ONE-DIMENSIONAL ISING MODEL WITH ANISOTROPY

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The one-dimensional Ising model, with $S = 1$ and the anisotropy of the single-ion type, is investigated. The correlation functions, specific heat and susceptibility in zero external field are calculated.

Properties of the Ising ferromagnet for higher spins in the presence of the single-ion anisotropy have received some attention recently [1–4].

In this note we shall present the results of a calculation of some thermodynamic quantities for the corresponding simple one-dimensional model, *i.e.* for the linear chain of the Ising spins ($S = 1$) with nearest-neighbour interaction. The total energy for such a system consisting of $2N$ spins $\mu_i = -1, 0, 1$, arranged in a ring, is given by

$$E_{2N} = -h \sum_{i=1}^{2N} \mu_i - 2J \sum_{i=1}^{2N} \mu_i\mu_{i+1} - K \sum_{i=1}^{2N} \mu_i^2, \quad (\mu_{2N+1} \equiv \mu_1) \tag{1}$$

where $J > 0$, K and h are the exchange, anisotropy and field parameters respectively.

At the beginning we discuss the problem of the ground state arrangement for $h = 0$. Let us divide all possible configurations of spins into classes C^m ($m = 0, \ldots, 2N$). A class C^m consist of all configurations for which strictly m spins have the zero projection. Of course, the class C^{2N} consists only of one configuration with zero energy. The minimal energy for the class C_0 is

$$\frac{E_{2N}^{\min}(C^0)}{4JN} = -(1+\varepsilon) \tag{2}$$

where $\varepsilon \equiv \dfrac{K}{2J}$, and corresponds to ferromagnetic ground state. On the other hand, the minimal energy for the class C^m, for $0 < m < 2N$, is

$$\frac{E_{2N}^{\min}(C^m)}{4JN} = -\left[\left(1-\frac{m+1}{2N}\right)+\varepsilon\left(1-\frac{m}{2N}\right)\right]. \tag{3}$$

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Thus, after additional minimization over the classes we obtain the ground state energy

$$E^{\min} = \begin{cases} -(1+\varepsilon) & \text{for } \varepsilon > -1 \\ & \text{(ferromagnetic order)} \\ 0 & \text{for } \varepsilon < -1 \\ & \text{(all } \mu_i = 0). \end{cases} \tag{4}$$

The ground state for $\varepsilon = -1$ is double degenerate for finite N and becomes undetermined in $N \to \infty$ limit.

The thermodynamic behaviour of the given system for $h = 0$, and the zero-field susceptibility can be calculated exactly by the direct application of the "generalized Bethe approximation" introduced by Obokata and Oguchi [5]. In this method the Bethe cluster consisting of some spin μ_0 with its two nearest neighbours μ_{-1}, μ_1 is considered and the corresponding reduced density matrix is introduced

$$\varrho_B = \sum{}' \exp\{-\beta E\}, \quad \left(\beta = \frac{1}{kT}\right) \tag{5}$$

where Σ' denotes the sum over all μ_i's except those in the Bethe cluster. Because of both the symmetry arguments and properties of μ_i

$$(\mu_i - 1)\mu_i(\mu_i + 1) = 0 \tag{6}$$

the general expression for the ϱ_B may be written as

$$\varrho_B = A[\exp[v\mu_0(\mu_{-1}+\mu_1)+u(\mu_{-1}^2+\mu_0^2+\mu_1^2)+ \\ +l(\mu_{-1}+\mu_0+\mu_1)]](1+\alpha\mu_{-1}+\gamma\mu_{-1}^2)(1+\alpha\mu_1+\gamma\mu_1^2) \tag{7}$$

where $v \equiv 2J\beta$, $u = K\beta$, $l = h\beta$ and A, α, γ are some functions of the temperature and field. For calculation of the thermodynamical averages

$$\langle \ldots \rangle \equiv \frac{\mathrm{Tr}\{\ldots \varrho_B\}}{\mathrm{Tr}\, \varrho_B} \tag{8}$$

the factor A is not needed. The functions α and γ can be determined from the consistency relations

$$\langle \mu_0 \rangle = \langle \mu_1 \rangle \tag{9}$$

$$\langle \mu_0^2 \rangle = \langle \mu_1^2 \rangle \tag{10}$$

after expanding them into the power series in l

$$\alpha = \alpha_1 \cdot l + \alpha_3 \cdot l^3 + \ldots \\ \gamma = \gamma_0 + \gamma_2 \cdot l + \ldots \tag{11}$$

(From the invariance of ϱ_B under the transformation $\mu_i \to -\mu_i$, $l \to -l$ it follows that α and γ must be odd and even functions of l, respectively.)

Strictly speaking, the formulae and calculations with α and γ independent on N are valid only in the thermodynamic limit for the translationally invariant system. For our case we obtain after corresponding calculations

$$\delta_0 \equiv 1+\gamma_0 = \frac{1}{4b}\cdot\{(a+a^{-1})b-1+\sqrt{[(a+a^{-1})b-1]^2+8b}\} \qquad (12)$$

where $a \equiv \exp v,\ b \equiv \exp u$,

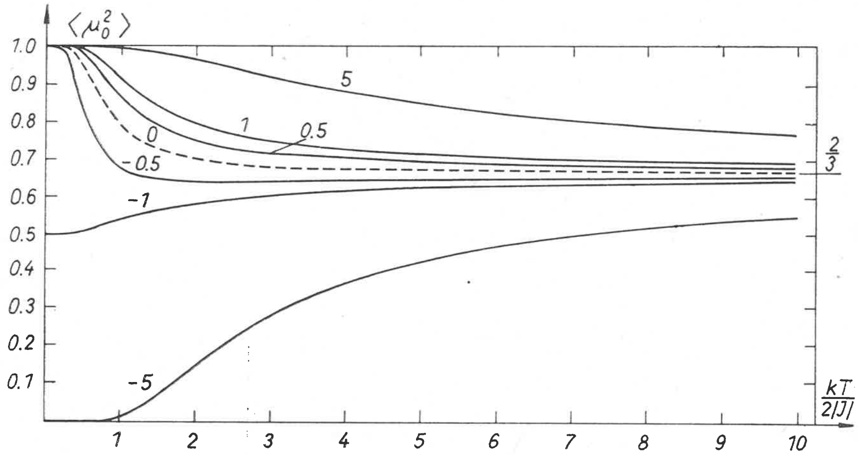

Fig. 1. Correlation function $\langle\mu_0^2\rangle$ *vs* reduced temperature $\frac{kT}{2|J|}$ for $\varepsilon = \frac{K}{2|J|} = -5.0;\ -1.0; -0.5;\ 0.0;\ 1.0; 5.0$ (for ferro- and antiferromagnetic interactions)

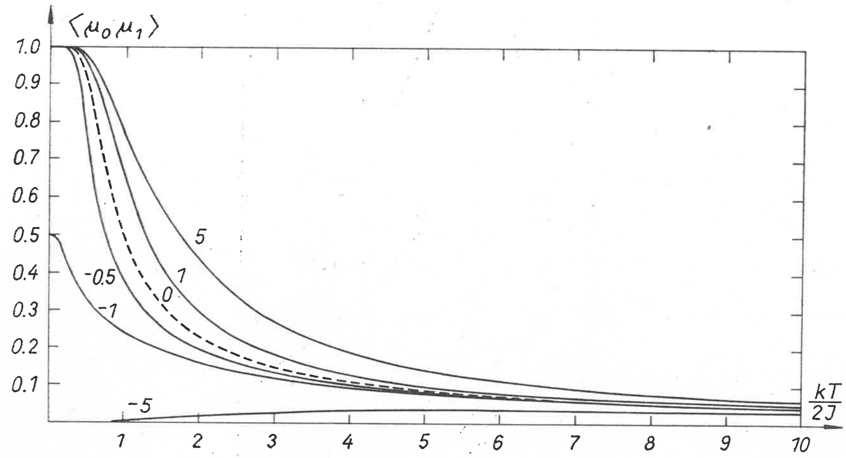

Fig. 2. Correlation function $\langle\mu_0\mu_1\rangle$ *vs* reduced temperature $\frac{kT}{2J}$ for $\varepsilon = 5.0;\ -1.0;\ -0.5;\ 0.0;$ $1.0; 5.0$ (correlation function $\langle\mu_0\mu_1\rangle$ for antiferromagnetic interaction as a function of the $\frac{kT}{2|J|}$ variable and the parameter $\varepsilon = \frac{K}{2|J|}$ have an opposite sign)

and

$$\alpha_1 = \delta_0 b(a-a^{-1})\frac{2\delta_0+a}{3b-a^2b+a+2\delta_0 b(a+2a^{-1}b^3)}. \tag{13}$$

Using (12) we may calculate the correlation functions in zero field

$$\langle\mu_0^2\rangle = 1-\frac{(2b\delta_0+1)^2}{\mathrm{Tr}'\varrho_B} \tag{14}$$

$$\langle\mu_0\mu_1\rangle = \frac{2b^2(a-a^{-1})\delta_0[\delta_0 b(a+a^{-1})+1]}{Tr'\varrho_B} \tag{15}$$

where

$$\mathrm{Tr}'\varrho_B \equiv A^{-1}\,\mathrm{Tr}\,\varrho_B = 2(\delta_0 b)^2(a^2b+a^{-2}b+2b+2)+ +4\delta_0 b(ab+a^{-1}b+1)+2b+1. \tag{16}$$

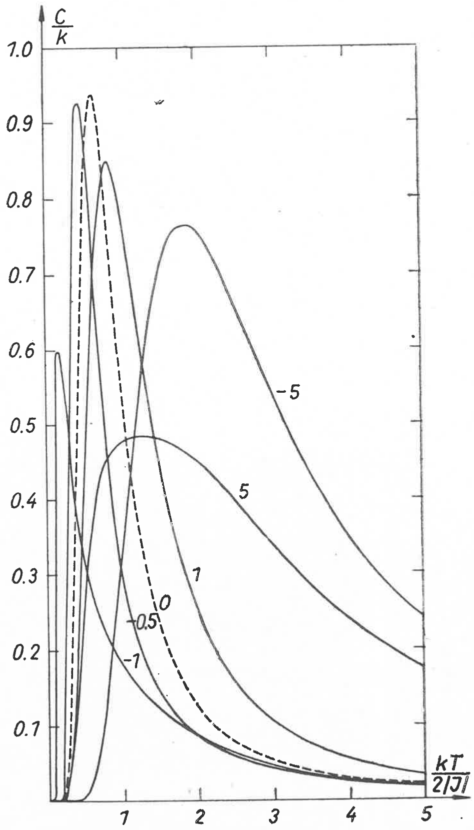

Fig. 3. Specific heat $\frac{C}{k}$ *vs* reduced temperature $\frac{kT}{2|J|}$ for $\varepsilon = \frac{K}{2|J|} = -5.0; -1.0; -0.5; 0.0; 1.0; 5.0$ (for ferro- and antiferromagnetic interactions)

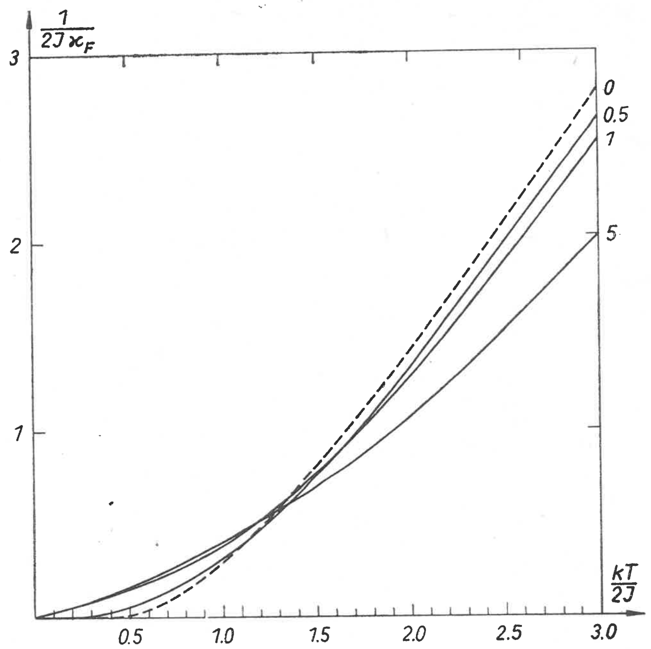

Fig. 4a. Inverse initial susceptibility $(2J\kappa)^{-1}$ *vs* reduced temperature $\frac{kT}{2J}$ for $\varepsilon = 0.0; 0.5; 1.0; 5.0$

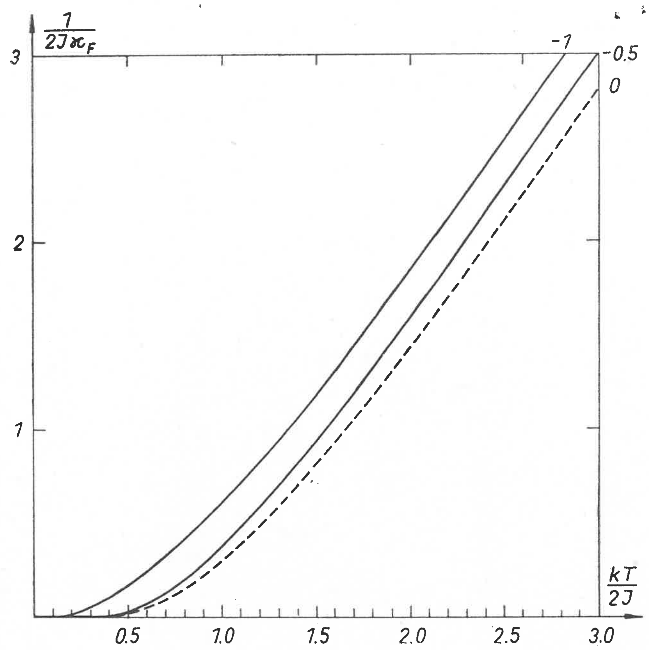

Fig. 4b. Inverse initial susceptibility $(2J\kappa)^{-1}$ *vs* reduced temperature $\frac{kT}{2J}$ for $\varepsilon = 0.0; -0.5; -1.0$

For $J = 0$ ($a = 1$), when the system consists of independent spins, we obtain from (14) and (15) $\langle \mu_0 \mu_1 \rangle = 0$, $\langle \mu_0^2 \rangle = \frac{2b}{2b+1}$ as may be expected. For $K = 0$ ($b = 1$) the results agree with those given in [5].

From (14) and (15) we may deduce the low- and high temperature behaviour of the correlation functions. We have

$$\lim_{T \to 0^+} \langle \mu_0^2 \rangle = \lim_{T \to 0^+} \langle \mu_0 \mu_1 \rangle = \begin{cases} 1 & \text{for } \varepsilon > -1 \\ \frac{1}{2} & \text{for } \varepsilon = -1 \\ 0 & \text{for } \varepsilon < -1 \end{cases} \tag{17}$$

and

$$\lim_{T \to +\infty} \langle \mu_0^2 \rangle = \tfrac{2}{3}, \qquad \lim_{T \to +\infty} \langle \mu_0 \mu_1 \rangle = 0. \tag{18}$$

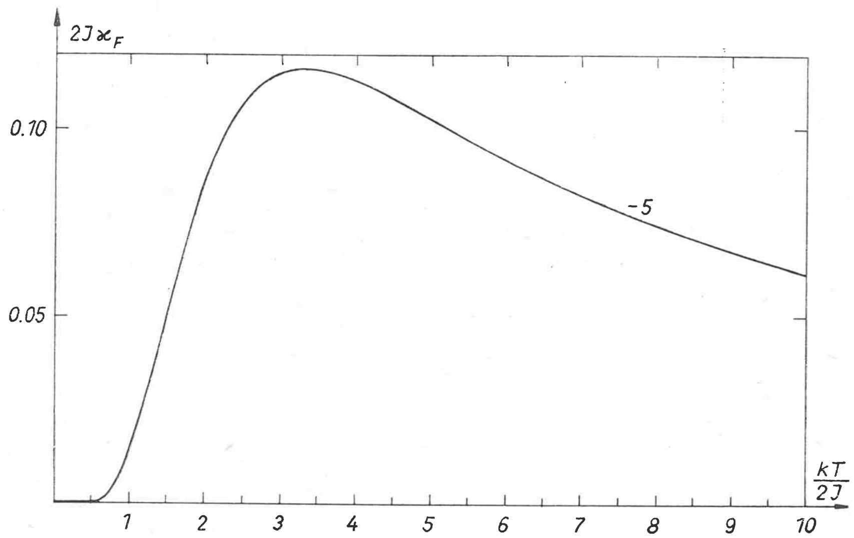

Fig. 5. Initial susceptibility $2J\kappa$ *vs* reduced temperature $\frac{kT}{2J}$ for $\varepsilon = -5$

Using (12) and (13) we may also calculate the initial susceptibility, according to definition

$$\kappa_F = \left. \frac{\partial \langle \mu_0 \rangle}{\partial h} \right|_{h=0}. \tag{19}$$

After corresponding calculations we obtain

$$2J\kappa_F = \frac{1}{x} \left[\langle \mu_0^2 \rangle + 2(\alpha_1' + 1) \langle \mu_0 \mu_1 \rangle \right] \tag{20}$$

where $x \equiv \frac{kT}{2J}$

and

$$\alpha_1' = \frac{b(a-a^{-1})(2\delta_0+a)}{3b-ba^2+a+2\delta_0 ba+4\delta_0 b^4 a^{-1}} = \frac{\alpha_1}{\delta_0}. \tag{21}$$

The susceptibility given by the above expression features interesting behaviour in the low temperature limit. Taking into account only leading terms in corresponding expansions, we obtain after long but standard considerations that

$$2J\kappa_F \underset{(\exp)}{\rightarrow} 0 \text{ for } \varepsilon < -1, \tag{22}$$

$$(2J\kappa_F)^{-1} \underset{(\exp)}{\rightarrow} 0 \text{ for } -1 \leqslant \varepsilon < \tfrac{2}{3}, \tag{23}$$

$$(2J\kappa_F)^{-1} \sim \frac{x}{5} \rightarrow 0 \text{ for } \varepsilon = \tfrac{2}{3}, \tag{24}$$

$$(2J\kappa_F)^{-1} \sim \frac{x}{3} \rightarrow 0 \text{ for } \varepsilon > \tfrac{2}{3}, \tag{25}$$

where the symbol (exp) denotes that the corresponding quantity behaves like $x^{-1} \cdot \exp(\text{const}/x)$.

The results of the numerical calculations for several values of the ratio $\varepsilon = \dfrac{K}{2J}$ are presented in Figs 1–5. The dotted curves for $K = 0$, which are known, are drawn for comparison.

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Note added in proof: Recently, the authors has been informed that equivalent model has been considered by Katsura and Tsujiyama (in "Critical Phenomena", *Proc. Conf.*, ed. M. S. Green, J. V. Sengers, Washington, 1966, p. 219—225) and also by A. Hintermann, F. Rys, (*Helv. Phys. Acta*, **42**, 608 (1969)). They use this model to examine the properties of an annealed Ising model (in this interpretation $\langle \mu_0^2 \rangle = p$ corresponds to concentration of magnetic ions and D to chemical potential). In our paper we investigate the system's behaviour, following Capel, with regard to anisotropy constant D, and thus our results are complementary to those given by quoted authors.

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