 &= (1/\eta_1)^2\sinh^2(\eta_1 c)\sinh(a/2)\cosh^3(a/2)f(x)|_{x=0} \\ K_6 &= (1/\eta_1)\sinh(\eta_1 c)\cosh(\eta_1 c)\sinh^4(a/2)f(x)|_{x=0} \\ K_7 &= (1/\eta_1)2\sinh^2(\eta_1 c)\sinh^3(a/2)\cosh(a/2)f(x)|_{x=0} \end{aligned} \tag{B.9}$$

and

$$\begin{aligned} L_1 &= (1/\eta_2)\sinh(\eta_2 b)\cosh^3(\eta_2 b)\cosh^2(c/2)F(x)|_{x=0} \\ L_2 &= \cosh^4(\eta_2 b)\sinh(c/2)\cosh(c/2)\cosh^4(\eta_2 b)F(x)|_{x=0} \end{aligned}$$

$$L_3 = (1/\eta_2)^3 \sinh^3(\eta_2 b) \cosh(\eta_2 b) \cosh^2(c/2) F(x)|_{x=0}$$
$$L_4 = (1/\eta_2)^2 \sinh^2(\eta_2 b) \cosh^2(\eta_2 b) \sinh(c/2) \cosh(c/2) F(x)|_{x=0} \tag{B.10}$$
$$L_5 = (1/\eta_2) \sinh(\eta_2 b) \cosh^3(\eta_2 b) \sinh^2(c/2) F(x)|_{x=0}$$
$$L_6 = (1/\eta_2)^4 \sinh^4(\eta_2 b) \cosh(c/2) \sinh(c/2) F(x)|_{x=0}$$
$$L_7 = (1/\eta_2)^3 \sinh^3(\eta_2 b) \cosh(\eta_2 b) \sinh(c/2) F(x)|_{x=0}$$

where η_1 and η_2 are given by

$$(\eta_1)^2 = d_1 = G(J_{AB}/2) \tag{B.11}$$

and

$$(\eta_2)^2 = d_3 = G(J_B \eta_0). \tag{B.12}$$

The coefficients Q_i ($i = 1$–7) in (32) are defined by

$$Q_1 = \cosh^4(\eta_2 b) \cosh^2(c/2) G(x)|_{x=0}$$
$$Q_2 = (1/\eta_2)^2 \sinh^2(\eta_2 b) \cosh(\eta_2 b) \cosh^2(c/2) G(x)|_{x=0}$$
$$Q_3 = (1/\eta_2) \sinh(\eta_2 b) \cosh^3(\eta_2 b) \sinh(c/2) \cosh(c/2) G(x)|_{x=0}$$
$$Q_4 = \cosh^4(\eta_2 b) \sinh^2(c/2) G(x)|_{x=0} \tag{B.13}$$
$$Q_5 = (1/\eta_2)^4 \sinh^4(\eta_2 b) \cosh^2(c/2) G(x)|_{x=0}$$
$$Q_6 = (1/\eta_2)^3 \sinh^3(\eta_2 b) \cosh(\eta_2 b) \sinh(c/2) \cosh(c/2) G(x)|_{x=0}$$
$$Q_7 = (1/\eta_2)^2 \sinh^2(\eta_2 b) \cosh^2(\eta_2 b) \sinh^2(c/2) G(x)|_{x=0}$$
$$Q_8 = (1/\eta)^4 \sinh^4(\eta_2 b) \sinh^2(c/2) G(x)|_{x=0}.$$

The coefficients U_i ($i = 7$–14) defined in (38) and (39) are given by

$$U_7 = (b_4/2)[4R_4 - 3R_1]$$
$$U_8 = (b_4/2)[2R_1 - R_4]$$
$$U_9 = (b_4/2)[2R_3 - 3R_2]$$
$$U_{10} = (b_4/2)[2R_2 - R_3] \tag{B.14}$$
$$U_{11} = b_2[4R_4 - 3R_1]$$
$$U_{12} = b_2[2R_1 - R_4]$$
$$U_{13} = a_2[4R_3 - 3R_2]$$
$$U_{14} = a_2[2R_2 - R_3].$$

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