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Critical Behavior in Magnetic Superlattices

by

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Critical behavior in magnetic superlattices

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Abstract

Based on the effective field theory with correlations, the critical behavior of a magnetic superlattice consisting of two different ferromagnets is examined. A simple cubic Ising model with nearest-neighbor coupling is assumed. It is found that there exists a critical value for the interface exchange coupling above which the interface magnetism appears. The critical temperature of the superlattice is studied as a function of the thickness of the constituents in a unit cell and of the exchange coupling energies in each material. A phase diagram is also given.

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I. Introduction

In recent years, there has been increasing interest in the nature of spin waves as well as critical phenomena in various magnetic layered structures and superlattices. Ma and Tsai[1] have studied the variation with modulation wavelength of the Curie temperature for a Heisenberg magnetic superlattice. Their results agree qualitatively with experiments on the Cu/Ni film.[2] Superlattice structures composed of alternating ferromagnetic and antiferromagnetic layers have been investigated by Hinchey and Mills,[3,4] using a localized spin model. A sequence of spin-reorientation transitions are found to be different for superlattices with the antiferromagnetic component consisting of an even or odd number of spin layers. In addition, the spin-wave spectrum and infrared absorption spectrum are calculated.

For a periodic multilayer system formed from two different ferromagnetic materials, Fishman et al[5] have discussed its statics and dynamics within the framework of the Ginzburg-Landau formulation. They have computed the transition temperature and spin-wave spectra. On the other hand, the Landau formalism of Camley and Tilley[6] has been applied to calculate the critical temperature in the same system.[7] Compared to Ref. 5, the formalism of Ref. 6 appears to be more general because it allows for a wider range of boundary conditions and includes the sign of exchange coupling across the interface.

For more complicated superlattices with arbitrary number of different layers in an elementary unit, Barnas[8] has derived some general dispersion equations for the bulk and surface magnetic polaritons. These equations are then applied to magnetostatic modes and to retarded wave propagation in the Voigt geometry.[9]

We study, in this article, the critical temperature in an infinite superlattice consisting of two ferromagnetic materials with different bulk

properties. In particular, we consider the two constituents A and B with different bulk transition temperatures as a simple model, i.e., $T_c^{(a)} \neq T_c^{(b)}$. The interface is in general different in nature from both bulks, even if the bulk critical temperatures are the same. We use the effective-field theory with correlations[10] in the present work, as it is believed to be far superior to the standard mean-field approximation.

Because of the periodicity of the superlattice structure, we restrict our discussions to a unit cell which interacts with its nearest-neighbor cells via interface couplings. Thus the system can be treated by extending the method developed for a magnetic slab.[11] Our major concerns are the dependence of the transition temperature on the thickness of individual constituents in the cell and the influence of the interface magnetic properties on the phase transition temperature. These questions, to our knowledge, have not been considered in the literature thus far.

In Sec. II. we outline the theory and derive the equation that determines the transition temperature. Numerical results are discussed in Sec. III where the existence of the interface magnetic phase transition is discovered and the critical value of the interface coupling relative the bulk coupling is determined. A brief conclusion is given in Sec. IV.

II. Theory

Consider an infinite superlattice consisting of two different ferromagnetic materials A and B. For simplicity, we restrict our attention to the case of simple cubic Ising-type structures. The periodic condition suggests that we only have to consider one unit cell which interacts with its nearest neighbors via the interface coupling. The situation is depicted in Fig. 1. The coupling strength between nearest-neighboring spins in A(B) is

denoted by $J_a(J_b)$, while J_{ab} stands for the exchange coupling between the nearest-neighbor spins across the interface. The corresponding number of atomic layers in A(B) is $L_a(L_b)$, and the thickness of the cell is $L = L_a + L_b$. The Hamiltonian of the system is given by

$$H = -\frac{1}{2}\sum_{i,j} J_{ij}S_iS_j \quad , \tag{1}$$

where the sum is taken over all the nearest-neighbor pairs only once, $S_i = \pm 1$ is the usual Ising variable, and J_{ij} stands for one of the three coupling constants depending on where the spin pair is located.

To evaluate the mean spin $<S_i>$, we start with the exact Callen identity,[12]

$$<S_i> = <\tanh (\beta \sum_j J_{ij} \; S_j)> \quad , \tag{2}$$

where $\beta = 1/k_BT$, $<...>$ indicates the usual canonical ensemble average for a given configuration of $\{J_{ij}\}$, and j runs over all nearest neighbors of site i. We now introduce the differential operator $D = \frac{\partial}{\partial x}$ and recall that the displacement operator $\exp(\alpha D)$ satisfies the relation

$$\exp(\alpha D)f(x) = f(x+\alpha) \quad . \tag{3}$$

Equation (2) can then be rewritten, with the help of (3), as

$$<S_i> = <\exp(D \sum_j J_{ij}S_j)> [\tanh(\beta x)]_{x=0}$$

$$= \langle | \prod_j [\cosh(DJ_{ij}) + S_j \sinh(DJ_{ij})] \rangle \tanh(\beta x) |_{x=0} \quad . \tag{4}$$

This equation represents a set of L coupled equations for the L spin layers in the unit cell. Each layer is only coupled to its nearest-neighbor layers. The multi-spin correlation function, however, must be decoupled before a practical calculation can be made. We follow the standard procedure[13] with the decoupling approximation $\langle x_1 x_2 .. x_\ell \rangle = \langle x_1 \rangle \langle x_2 \rangle \ldots \langle x_\ell \rangle$. Thus the average atomic magnetization of each layer is given by

$$m_1 = [\cosh(DJ_{ab}) + m_o \sinh(DJ_{ab})][\cosh(DJ_a) + m_1 \sinh(DJ_a)]^4$$

$$\times [\cosh(DJ_a) + m_2 \sinh(DJ_a)] f(x) \Big|_{x=0} \tag{5a}$$

$$\vdots$$

$$m_i = [\cosh(DJ_a) + m_{i-1} \sinh(DJ_a)][\cosh(DJ_a) + m_i \sinh(DJ_a)]^4$$

$$\times [\cosh(DJ_a) + m_{i+1} \sinh(DJ_a)] f(x) \Big|_{x=0} \qquad 2 \le i \le L_a \tag{5b}$$

$$\vdots$$

$$m_{L_a} = [\cosh(DJ_a) + m_{L_a-1} \sinh(DJ_a)][\cosh(DJ_a) + m_{L_a} \sinh(DJa)]^4$$

$$\times [\cosh(DJ_{ab}) + M_{L_a+1} \sinh(DJ_{ab})] f(x) \Big|_{x=0} \tag{5c}$$

$$m_{L_a+1} = [\cosh(DJ_{ab}) + m_{L_a} \sinh(DJ_{ab})][\cosh(DJ_b) + m_{L_a+1} \sinh(DJ_b)]^4$$

$$\times [\cosh(DJ_b) + m_{L_a+2} \sinh(DJ_{ab})] f(x) \Big|_{x=0} \tag{5d}$$

$$\vdots$$

$$m_j = [\cosh(DJ_a) + m_{j-1}\sinh(DJ_b)][\cosh(DJ_b) + m_j\sinh(DJ_b)]^4$$

$$[\cosh(DJ_b) + m_{j+1}\sinh(DJ_b)]f(x)\Big|_{x=0} \qquad L_a \le j \le L-1 \tag{5e}$$

$$\vdots$$

$$m_L = [\cosh(DJ_b) + m_{L-1}\sinh(DJ_b)]\cosh(DJ_b) + m_L\sinh(DJ_b)]^4$$

$$[\cosh(DJ_{ab}) + m_{L+1}\sinh(DJ_{ab})]f(x)\Big|_{x=0} \quad , \tag{5f}$$

where we have defined

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

on which the operator D applies. The variable x is set to zero at the end of the calculation in each equation. It is observed that the periodic condition of the superlattice is indeed satisfied, namely, $m_o = m_L$ and $m_1 = m_{L+1}$. As the temperature becomes higher than the critical temperature, the whole system becomes demagnetized. Thus, we can determine T_c from Eq. (5) by requiring that the mean atomic magnetization in every spin layer approaches zero. Consequently, all terms of the order higher than linear in Eqs. (5) can be neglected. This leads to a set of simultaneous equations

$$(1-4A_1)m_1 - A_2m_o - A_1m_2 = 0$$

$$\vdots$$

$$(1-4A_3)m_i - A_3(m_{i-1}+m_{i+1}) = 0$$

$$\vdots$$

$$(1-4A_1)m_{L_a} - A_1m_{L_a-1} - A_2m_{L_a+1} = 0$$

$$\begin{aligned}
&\vdots \\
&(1-4A_4)m_{L_a+1} - A_5 m_{L_a} - A_4 m_{L_a+2} = 0 \\
&\vdots \\
&(1-4A_6)m_j - A_6(m_{j-1} - m_{j+1}) = 0 \\
&\vdots \\
&(1-4A_4)m_L - A_4 m_{L-1} - A_5 m_{L+1} = 0 \quad ,
\end{aligned} \tag{7}$$

where the coefficients are given by

$$\begin{aligned}
A_1 &= \cosh^4(DJ_a)\sinh(DJ_a)\cosh(DJ_{ab})f(x)\Big|_{x=0} \\
A_2 &= \cosh^5(DJ_a)\sinh(DJ_{ab})f(x)\Big|_{x=0} \\
A_3 &= \cosh^5(DJ_a)\sinh(DJ_a)f(x)\Big|_{x=0} \\
A_4 &= \cosh^4(DJ_b)\sinh(DJ_b)\cosh(DJ_{ab})f(x)\Big|_{x=0} \\
A_5 &= \cosh^5(DJ_b)\sinh(DJ_{ab})f(x)\Big|_{x=0} \\
A_6 &= \cosh^5(DJ_b)\sinh(DJ_b)f(x)\Big|_{x=0} \quad .
\end{aligned} \tag{8}$$

The secular equation of this set of coupled equations is

$$
\begin{vmatrix}
a_1 & -1 & & & & & & & & & b_1 \\
-1 & c_1 & -1 & \cdots & & & & & & & \\
 & & \vdots & \ddots & & & & & & & \\
 & & & \cdots & -1 & a_1 & b_1 & & & & \\
 & & & & & b_2 & a_2 & -1 & & & \\
 & & & & & & -1 & c_2 & -1 & \cdots & \\
 & & & & & & & & \vdots & \ddots & \\
 & & & & & & & & \cdots & -1 & c_2 & -1 \\
b_2 & & & & & & & & & & -1 & a_2
\end{vmatrix} = 0 \quad , \tag{9}
$$

where we have defined

$$
\begin{aligned}
a_1 &= (1-4A_1)/A_1 & \qquad a_2 &= (1-4A_4)/A_4 \\
b_1 &= -A_2/A_1 & \qquad b_2 &= -A_5/A_4 \\
c_1 &= (1-4A_3)/A_3 & \qquad c_2 &= (1-4A_6)/A_6 \quad .
\end{aligned} \tag{10}
$$

The $L \times L$ determinant in (9) can only be evaluated numerically for a given set of coupling constants J_{ij}. As all the coefficients A_ν involve β through (6), T_c can be obtained as a function of the J's. The results of this calculation are discussed in the following section.

III. Results and discussion

Throughout this paper, we take J_b as the unit of energy, and the length is measured in the unit of the lattice constant in our numerical work. We first show the critical temperature as a function of the unit cell width L in

Fig. 1. Four cases of different L_a values are plotted for fixed J_a and J_{ab}. We first note that T_c decreases with increasing L_a, in general. This is because we have assumed $J_a < J_b$ in our calculation, and it is well known that the bulk transition temperature is approximately proportional to the exchange coupling if the spin and lattice structure are specified. For a given L_a, it is observed that T_c increases steadily as L increases indefinitely. All the curves approach the same limiting value $T_c = 5.073\ J_b/k_B$, which is simply $T_c^{(b)}$. This is of course easily understood.

To study the effects of the interface exchange coupling on the transition temperature of the superlattice, T_c is calculated for various J_{ab} but fixed J_a and L_a. Figure 3 shows the results for $J_a = J_b$. Curve c corresponds to the case $J_{ab} = J_b$ and appears like that of a slab of material B. It is very interesting to see that there exists a critical interface coupling $J_{ab}^c = 1.46\ J_b$ such that T_c remains constant for any L_b, as represented by curve b. For J_{ab}^c larger than this critical value, we find that T_c is higher than both $T_c^{(a)}$ and $T_c^{(b)}$. Curve a illustrates one such particular case $J_{ab} = 2J_b$. This suggests that there exists an interface magnetism in the system. For $J_{ab} > J_{ab}^c$, the system may order in the interface layers before it orders in other layers. The situation does not change for $J_a \neq J_b$. The results for $J_a = 0.5\ J_b$ are plotted in Fig. 4, whose curves are very similar except that the critical interface coupling J_{ab}^c in this case is bigger than in Fig. 3. This is because the lower $T_c^{(a)}$ needs a stronger, compensating interface exchange coupling in order to reach the interface phase transition.

Figure 5 demonstrates that as long as $J_a = J_b$, the critical coupling $J_{ab}^c = 1.46\ J_b$ does not depend upon the thickness L_a. Curve d remains the same for all three cases calculated, while for $J_{ab} = 2.0\ J_b$ and $0.1\ J_b$, T_c behaves very differently when L_a is varied. Curves (a,a'), (b,b') and (c,c') correspond to

$L_a = 3$, 5 and 10 respectively. For $J_{ab} > J_{ab}^c$ when the interface magnetism appears, T_c decreases as L increases. For the a and b cases, material B dominates the system for $L > 13$. For the case c, $L_a = 10$, and T_c drops quickly at the beginning and approaches $T_c^{(b)}$ for $L \geq 20$. On the other hand, the transition temperature increases with L for $J_{ab} < J_{ab}^c$. The apparently anomalous behavior of curve c' can be understood in the following manner. As $J_{ab} = 0.1\ J_b$, T_c is mainly determined by material A(B) if $L_a(L_b)$ is larger than $L_b(L_a)$. Hence, T_c changes little until L approaches 18, because $L_a = 10$ in this case.

Figure 6 shows the phase diagram of the system by plotting the critical interface exchange coupling as a function of J_a. Three different thicknesses L_a are plotted. It is interesting to note that the three curves meet when $J_a = J_b$, suggesting that the critical interface exchange is independent of the relative thickness of the constituents in the unit cell as long as their exchange couplings are the same. This is of course in agreement with the above results in Fig. 5.

We have considered ferromagnetic interface coupling in our discussion. The critical temperature of the system, however, remains the same if the interface exchange coupling becomes antiferromagnetic. This is consistent with the discussion in Ref. 7.

IV. Conclusions

We have investigated the criticality of a two-component ferromagnetic superlattice by considering one unit cell, assuming nearest-neighbor spin exchange couplings. The interface exchange energy is, in general, different from either of the bulk ones. For the first time, the critical value J_{ab}^c is introduced. When J_{ab} is larger than this critical value, the interface

magnetism appears, and T_c for the system is higher than either T_c^a or T_c^b. When J_{ab} is smaller than the critical value, $T_c < T_c^a, T_c^b$.

Finally, we remark that the method is general and can be used to treat the ferromagnetic/antiferromagnet and antiferromagnet/antiferromagnet superlattices. With modifications in spatial fluctuations of the coupling J's, the method can easily be generalized to superlattices involving certain type of amorphous magnetic materials.

Acknowledgments

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Figure captions

1. Unit cell of the superlattice composed of ferromagnetic materials A and B, where $L = L_a + L_b$ is the thickness of the cell. The solid and dashed lines represent the nearest-neighbor exchange coupling energies between spins in one material and in the interface, respectively.
2. Dependence of T_c on the thickness L. The interface coupling is chosen as $J_{ab} = 0.9\ J_b$ and $J_a = 0.8\ J_b$. Number of spin layers of material A is (a) 3, (b) 4 and (c) 5, (d) 6.
3. T_c as a function of L for $L_a = 3$ and $J_a = J_b$ but various interface coupling strengths. (a) $J_{ab} = 2.0\ J_b$, (b) $J_{ab} = 1.46$ and (c) $J_{ab} = J_b$.
4. Same as Fig. 3 except that $J_a = 0.5\ J_b$. (a) $J_{ab} = 3.0\ J_b$, (b) $J_{ab} = 2.51\ J_b$ and (c) $J_{ab} = 1.9\ J_b$.
5. T_c as a function of L for $J_a = J_b$ but different J_{ab} and L_a. $J_{ab} = 2.0\ J_b$ for curves a, b and c, and $J_{ab} = 0.1\ J_b$ for a', b' and c'. The number of spin layers L_a is 3 for a, a', 5 for b, b', and 10 for c, c'.
6. Phase diagram in terms of the coupling J_{ab} and J_a for L_a = (a) 3, (b) 4 and (c) 10.

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Fig. 1

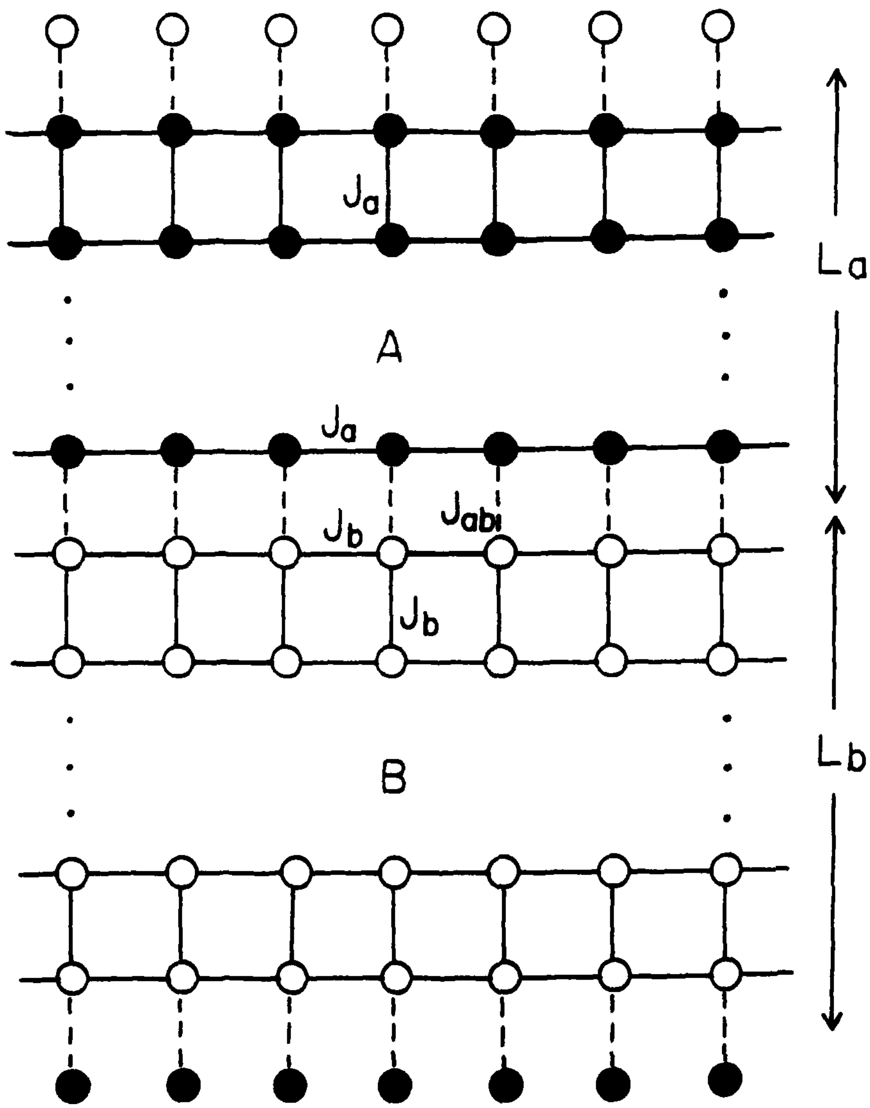


Fig. 2

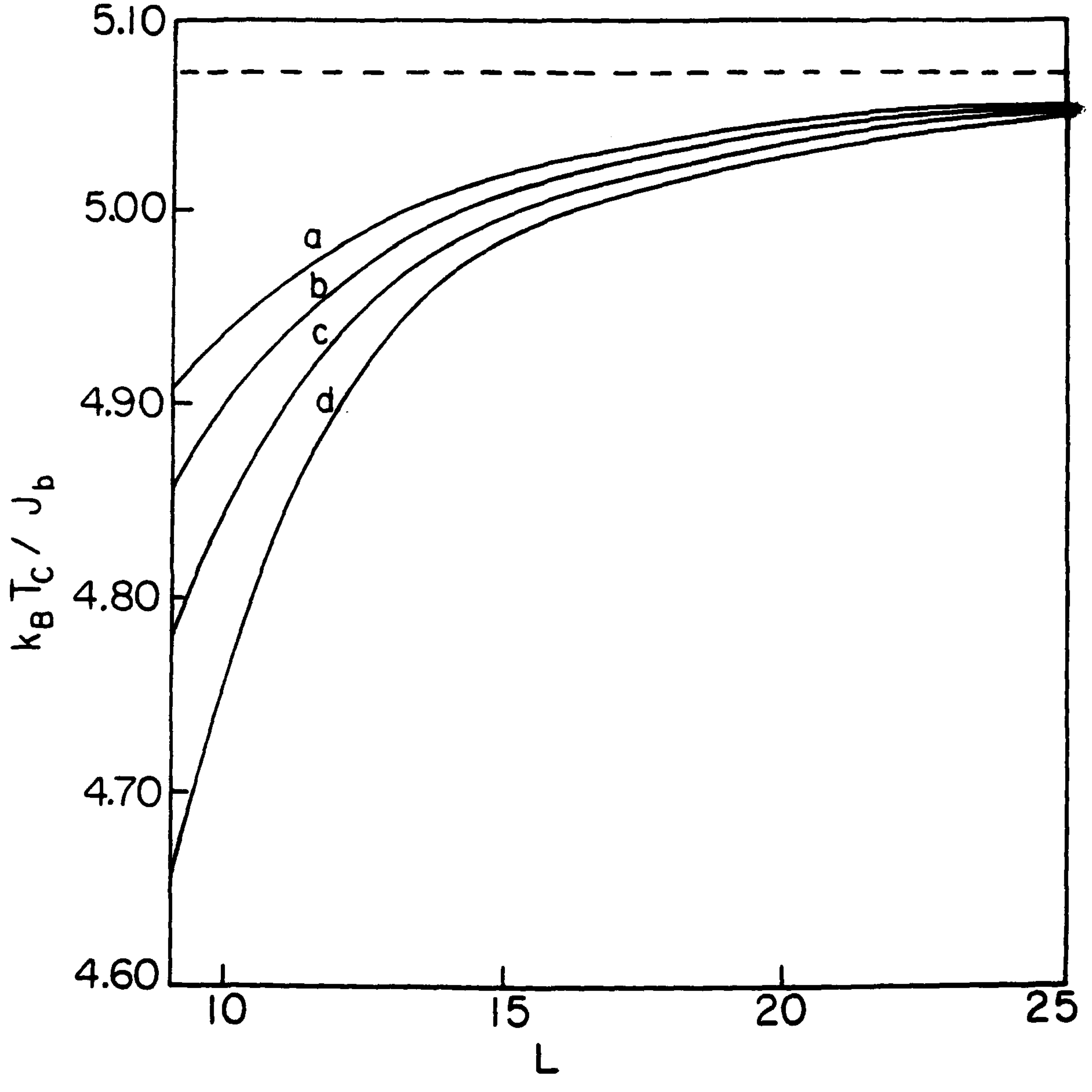


Fig 3

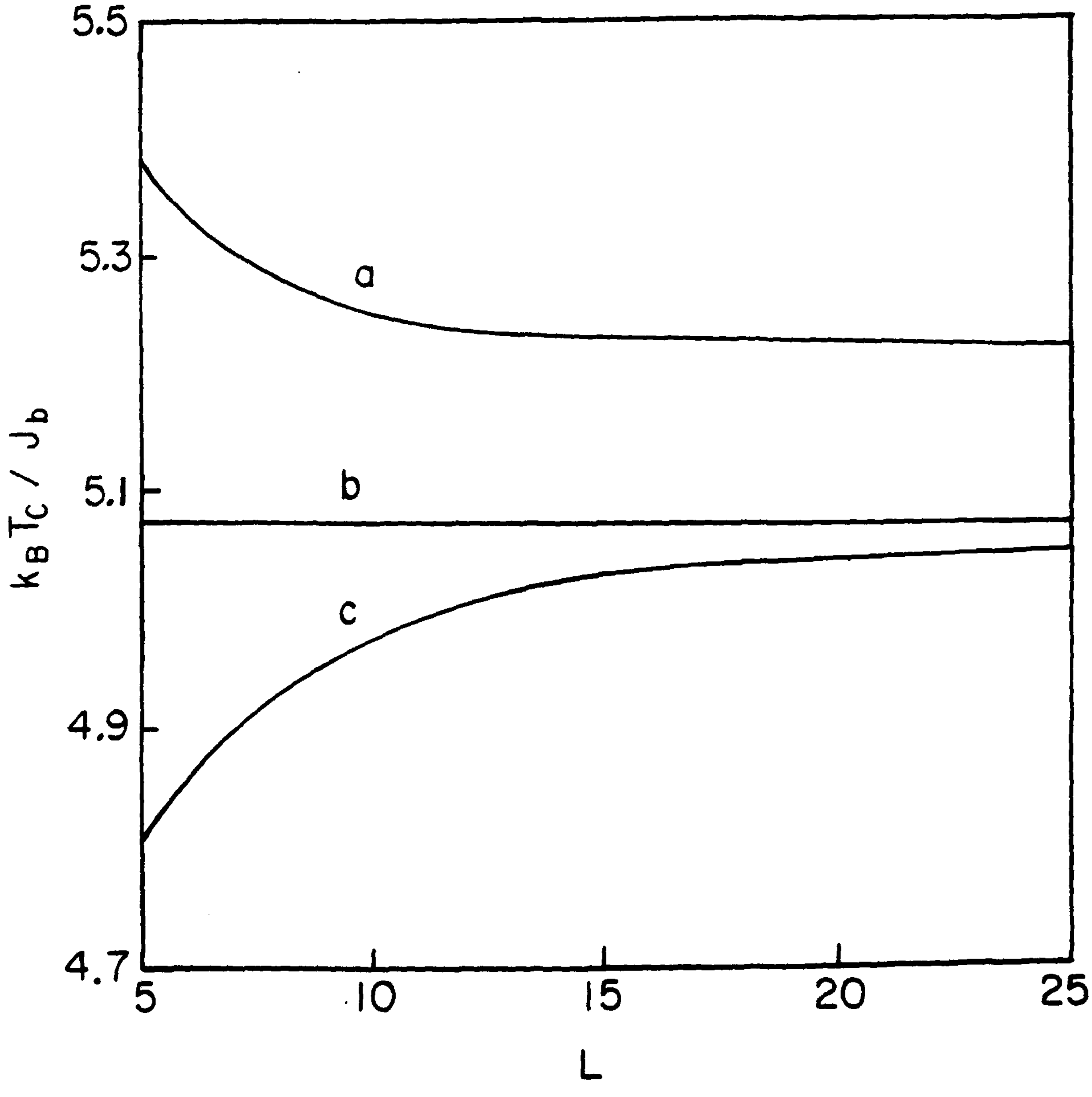


Fig. 4

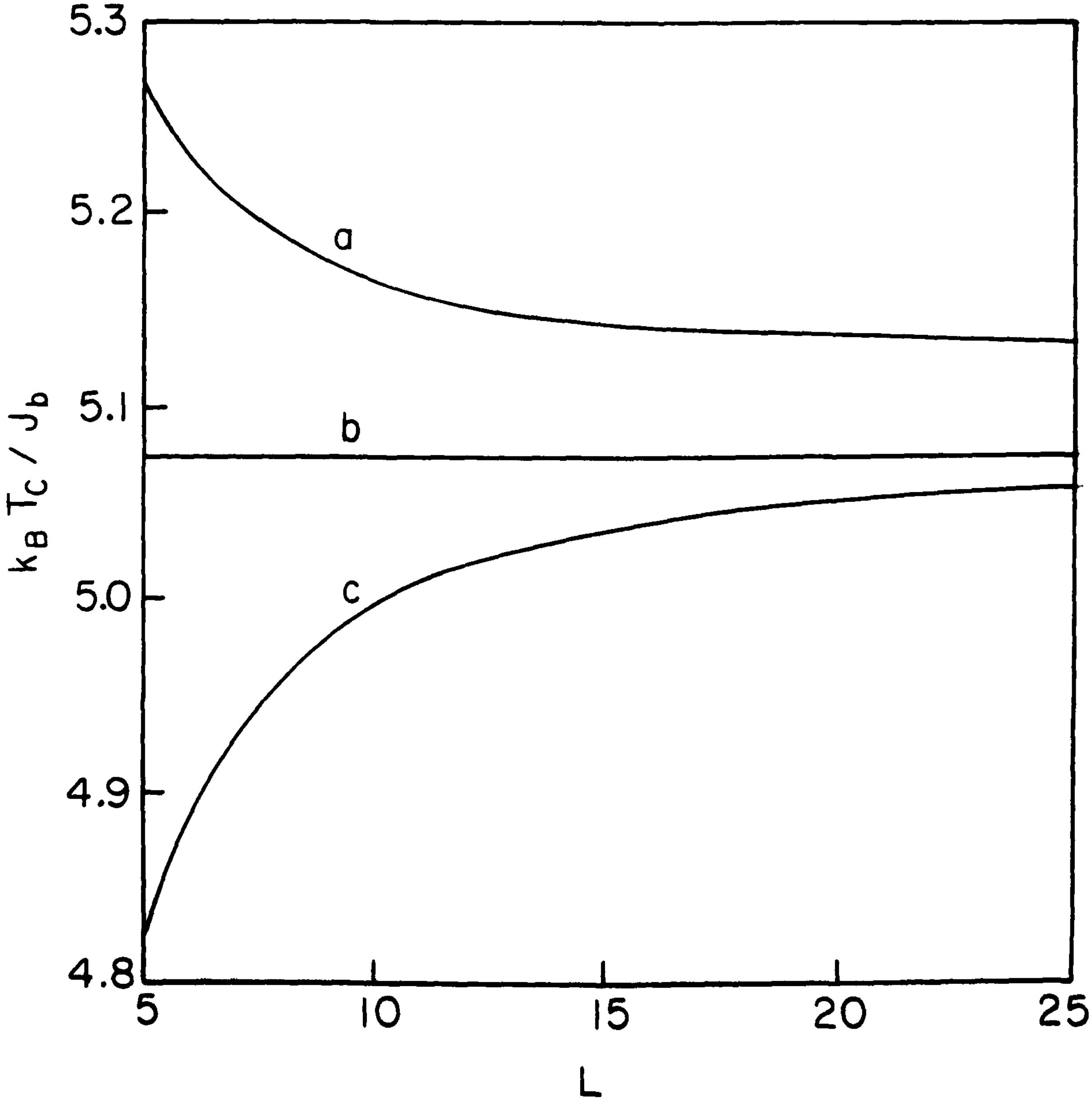


Fig. 5

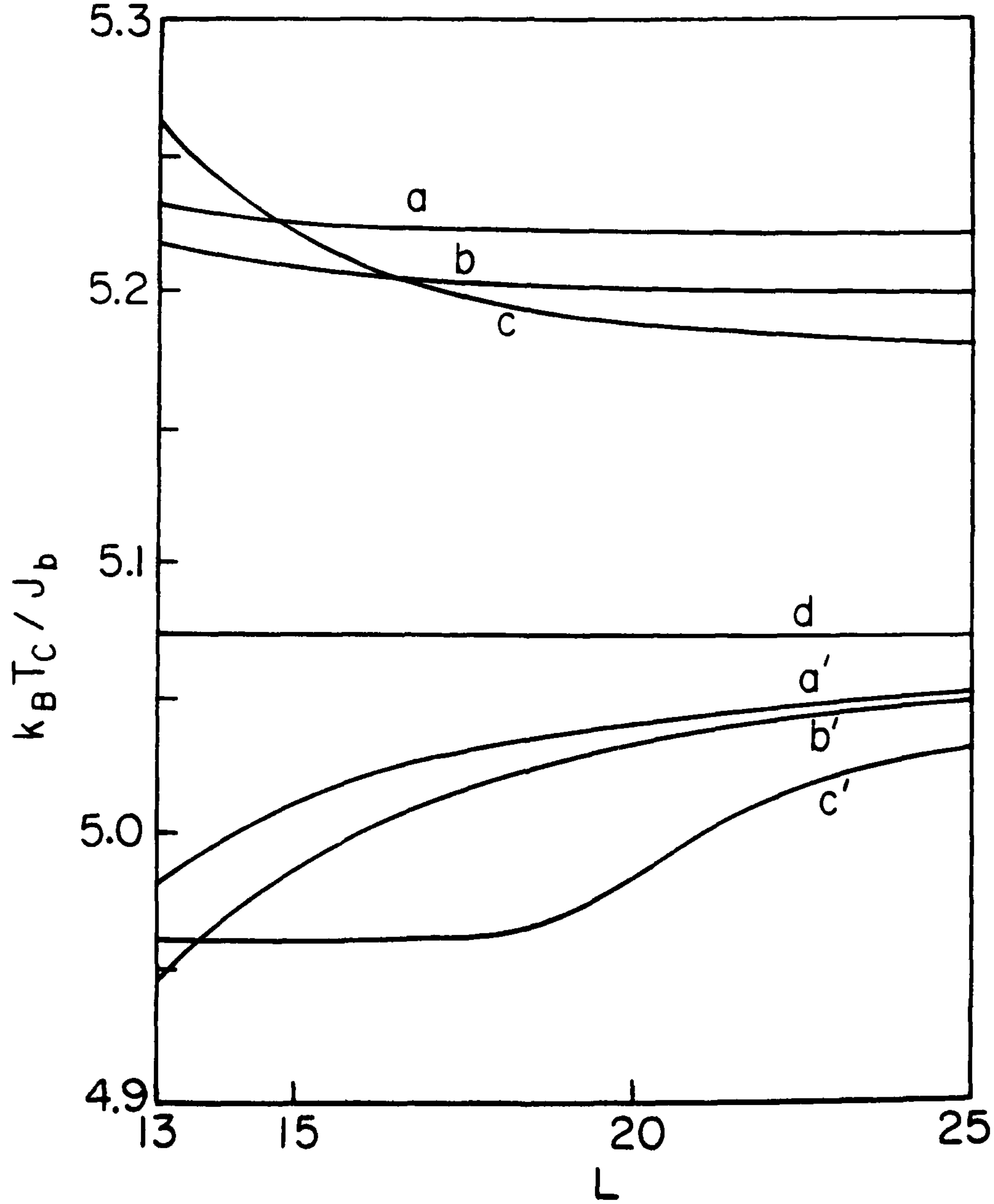
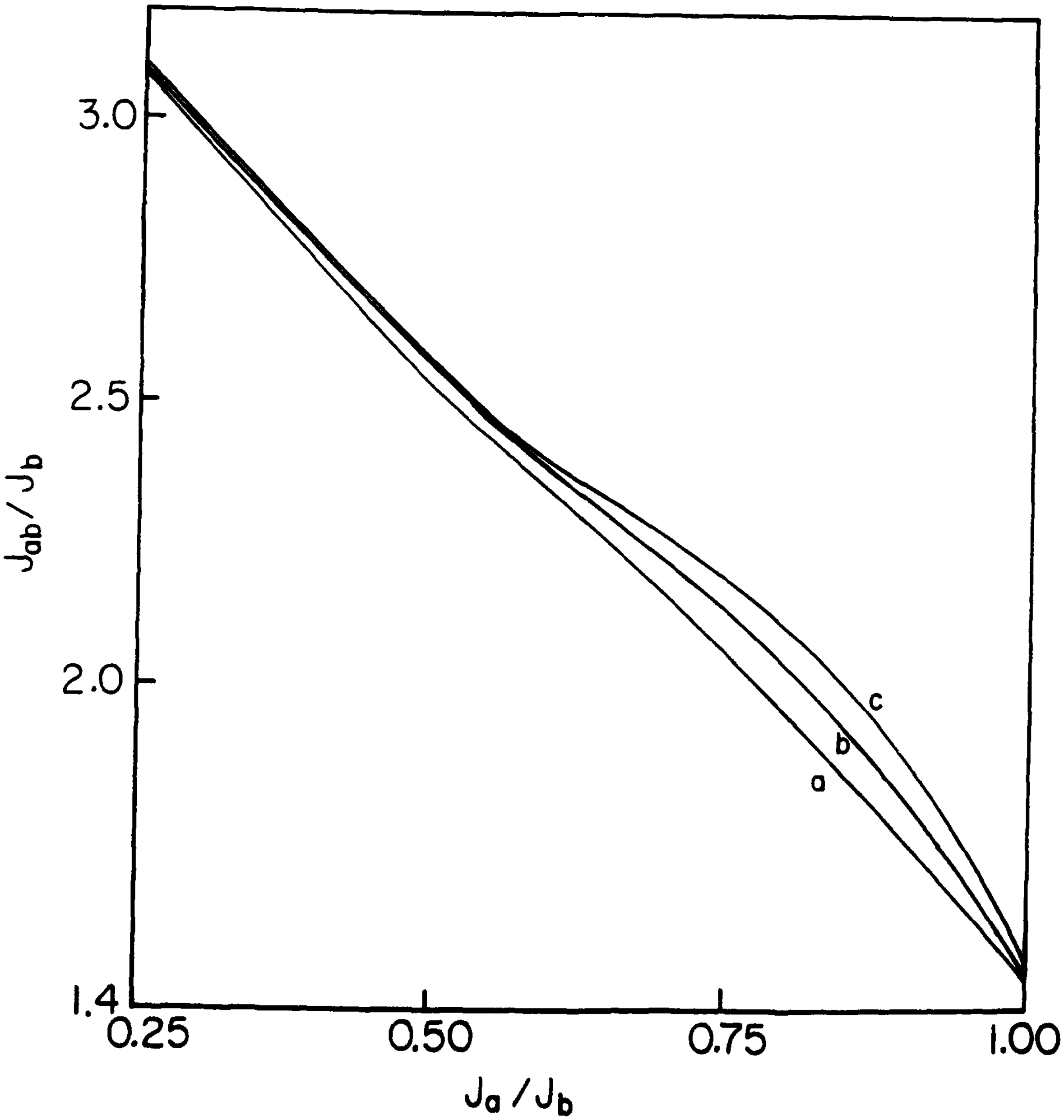


Fig. 6



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