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FLUCTUATIONS OF THE MOLECULAR FIELD IN THE ISING MODEL WITH SINGLE-ION ANISOTROPY

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A new approximation including Gaussian fluctuations of the molecular field is applied to an Ising model with a single-ion anisotropy. The free energy, the magnetization, $\langle (S^z)^2 \rangle$ as well as the mean squares of fluctuations have been calculated. Our results are then compared with those obtained by various other approximations.

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1. Introduction

The problem of the easy-axis ferromagnet with single-ion anisotropy has arisen great interest in recent years because of quite obvious reasons. First of all, the single-ion anisotropy prevails in almost all magnetic crystals and thus its effects are of a great importance. For a $S = 1$ system, the single-ion anisotropy is of a second-order, in terms of spin variables, and can be simplified further, if the system possesses a uniaxial symmetry.

In the present paper we apply a new method of approximation proposed in the papers [1, 2] for studying the thermodynamical properties of the $S = 1$ Ising model with a single-ion anisotropy. Within the framework of the method, one obtains the results including Gaussian fluctuations of molecular field. Contrary to the previous papers [3–5], the results are valid in the entire range of temperatures.

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We consider the following model of a ferromagnet:

$$\mathscr{H} = -\tfrac{1}{2}\sum_{j\neq j'} I_{jj'}S_j^zS_{j'}^z + D\sum_j (S_j^z)^2, \tag{1}$$

where $S = 1$. The terms on the right-hand side of Eq. (1) are the Ising term and the single--ion anisotropy, respectively.

2. *Gaussian fluctuations of the molecular field*

With the aid of the method proposed in the papers [1, 2], we now proceed to study the influence of fluctuations of the molecular field on the thermodynamical properties of our model. In this aim, let us rewrite the Hamiltonian (1) as

$$\mathscr{H} = \mathscr{H}_0 + \mathscr{H}_1, \tag{2}$$

where

$$\mathscr{H}_0 = \tfrac{1}{2} zNI\langle S^z\rangle^2 + D\sum_j (S_j^z)^2 - zI\langle S^z\rangle \sum_j S_j^z \tag{3}$$

is the molecular field Hamiltonian, whereas

$$\mathscr{H}_1 = -\tfrac{1}{2}\sum_{j\neq j'} I_{jj'}\delta S_j^z\delta S_{j'}^z \tag{4}$$

is the perturbing term and

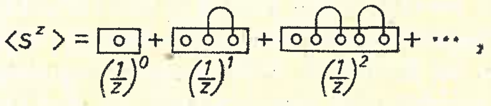
$$\delta S_j^z = S_j^z - \langle S^z\rangle \tag{5}$$

is the operator of the fluctuation of the j-th spin.

According to the rules of the thermodynamical perturbation expansion [6] we can write

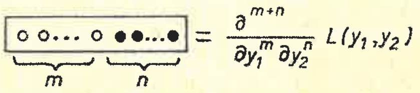
$$\langle S^z\rangle = \frac{\langle S^z e^{-\beta\mathscr{H}_1}\rangle_0}{\langle e^{-\beta\mathscr{H}_1}\rangle_0}. \tag{6}$$

The right-hand side of Eq. (6) can be expanded into a series with respect to the perturbing term $\mathscr{H}_1$. From such an infinite series we now choose a certain partial sum of the subseries with increasing power of the high-density parameter $1/z$ [6] which can be represented graphically as



(7)

where



$$= \frac{\partial^{m+n}}{\partial y_1^m \partial y_2^n} L(y_1, y_2) \tag{8}$$

and

$$L(y_1, y_2) = \ln(2e^{y_2}\cosh y_1 + 1). \tag{9}$$

and moreover,

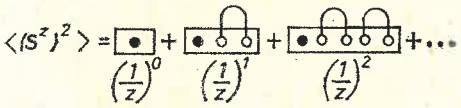
$$y_1 = \beta z I \langle S^z \rangle, \tag{10}$$

$$y_2 = -\beta D, \tag{11}$$

$$\sqcap = \frac{1}{N}\sum_k \tilde{I}(k), \tag{12}$$

where $\tilde{I}(k)$ is the Fourier transform of the effective exchange parameter. An open circle in symbol (8) stands for a site S^z, whereas a full dot denotes a site $(S^z)^2$.

Similarly as for $\langle S^z \rangle$, we can write a partial sum of the series of the high-density expansion for $\langle (S^z)^2 \rangle$ as



(13)

The series (7) and (13) can be rewritten in the explicit analytical form as

$$\langle S^z \rangle = \overline{\frac{\partial L(y_1, y_2)}{\partial y_1}}, \tag{14}$$

$$\langle (S^z)^2 \rangle = \overline{\frac{\partial L(y_1, y_2)}{\partial y_2}}, \tag{15}$$

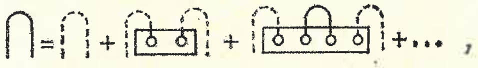
where the bar denotes the average with the Gaussian distribution

$$\overline{\frac{\partial^{m+n} L(y_1, y_2)}{\partial y_1^m \partial y_2^n}} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{-\frac{1}{2}x^2} \frac{\partial^{m+n}}{\partial y_1^m \partial y_2^n} L(y_1 + \delta y_1 x, y_2) dx \tag{16}$$

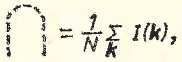
and

$$\delta y_1 = \sqrt{\sqcap}. \tag{17}$$

On the basis of Eq. (16) δy_1 can be interpreted as a root of the mean square fluctuation of the molecular field. As in the papers [1, 2], δy_1 is calculated by means of the following self-consistent renormalization of the interaction line



(18a)



(18b)

from which

$$(\delta y_1)^2 = z\beta^2 I^2 \overline{\frac{\partial^2 L(y_1, y_2)}{\partial y_1^2}}. \tag{19}$$

Eqs (14) and (19) form a closed set of equations for $\langle S^z \rangle$ and δy_1. Within the framework of the approximation (18), we can also easily write an expression for the free energy F fulfilling the following stability conditions

$$\frac{\partial F}{\partial \langle S^z \rangle} = \frac{\partial F}{\partial (\delta y_1)} = 0 \tag{20}$$

and the condition

$$\lim_{\delta y_1 \to 0} F = F_{\mathrm{MFA}}, \tag{21}$$

which means that for small fluctuations our formulae go over into the MFA. Therefore,

$$\frac{F}{N} = \tfrac{1}{2} Iz \langle S^z \rangle^2 - \frac{1}{\beta} \overline{L(y_1, y_2)} + \tfrac{1}{4}\, \delta y^4 (z\beta^3 I^2)^{-1}. \tag{22}$$

Equations (14)–(22) comprise the total information about the thermodynamical properties of our system within the framework of the approximation comprising the Gaussian fluctuations of the molecular field.

3. *Numerical results*

The analysis of Eqs (14)–(22) can be performed only numerically. For this aim it seems to be convenient to introduce the following relative units:

$$t = \frac{k_B T}{Iz}, \quad d = \frac{D}{Iz}, \quad f = \frac{F}{NIz}. \tag{23}$$

In terms of the new units the respective equations of the previous section take the following form:

$$(\delta y_1)^2 = \frac{1}{z} \frac{1}{t^2} \overline{\frac{\partial^2 L(y_1, y_2)}{\partial y_1^2}}, \tag{24}$$

$$f = \tfrac{1}{2} \langle S^z \rangle^2 - t\overline{L(y_1, y_2)} + \tfrac{1}{4} z t^3 \delta y_1^4, \tag{25}$$

TABLE I

Values of the critical temperature t_c of the spin -1 Ising model ($d = 0$) from various calculations SC

MFA	0.667
RPA [7]	0.528
HTS [8]	0.532
Variational approximation [8]	0.481
Present paper	0.593

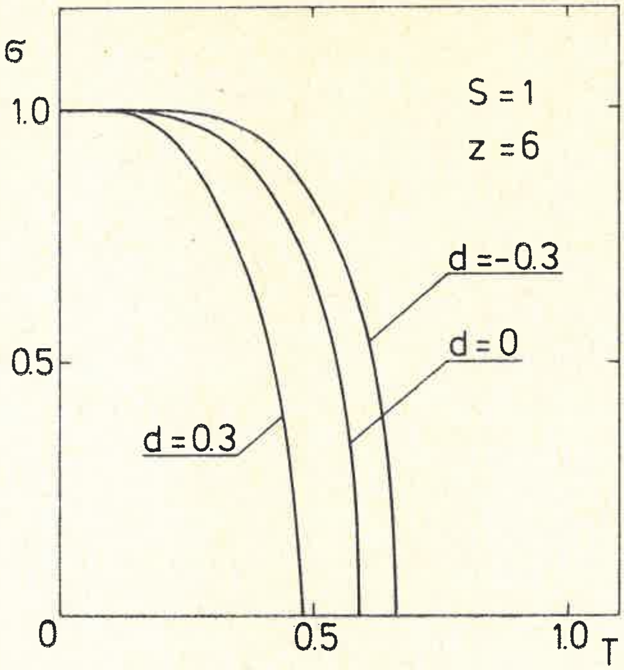


Fig. 1. Relative spontaneous magnetization σ of sc ferromagnet versus relative temperature t

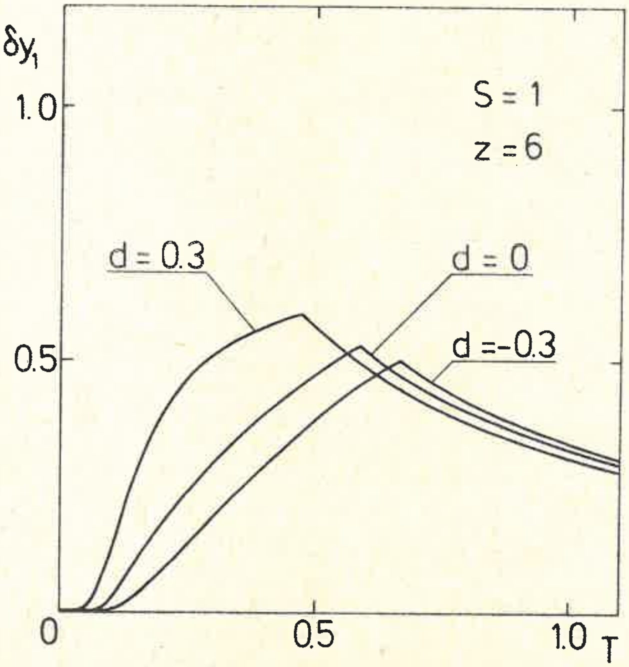


Fig. 2. Mean fluctuations of the molecular field δy_1 plotted against temperature for sc ferromagnet

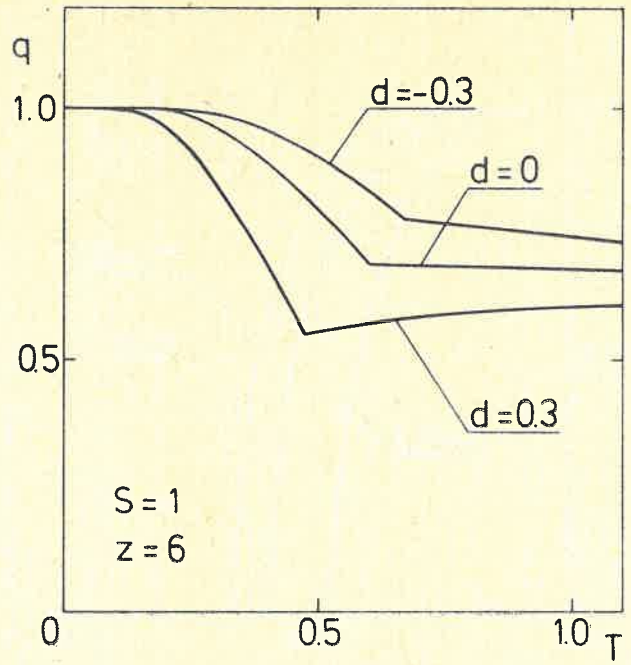


Fig. 3. Temperature dependences of $q = \langle (S^z)^2 \rangle$ for sc ferromagnet

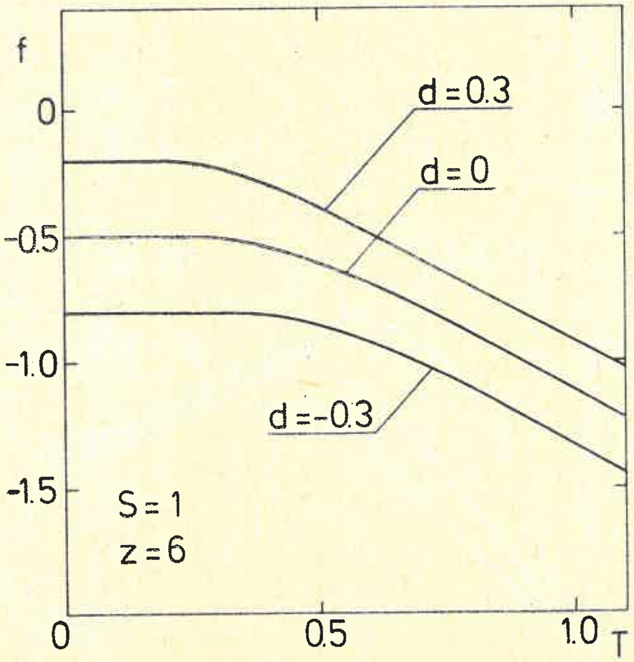


Fig. 4. Temperature dependences of the free energy f for sc ferromagnet

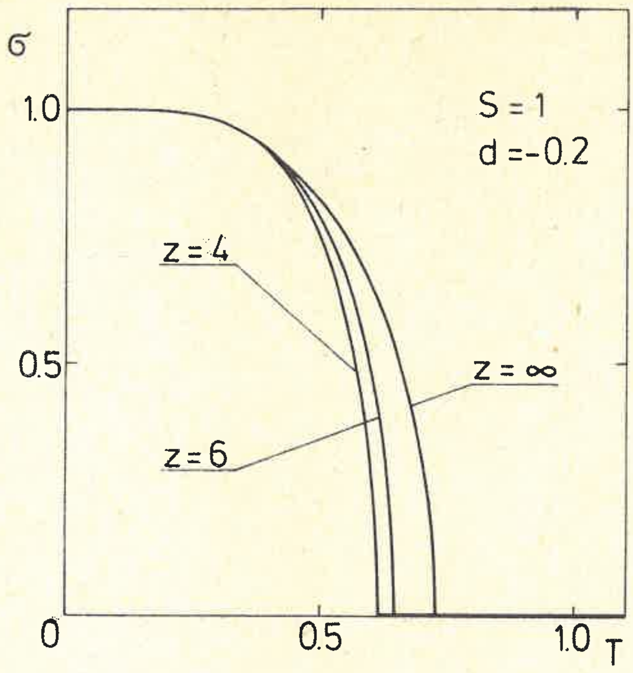


Fig. 5. Relative spontaneous magnetization σ versus relative temperature t

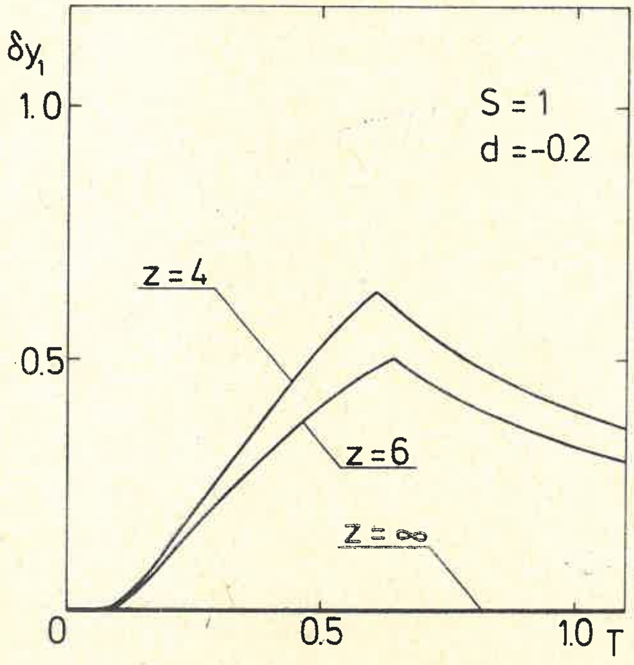


Fig. 6. Mean fluctuations of the molecular field δy_1 plotted against temperature

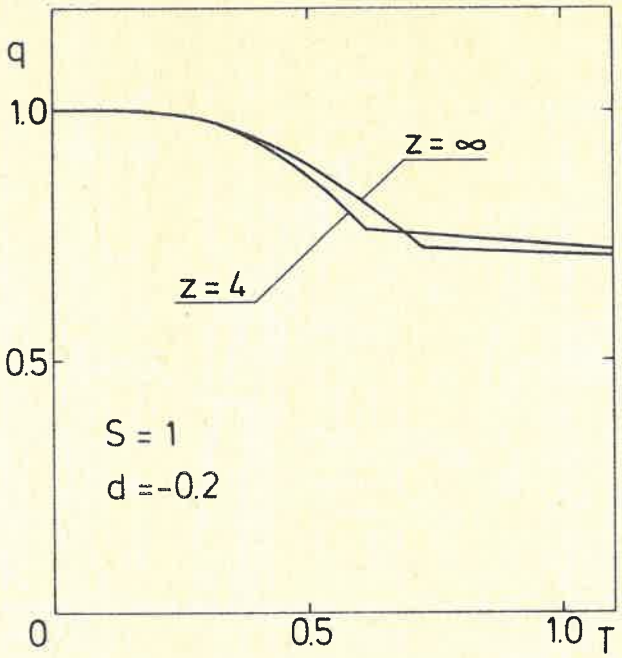


Fig. 7. Temperature dependences of $q = \langle (S)^2 \rangle$

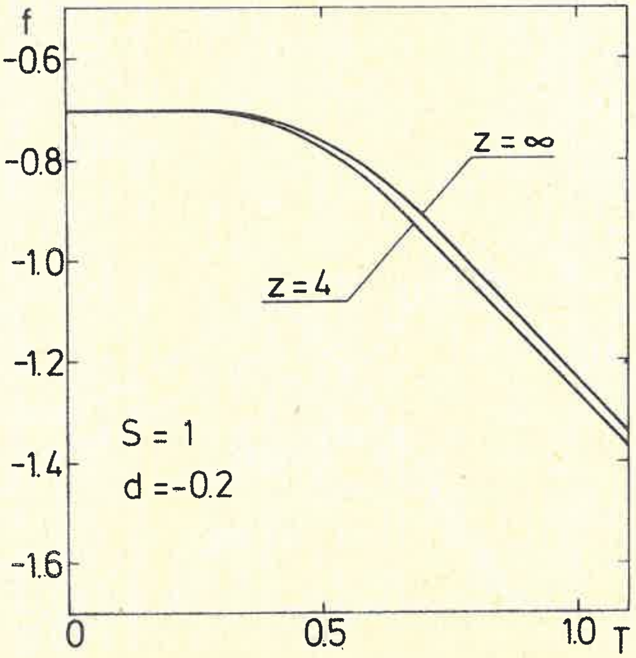


Fig. 8. Temperature dependences of the free energy *f*

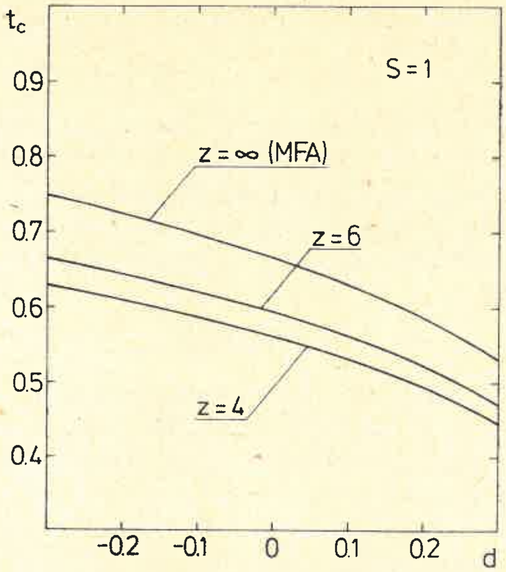


Fig. 9. Relative Curie temperature t_c plotted against the parameter d

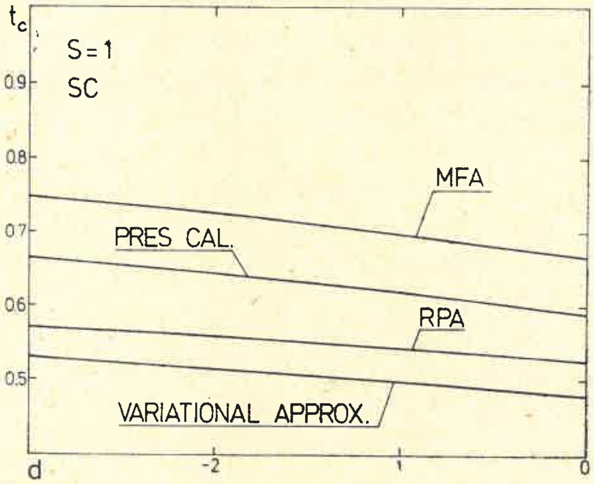


Fig. 10. Curie temperature t_c as a function of anisotropy d calculated by MFA, RPA [7] variational approximation [8] and from Eq. (28)

where

$$y_1 = t^{-1}\langle S^z\rangle, \tag{26}$$

$$y_2 = -t^{-1}d. \tag{27}$$

From Eqs (14) and (26), with the assumption that $\langle S^z\rangle \to 0$, we can obtain the following expression for the Curie temperature

$$t_c = \left(\frac{\partial^2 L(y_1, y_2)}{\partial y_1^2}\right)_{y_1=0}. \tag{28}$$

From Eq. (25) one can easily derive a value of the free energy at absolute zero:

$$f(t = 0) = -\tfrac{1}{2}+d. \tag{29}$$

The results of our numerical calculations are presented in Figs 1–10. We have shown there temperature variations of the magnetization, $\langle (S^z)^2 \rangle$ and the free energy. Moreover, the dependence of the Curie temperature upon the parameter d is plotted. In Table I the values of the Curie temperature for the Ising model obtained in the present paper and those calculated using the other methods, are gathered for comparison.

4. Conclusions

The most essential conclusion of the present paper is an ascertainment that the approximation proposed in the paper [1] can be successfully applied for studying spin models including crystal-field effects. We have just obtained the results which, in comparison with those of other methods, are really good in the entire temperature range. It is worthwhile to note moreover, that our results have been derived by solving Eqs (14) and (19) which possess a much simpler analytical form than the analogous equations derived within the framework of other competitive approximations. This is an essential advantage of the approximation proposed by us.

Moreover, the important result of our paper consists in obtaining, for the first time, the temperature-dependence of the mean square fluctuation of the molecular field for the model comprising the single-ion anisotropy.

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