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INDUCED MAGNETISM IN A SYSTEM CONSISTING OF VAN VLECK IONS COUPLED TO AN ELECTRON GAS, IN THE NARROW BAND LIMIT.

by

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A B S T R A C T

The magnetic properties of a model consisting of an electron gas, interacting by exchange with van Vleck ions, under the action of a crystal field, is studied in the narrow band limit. Iso-T_c curves (in the plane of the interaction parameters), ionic and electronic magnetizations and susceptibilities versus temperature, as well as the magnetic specific heat, are obtained for several values of exchange and crystal field paramaters.

Les proprietés magnétiques d'un modèle dans lequel un gaz d'électrons se couple par échange avec des ions van Vleck dans un champ cristallin sont etudiés dans la limite de bande étroite. Dans le plan des paramètres des interactions, on obtient des courbes iso-T_c. Les aimantations, susceptibilités et chaleurs specifiques magnétiques, ionique et électronique, sont étudiés en fonction de la temperature pour plusieurs valeur des paramètres d'échange et de champ cristallin.

1. INTRODUCTION

The possibility of onset of magnetic order in a system of rare-earth ions, which under the action of a crystal field have the ground state splitted into two singlet levels, interacting by direct exchange, has been studied in several approximations (molecular field, RPA, etc.) in the literature [1,2].

Explicit consideration for the magnetic role of the conduction electrons is usually emphasized in the heavy rare-earth intermetallics, where however crystal field effects are less relevant than in the case of light ones [3,4].

In this work we discuss the magnetic behaviour of singlet-singlet levels coupled via exchange to an electron gas in the narrow band limit. This limit seems interesting in the sense that it represents the opposite limit of the parabolic electronic density of states considered in previous works [5,6].We concentrate on the temperature dependence of the magnetizations, susceptibilities and magnetic specific heats of the ionic and electronic counterparts. The paper goes as follows: in section 2, we introduce the Hamiltonian and specify the physical quantities to be computed; in section 3 the magnetic state equations, from which the critical temperature, magnetizations versus temperaturo ($T \leq T_c$) and susceptibilities are presented, and expressions for the magnet-specific heats are obtained.Finally (section), numerical results are presented and commented.

2. FORMULATION OF THE PROBLEM

The model Hamiltonian is

$$\mathcal{H} = \sum_{k\sigma} E_k C^{+}_{k\sigma} C_{k\sigma} - \Delta \sum_i S^x_i - J \sum_i S^z_i \sigma^z_i - 2\mu_B H \sum_i (g\alpha S^z_i + \sigma^z_i) \qquad (1)$$

The first term refers to the conduction electrons, the second to the ions (where Δ is the energy difference between the two levels), the third is the exchange interaction and the last is the magnetic interaction. A more detailed description is given in [5].

We want to compute (in the narrow band limit):

1 - the dependency of the critical temperature on the exchange and crystal field parameters;

2 - the temperature dependence of the ionic and electronic magnetizations and susceptibilities;

3 - the temperature dependence of the magnetic specific heats of the electronic and ionic counter-parts.

3. MAGNETIC STATE EQUATIONS

In the molecular field approximation, the system of equations which relate the magnetizations and the chemical potential to the temperature, to the external magnetic field, and to the parameters of the model were derived in [5].

$$\langle S^z \rangle = \frac{1}{2} \frac{J\zeta + 4(g\alpha)^2 \mu_B H}{\left[(J\zeta)^2 + 4\Delta^2\right]^{1/2}} \tanh \frac{\left[(J\zeta)^2 + 4\Delta^2\right]^{1/2}}{4k_B T} \qquad (2)$$

$$\langle \delta^z \rangle = \frac{1}{2N} \sum_k f(E_{k\uparrow}) - f(E_{k\downarrow}) \tag{3}$$

$$N = \sum_k f(E_{k\uparrow}) + f(E_{k\downarrow}) \tag{4}$$

where $E_{k\sigma} = E_k - J\sigma\langle S^z \rangle - \sigma\mu_B H$ ($\sigma = \uparrow$ or $\downarrow$ when used as indice and $\pm$ as coefficient), J and Δ are the exchange and the crystal field parameters, α is the non-diagonal matrix element of the angular momentum between the two singlet levels, $\langle \delta^z \rangle$ and $\langle S^z \rangle$ are the electronic and the ionic spin magnetization and $\zeta = 2\langle \delta^z \rangle$.

In the limit $E_k = E_o$ for every k of the Brillouin zone, equations 2 and 3 reduce to

$$\zeta = \frac{1}{\exp\beta\left[E_o - (\mu + J\langle S^z \rangle + \mu_B H)\right] + 1} - \frac{1}{\exp\beta\left[E_o - (\mu + J\langle S^z \rangle - \mu_B H)\right] + 1} \tag{5}$$

$$1 = \frac{1}{\exp\beta\left[E_o - (\mu + J\langle S^z \rangle + \mu_B H)\right] + 1} + \frac{1}{\exp\beta\left[E_o - (\mu + J\langle S^z \rangle - \mu_B H)\right] + 1} \tag{6}$$

A physical solution ($\zeta \leq 1$) of (5) and (6) is given by

$$\zeta = \tanh\left(\frac{J\langle S^z \rangle + \mu_B H}{2k_B T}\right) \tag{7}$$

Equations (2) and (7) allow us to obtain $\langle S^z \rangle$ and ζ versus T as a function of the magnetic field and the parameters Δ and J. In other words (2) and (7) are our margnetic state equations.

For H=0, in the limit $T \to T_c$, one obtains

$$8\left(\frac{k_B T_c}{J}\right)\frac{\Delta}{J} = \tanh\frac{\Delta}{2k_B T_c} \tag{8}$$

From equation (8) we can compute iso-T_c curves in the plane ΔxJ(see next section).

For $T \geq T_c$, in the limit $H \to 0$, one has

$$\frac{\mu_B H}{J(2\langle S^z\rangle)} = \frac{4\frac{k_B T}{J} - \frac{1}{2\Delta/J}\tanh\frac{\Delta/J}{2k_B T/J}}{\left[8(g\alpha)^2\frac{k_B T/J}{\Delta/J} + \frac{2}{\Delta/J}\right]\tanh\frac{\Delta/J}{2k_B T/J}} \tag{9}$$

$$\frac{\mu_B H}{J\zeta} = \frac{4\frac{k_B T}{J} - \frac{1}{2\Delta/J}\tanh\frac{\Delta/J}{2k_B T/J}}{4 + \frac{2(g\alpha)^2}{\Delta/J}\tanh\frac{\Delta/J}{2k_B T/J}} \tag{10}$$

The magnetic specific heat for the electronic and ionic counterparts are derived from the relation $C_H = -T\left(\frac{\partial^2 F}{\partial T^2}\right)_H$, $F = -k_B T \ln Z$. The ionic specific heat expression (derived in [5]) is

$$C_H^i = \frac{J^2\zeta^2 + 4\Delta^2}{16 k_B T^2}\,\mathrm{sech}^2\,\frac{(J^2\zeta^2+4\Delta^2)^{1/2}}{4k_B T} \tag{11}$$

The electronic specific heat is obtained using

$$Z_e = \exp[-\beta J\langle S^z\rangle] + \exp[\beta J\langle S^z\rangle] \tag{12}$$

one obtains

$$C_H^e = \frac{(J\langle S^z\rangle)^2}{k_B T^2}\,\mathrm{sech}^2\,\frac{J\langle S^z\rangle}{k_B T} \tag{13}$$

Expressions 8, 9, 10, 11 and 13 are numerically analyzed in the next section.

4. NUMERICAL RESULTS AND COMMENTS

The relative role of Δ and J on the critical temperature is conveniently displayed by equal-T_c curves in the J x Δ plane. Fig.1 shows these curves for $k_B T_C$=0.1 eV, 0.5 eV and 1.0 eV. One notes that these curves are quite insensitive to the parameter Δ.

The temperature dependence of magnetizations and inverse of the susceptibilities for several values of Δ/J are given in figures 2a, 2b and 2c. One notes that the ionic magnetization $2\langle S^z \rangle$ is always less than 1.0, and decreases when Δ/J increases. Deviations of Curie-Weiss law increases for greater values of Δ/J. Figure 2d compares the electronic magnetization and susceptibility of our results with the pure Stoner model, in the narrow band limit, for the same T_c and shows that in our case the electronic magnetizations is never greater than the corresponding pure Stoner model.

Figure 3a and 3b show the temperature dependence of the magnetic specific heat (MSH) for the ionic and electronic counter parts for several values of Δ/J. It is interesting to note that the maximum value of the MSH is independent of Δ/J; for $T \geq T_c$ MSH is zero for the electronic, but not for the ionic MSH. The width in temperature in which the MSH is relevant depends on the Δ/J, particularly in the ionic case.

FIGURE CAPTION

Fig.1 - Equi-T_c curves in the plane $J \times \Delta$ for $k_B T_c = 0.1$ eV, 0.5 eV and 1.0 eV.

Fig.2a - Temperature dependence of the electronic magnetization and inverse of suscepbility for $\frac{\Delta}{J} = 1.0$ (curve 1), $\frac{\Delta}{J} = 0.5$ (curve 2) and $\Delta/J = 0.1$ (curve 3).

Fig.2b - Temperature dependence of the ionic magnetization and inverse of susceptibility for the same values of Δ/J of Fig.2a.

Fig.2c - Temperature dependence of the total magnetization and inverse of the total susceptibility. The drawing was done using $(g\alpha)^2 = 2$.

Fig.2d - Temperature dependence of electronic magnetization and inverse of susceptibility of a pure stones model with $\frac{k\theta'}{J} = 0.42$ (curve 2) and for our case with $\Delta/J = 0.5$ (curve 1). The choice of the parameters was done in order that curves 1 and 2 have the same T_c.

Fig.3a - Ionic magnetic specific heat versus temperature for $\Delta/J = 0.5$ (curve 1) and $\Delta/J = 0.1$ (curve 2).

Fig.3b - Electronic magnetic specific heat versus temperature for $\Delta/J = 1.0$ (curve 1), $\Delta/J = 0.5$ (curve 2) and $\Delta/J = 0.1$ (curve 3).

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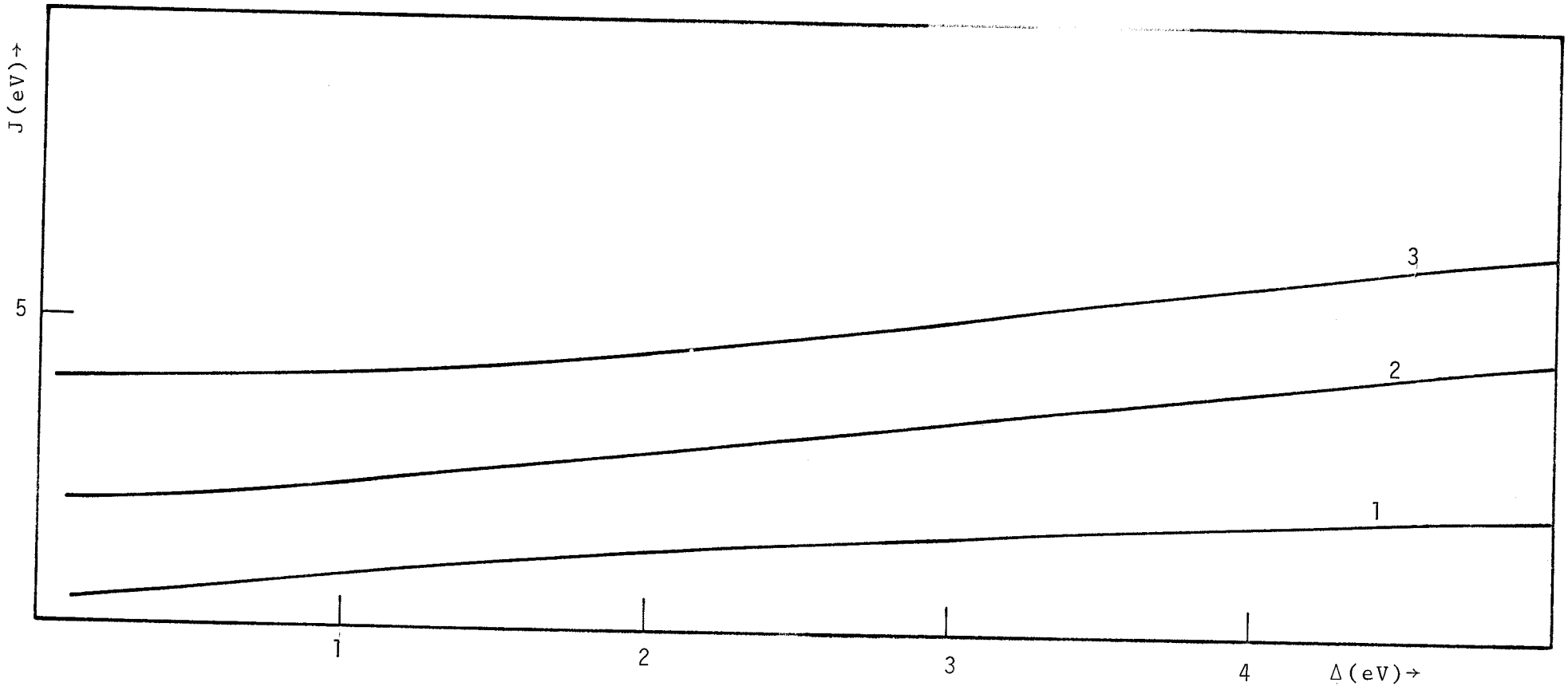


Fig. 1

Fig. 2a

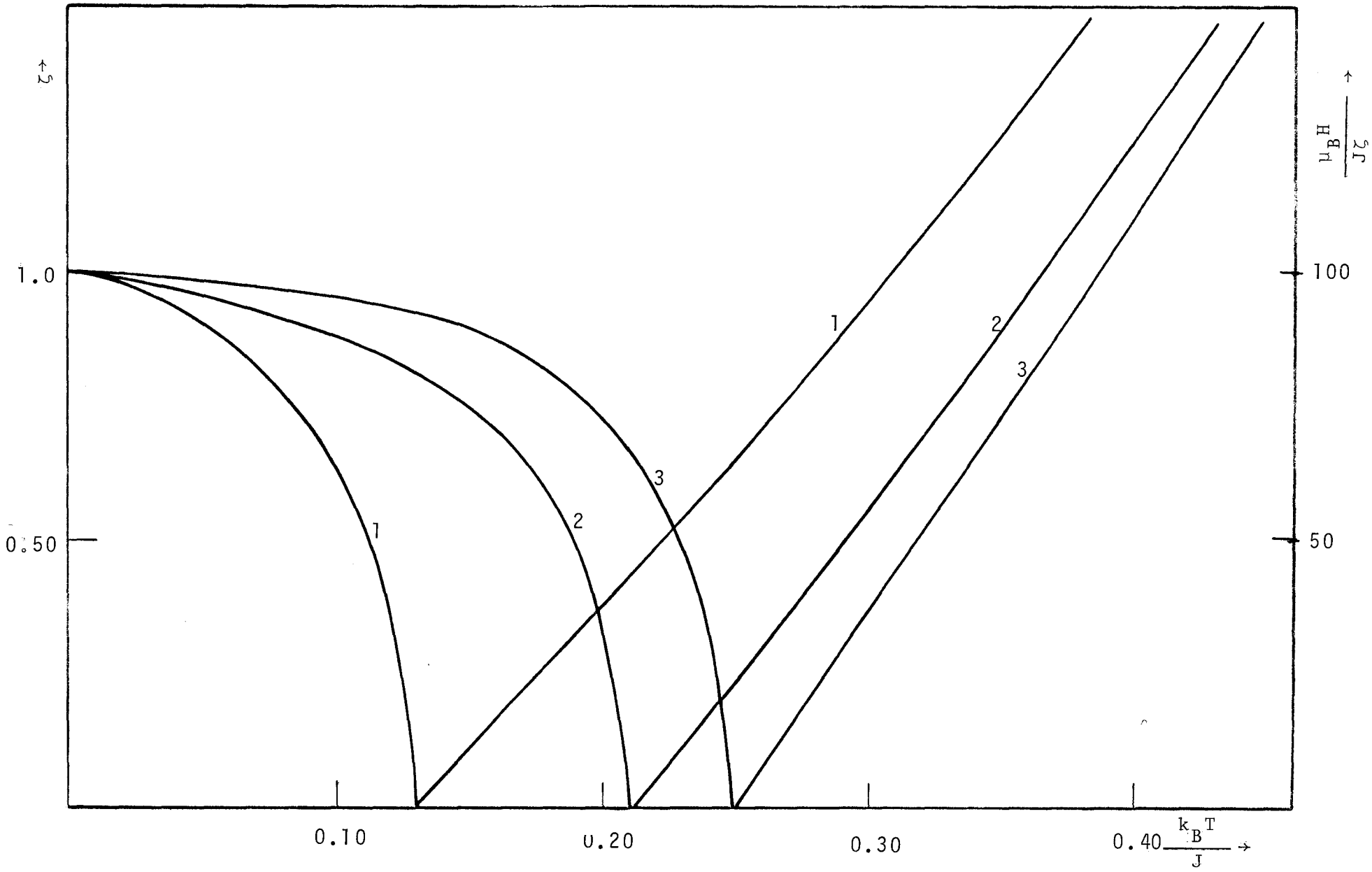


Fig. 2b

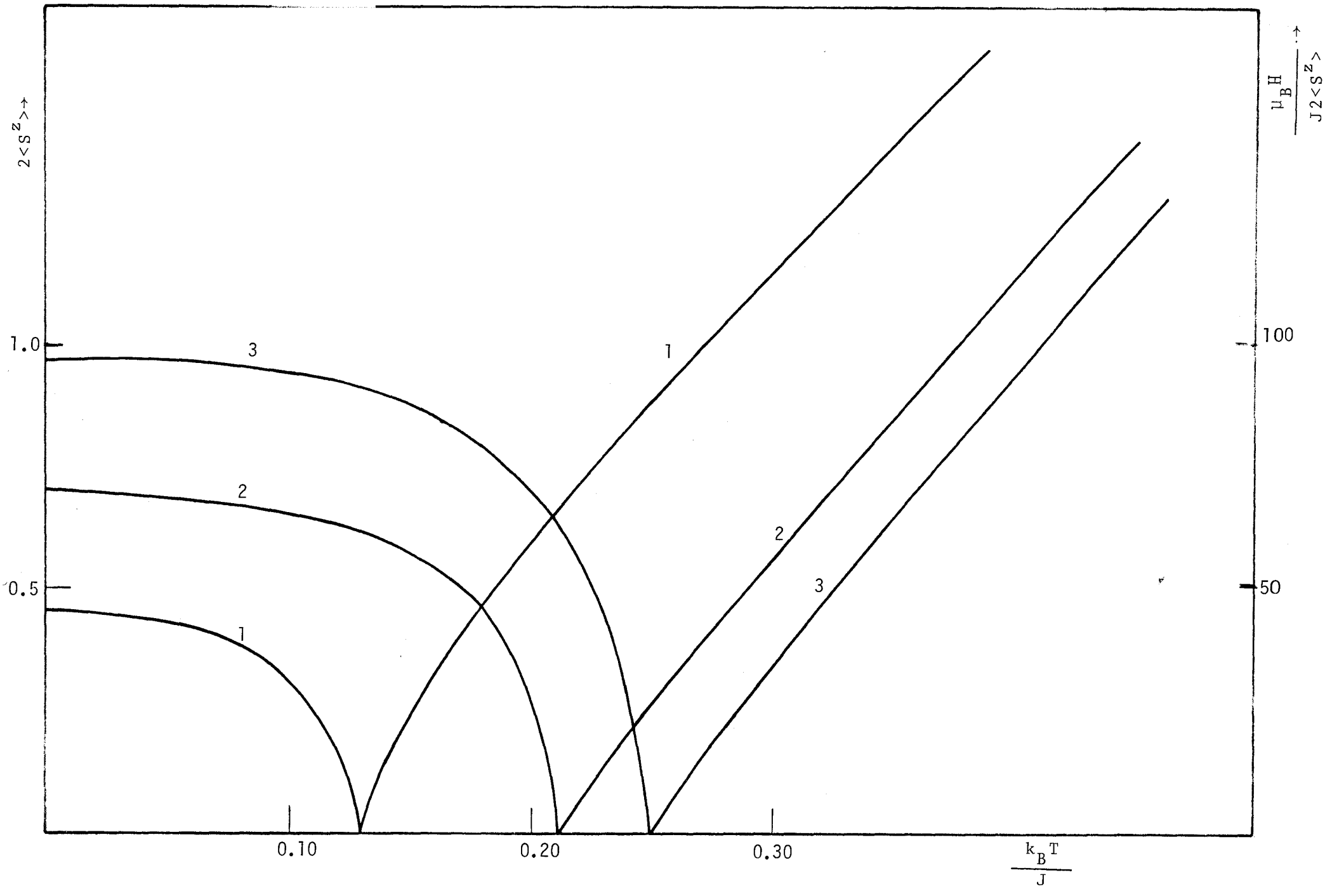

$2\langle S^z \rangle \rightarrow$
1.0
0.5
3
2
1
0.10
0.20
0.30
$\frac{k_B T}{J}$
1
2
3
100
50
$\frac{\mu_B H}{J 2\langle S^z \rangle} \rightarrow$

Fig. 2c

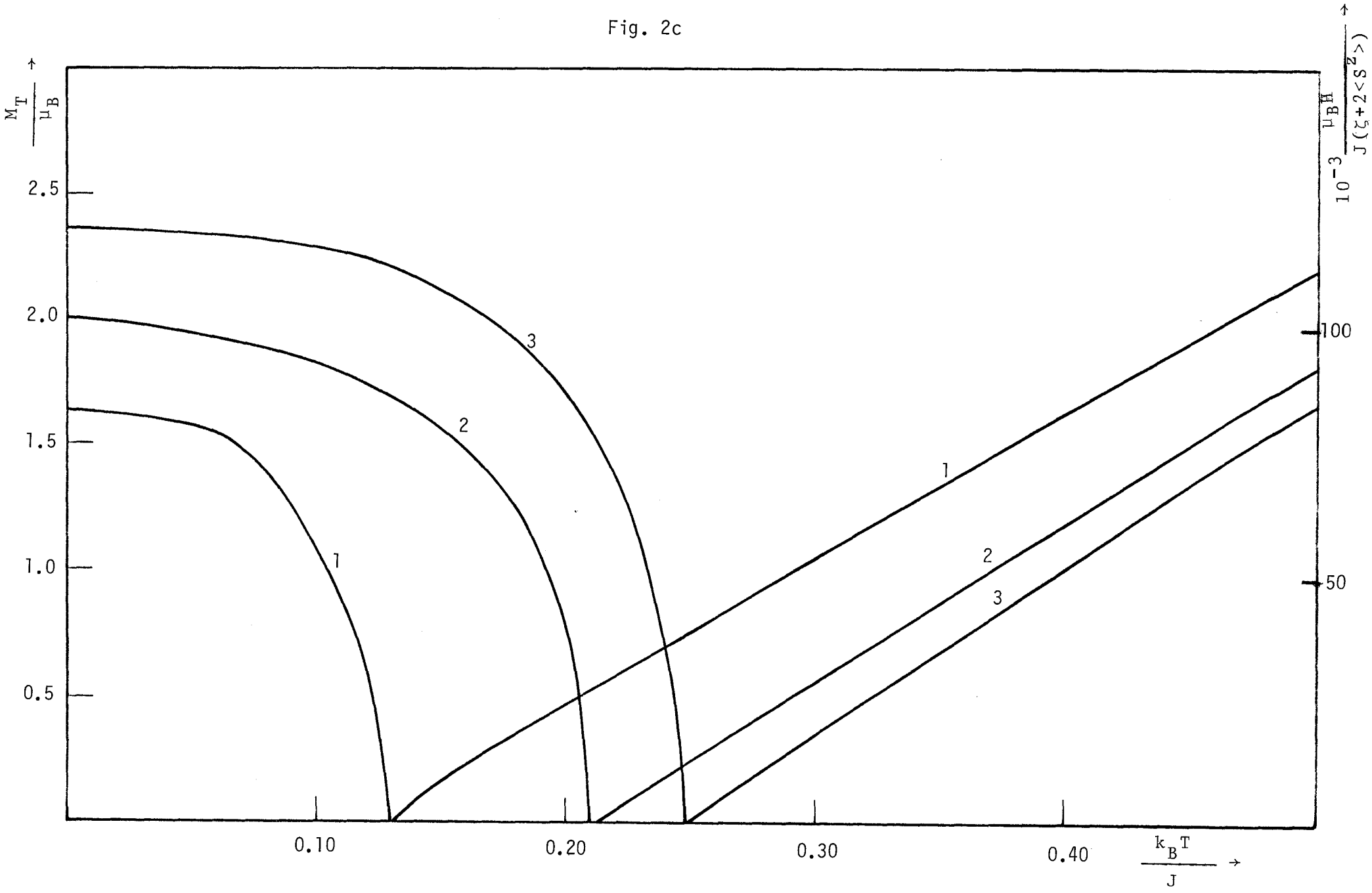
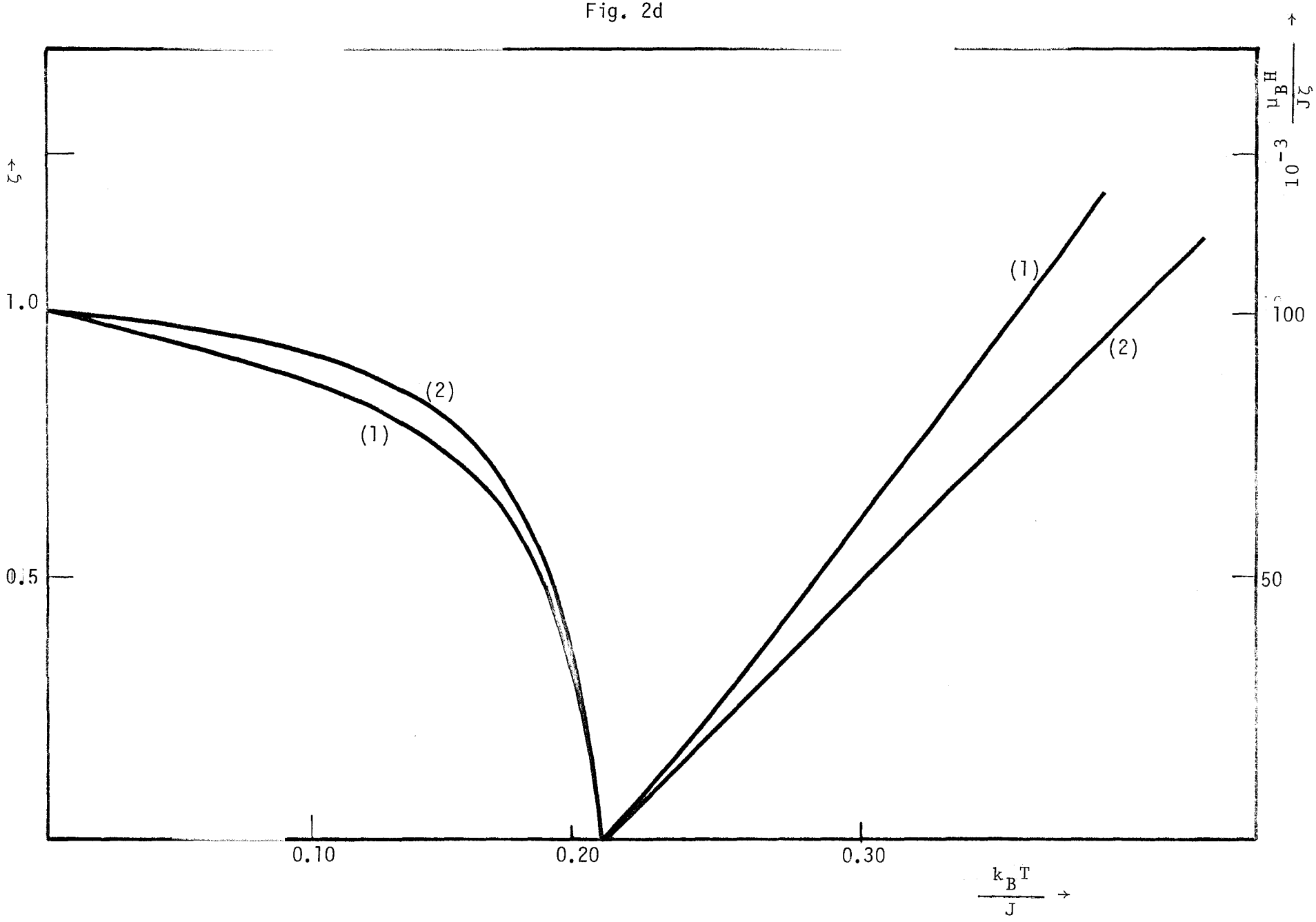

$\frac{M_T}{\mu_B}$ →
2.5
2.0
1.5
1.0
0.5
1
2
3
0.10
0.20
0.30
0.40
$\frac{k_B T}{J}$ →
$10^{-3}\frac{\mu_B H}{J(\zeta+2<S^z>)}$ →
100
50

Fig. 2d



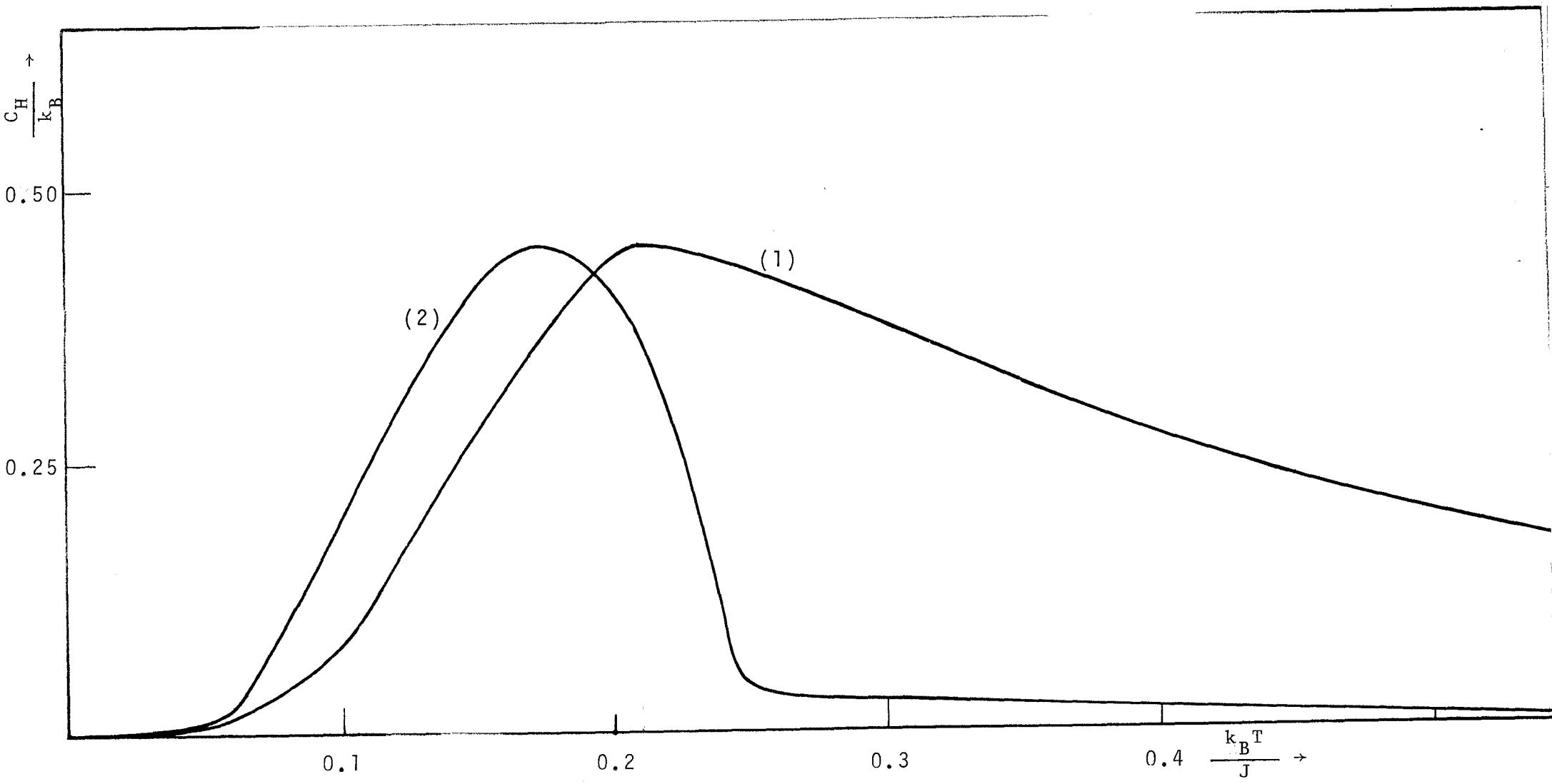


Fig. 3a

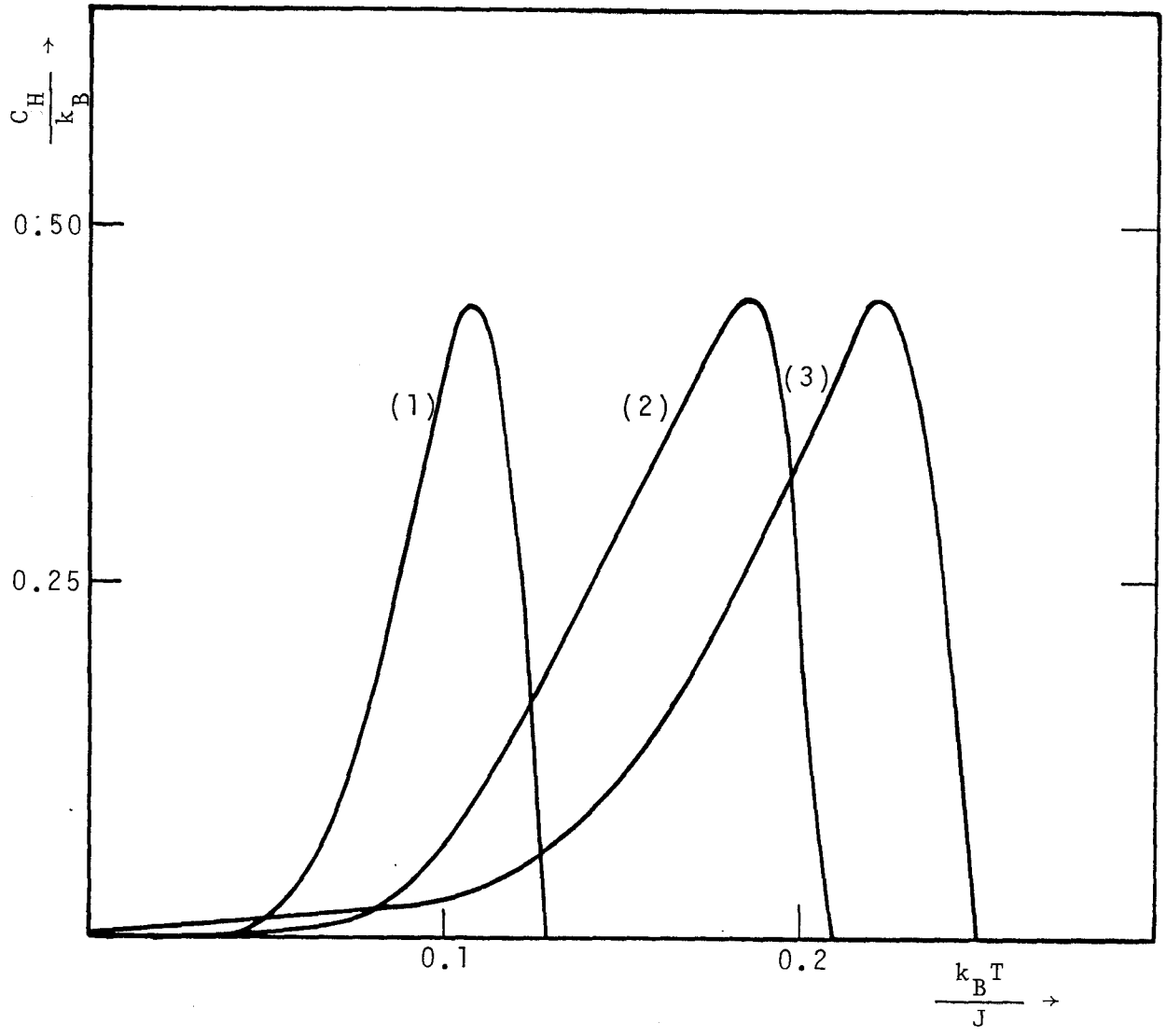


Fig. 3b