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HTS EXPANSION METHOD

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EFFECT OF CRYSTAL-FIELD ANISOTROPY ON CURIE TEMPERATURE OF ISING FERROMAGNET. HTS EXPANSION METHOD

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I. Introduction

The influence of single-ion anisotropy on the ferromagnetic Curie temperature is an important problem for many magnetic materials (e.g., R.E. and actinide compounds) and was extensively studied in molecular field approximation (MFA) (see [1,2]) and by Green function method with various decoupling procedures (see [3,4]). Results of those papers differ from each other considerably, especially for high anisotropies, and it seems to us useful to analyse this problem by means of the exact high temperature series expansion (HTSE). (For references about the method and use of the series we refer the reader to the review articles by Fischer [5]). In the present paper we will discuss the problem on the example of Ising ferromagnetic with single-ion anisotropy term.

II. HTSE for Zero Field Susceptibility

We will consider the Hamiltonian

$$H = H_z + H_I + H_0 , \tag{1}$$

where

$$H_z = -\frac{\mu_B}{S} \mathcal{H} \sum_{i=1}^{N} S_i^z , \tag{2}$$

$$H_I = -\frac{1}{S^2} \sum_{i,l} J_{il} S_i^z S_l^z , \tag{3}$$

$$H_0 = -\frac{D}{S^2} \sum_i (S_i^z)^2 \tag{4}$$

with exchange interaction restricted to the nearest neighbours. The zero field susceptibility is computed from

$$\left(\frac{S^2}{\beta\mu^2}\right)\chi_0 = \frac{1}{N}\sum_{i,j} \langle S_i^z S_j^z \rangle \Big|_{\mathcal{H}=0} \qquad \left(\beta = \frac{1}{kT}\right), \tag{5}$$

where

$$\langle A \rangle \equiv \frac{Tr(e^{-\beta H} A)}{Tr e^{-\beta H}}. \tag{6}$$

Since H_1 and H_0 commute we may write

$$\langle A \rangle \Big|_{\mathcal{H}=0} = \frac{Tr[(A e^{-\beta H_1}) e^{-\beta H_0}]}{Tr[(e^{-\beta H_1}) e^{-\beta H_0}]} \equiv \frac{\langle A e^{-\beta H_1} \rangle_0}{\langle e^{-\beta H_1} \rangle_0} \tag{7}$$

and all quantities will be determined in terms of averages over the states of H_0. Thus, in deriving HTSE we will expand only exchange part, but crystal-field contribution will be calculated in each step exactly. In such a way we obtain the following expansion for susceptibility

$$\left(\frac{kT}{\mu^2 \sigma_2}\right)\chi_0 = \sum_{n=0}^{\infty} a_n y^n, \tag{8}$$

where

$$y \equiv 2z\sigma_2 \beta J, \tag{9}$$

$$a_0 = a_1 = 1, \tag{10}$$

$$a_2 = 1 - \frac{1}{2z}\left(3 - \frac{\sigma_4}{\sigma_2^2}\right), \tag{11}$$

$$a_3 = 1 - \frac{1}{z}\left(3 - \frac{\sigma_4}{\sigma_2^2}\right) + \frac{1}{2z^2}\left[\frac{1}{3}\left(3 - \frac{\sigma_4}{\sigma_2^2}\right)^2 - x\left(3 - \frac{\sigma_4}{\sigma_2^2}\right)\right], \tag{12}$$

$$a_4 = 1 - \frac{3}{2z}\left(3 - \frac{\sigma_4}{\sigma_2^2}\right) + \frac{1}{4z^2}\left[3\left(3 - \frac{\sigma_4}{\sigma_2^2}\right)^2 - 3 + \frac{1}{2}\frac{\sigma_4}{\sigma_2^2} + \frac{1}{2}\frac{\sigma_6}{\sigma_2^3} - \frac{2}{3}\frac{\sigma_4^2}{\sigma_2^4} - 4x\left(3 - \frac{\sigma_4}{\sigma_2^2}\right)\right] + \frac{1}{8z^3}\left(3 - \frac{\sigma_4}{\sigma_2^2}\right)\left[5\frac{\sigma_4}{\sigma_2^2} - 6 - \frac{1}{3}\frac{\sigma_6}{\sigma_2^3} + 4x\left(3 - \frac{\sigma_4}{\sigma_2^2}\right) - 4v\right], \tag{13}$$

$$
\begin{aligned}
a_5 = {} & 1 - \frac{2}{z}\left(3 - \frac{\sigma_4}{\sigma_2^2}\right) + \frac{1}{4z^2}\left[51 - 37\frac{\sigma_4}{\sigma_2^2} + 5\frac{\sigma_4^2}{\sigma_2^4} + \frac{\sigma_6}{\sigma_2^3} - 6x\left(3 - \frac{\sigma_4}{\sigma_2^2}\right)\right] + \\
& + \frac{1}{4z^3}\left[-42 + 47\frac{\sigma_4}{\sigma_2^2} - 11\frac{\sigma_4^2}{\sigma_2^4} - 3\frac{\sigma_6}{\sigma_2^3} + \frac{\sigma_6\sigma_4}{\sigma_2^5} + x\left(63 - 47\frac{\sigma_4}{\sigma_2^2} + 7\frac{\sigma_4^2}{\sigma_2^4} + \frac{\sigma_6}{\sigma_2^3}\right) - \right. \\
& \left. -4v\left(3 - \frac{\sigma_4}{\sigma_2^2}\right)\right] + \frac{1}{z^4}\left[3 - \frac{9}{2}\frac{\sigma_4}{\sigma_2^2} + \frac{11}{8}\frac{\sigma_4^2}{\sigma_2^4} + \frac{1}{2}\frac{\sigma_6}{\sigma_2^3} - \frac{1}{4}\frac{\sigma_6\sigma_4}{\sigma_2^5} + \frac{1}{120}\frac{\sigma_6^2}{\sigma_2^6} + \right. \\
& + x\left(-12 + 16\frac{\sigma_4}{\sigma_2^2} - 5\frac{\sigma_4^2}{\sigma_2^4} + \frac{1}{3}\frac{\sigma_4^3}{\sigma_2^6} - \frac{1}{2}\frac{\sigma_6}{\sigma_2^3} + \frac{1}{6}\frac{\sigma_6\sigma_4}{\sigma_2^5}\right) + \\
& \left. + \frac{1}{2}(v+u)\left(3 - \frac{\sigma_4}{\sigma_2^2}\right)^2 - \frac{1}{2}w\left(3 - \frac{\sigma_4}{\sigma_2^2}\right)\right], \qquad (14)
\end{aligned}
$$

and

$$\sigma_n \equiv \frac{1}{S^n} \langle (S^z)^n \rangle_0 . \qquad (15)$$

Parameters x, v, z, u, w for cubic lattices are given in Table I.

Table I

	s.c.	b.c.c.	f.c.c.
x	0	0	4
v	4	12	22
z	6	8	12
u	0	0	12
w	0	0	140

In contrast to usual HTSE our coefficients a_n are not constant but depend on D/kT. It appeared, however, that at least up to the 5th order, they are positive, decreasing monotonically with D and limited. Since they depend on D and T only through the moments σ_n and, as it follows from our analysis, the structure of the series closely resembles that of pure Ising model we think that this property will be conserved also for higher order approximations.

III. Determination of T_c

In order to evaluate the Curie temperature we used the ratio method. We assume that susceptibility χ_0 has a singularity at T_c of the form $(T-T_c)^{-\gamma}$ and we are looking for the convergency radius of (8). Using the d'Alambert criterion we obtain the sequence of equations

$$a_n y^n / a_{n-1} y^{n-1} = 1 \tag{16}$$

and solving them for βJ we get the sequence of Curie temperatures

$$\frac{kT_c^{(n)}}{2zJ} = \sigma_2 \frac{a_n}{a_{n-1}} \Big|_{T=T_c^{(n)}} . \tag{17}$$

IV. Results and Discussion

Eqs. (16) have been solved by a computer for three cubic lattices in the whole range of D/J and for different values of S. The results are illustrated on Figures 1-4 and in Tables. Figure 1 presents

$\theta_c = \frac{kT_c}{2zJ}$ versus $1/n$ for a few different values of D/J and

$S = 1{\cdot}5$ for s.c., b.c.c. and f.c.c lattices. We indicated used extrapolation method on Fig. 1 for $D=0$ and $D=\infty$. All the curves closely resemble those of pure Ising model ($D=0$) being only, almost parallelly, shifted with respect to the latter and we see that only very little, if any increase of the slope may be expected for very large D/J. $T_c^{(n)}(0)$ and $T_c^{(n)}(\infty)$ provide, respectively, the lower and the upper limit of $T_c^{(n)}(D/J)$. Comparison with Ising model shows that we may expect in our case the same accuracy of extrapolation i.e. 1%.

The values of θ_c are given for few values of D/J and different S in Table 2 (for f.c.c. lattice). θ_c^{MFA} denotes that of MFA approximation, $\theta_c^{(5)}$ – that obtained from the ratio of the 5th and 4th coefficients and θ_c^{ex} is our extrapolated value. These differ from those obtained from the best extrapolation (see [5]) less than 1%. Another interesting feature of our results is visualized on Figs. 3 and 4 and in Table 3. The Figures contain plot of the ratio $T_c(D)/T_c(0)$ as a function of D/J. We see that for D/J as large as 10, $T_c^{MFA}(D)/T_c^{MFA}(0)$ coincide with $T_c^{ex}(D)/T_c^{ex}(0)$. In Table 3 the ratio $T_c^{ex}(D)/T_c^{MFA}(D)$ is given and we see that this ratio does not depend on D within 1% error up to $D/J = 10$. For $D = \infty$ this ratio deviates from that constant value less than 5%. If we compare this result with those obtained in [3,4] for the Heisenberg model it may be an indication that, in this respect, MFA works better than various decoupling procedures for Green function theories.

We tried to determine the slope of the curves $T_c^{(n)}$ versus $1/n$ (Fig. 1) and find a change of the critical index γ. However, these values may be estimated with smaller accuracy than T_c alone, in our case we were able to determine the slope with 20% error, which gives ~ 4% error for γ. Therefore we cannot definitely conclude does its value change in comparison with pure Ising model or not. It is however remarkable that the slopes estimated in different approximations lie systematically higher than those for $D = 0$ and some small increase in γ may be expected. In Table 4 we give a few numbers to visualize the situation. $\gamma^{(n,m)}$ denote index γ estimated from the slope between n-th and m-th order of approximation.

We see again that no change is observed for D/J as large as 10, a systematic increase of γ for very high D/J, but still within the accuracy of our extrapolation.

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Table 2

Values of $\theta_c = \frac{kT_c}{2zJ}$ for f.c.c. lattice. $\theta_c^{(5)}$ are obtained from a_5/a_4, θ_c^{ex} denotes extralopated values.

S	$\mathcal{D}/J$	0	0.05	0.I	0.5	I	5	I0	50	I00	∞
1	θ_c^{MFA}	0.667	0.667	0.668	0.674	0.680	0.727	0.774	0.947	0.993	I.000
	$\theta_c^{(5)}$	0.594	0.595	0.595	0.600	0.606	0.647	0.688	0.826	0.854	0.857
	θ_c^{ex}	0.570	0.57I	0.572	0.576	0.582	0.622	0.66I	0.790	0.8I4	0.8I6
1.5	θ_c^{MFA}	0.556	0.556	0.557	0.563	0.570	0.62I	0.675	0.899	0.980	I.000
	$\theta_c^{(5)}$	0.50I	0.50I	0.502	0.507	0.5I4	0.560	0.607	0.794	0.848	0.857
	θ_c^{ex}	0.482	0.483	0.483	0.489	0.495	0.539	0.585	0.762	0.809	0.8I6
3	θ_c^{MFA}	0.444	0.445	0.446	0.45I	0.458	0.507	0.560	0.8I0	0.937	I.000
	$\theta_c^{(5)}$	0.404	0.405	0.405	0.4I0	0.4I6	0.46I	0.509	0.726	0.822	0.857
	θ_c^{ex}	0.390	0.39I	0.39I	0.396	0.402	0.446	0.492	0.70I	0.787	0.8I6

Table 3

$T_c^{ex}(\mathcal{D}/J)/T_c^{MFA}(\mathcal{D}/J)$ for cubic lattices

S=1

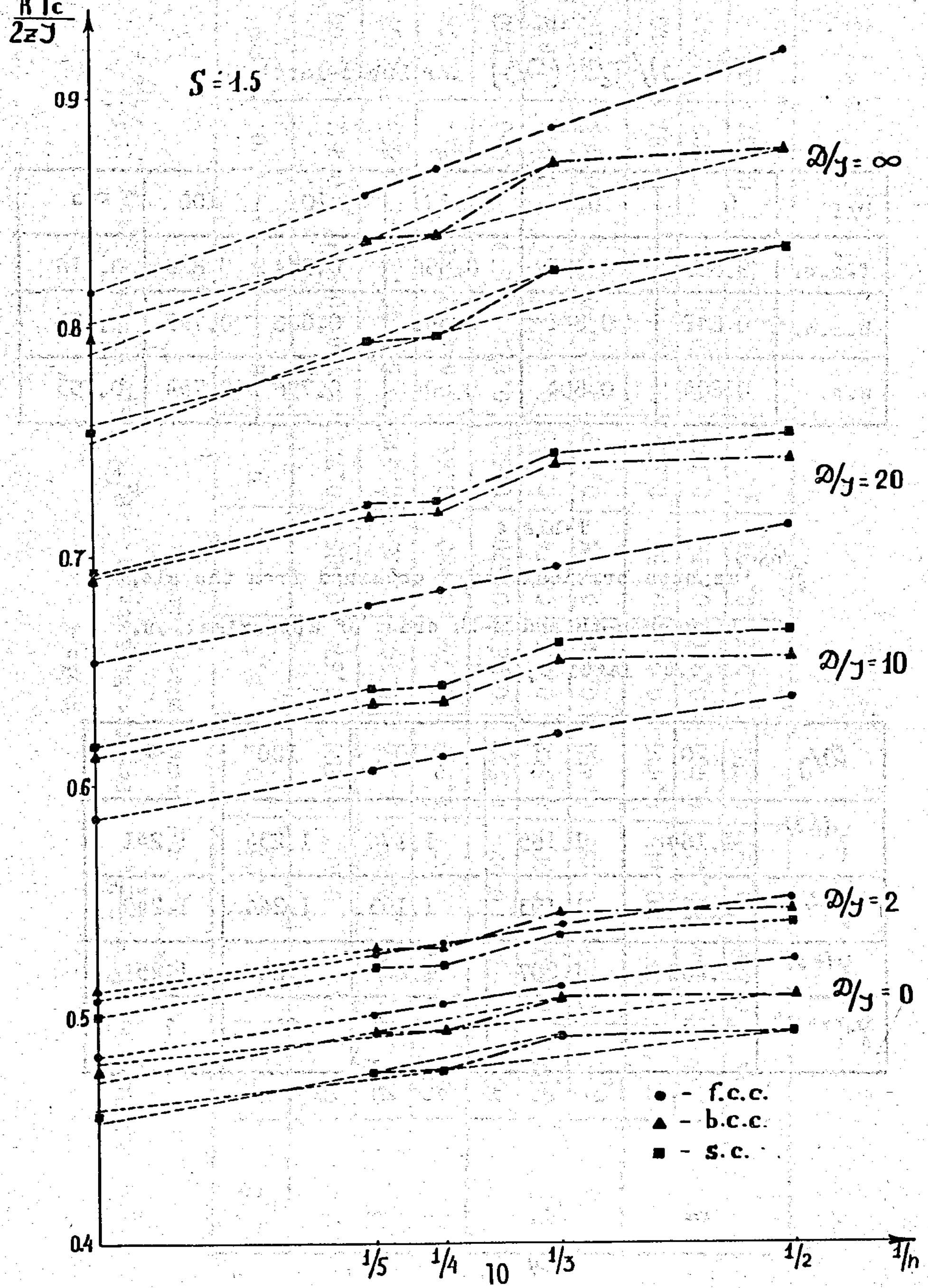
D/I	0	0.I	I	I0	I00	∞
f.c.c.	0.855	0.855	0.856	0.854	0.820	0.8I6
b.c.c.	0.84I	0.84I	0.84I	0.836	0.795	0.795
s.c.	0.804	0.804	0.804	0.796	0.754	0.753

Table 4

$\gamma^{(n,m)}$ denotes critical index obtained from the slope between n-th and m-th order of approximation. F.c.c. lattice, S=1.

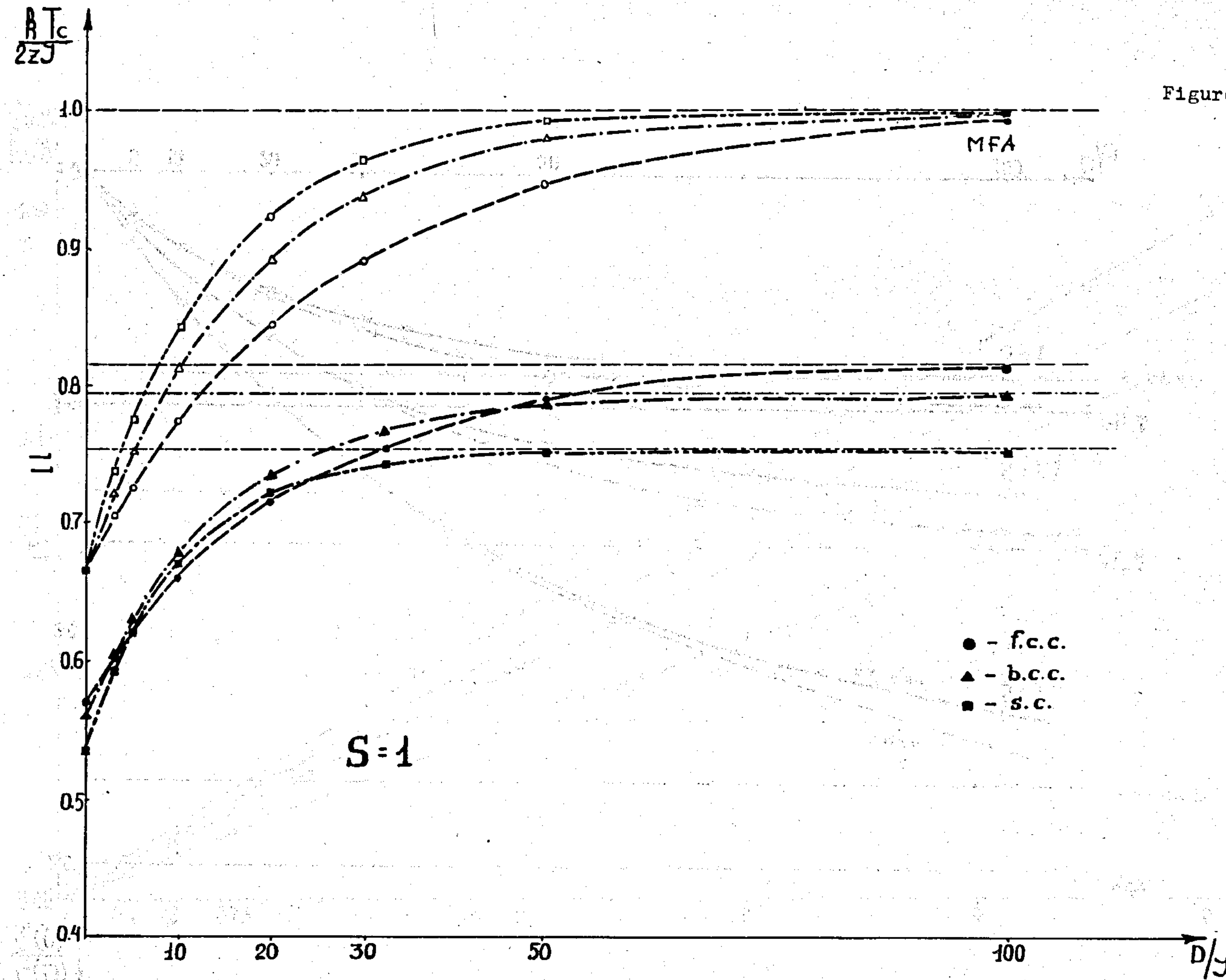
$\mathcal{D}/J$	0	I	I0	I00	∞
$\gamma^{(2,3)}$	I.I64	I.I65	I.I74	I.234	I.24I
$\gamma^{(3,4)}$	I.I93	I.I93	I.I93	I.244	I.249
$\gamma^{(4,5)}$	I.208	I.207	I.204	I.247	I.25I
γ"exact"	I.250	?	?	?	?

Figure 1.

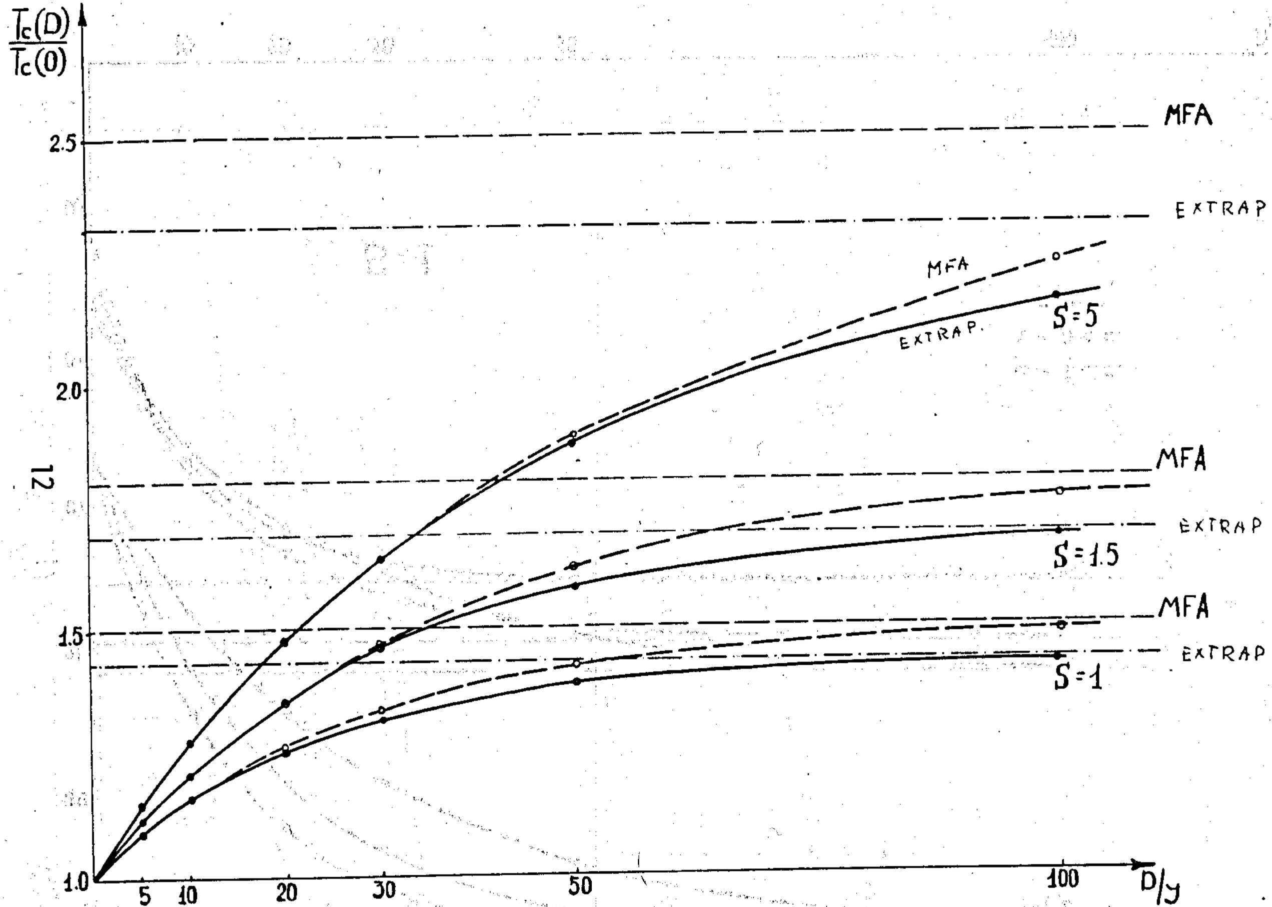


$\frac{k T_c}{2zJ}$
S = 1.5
0.9
0.8
0.7
0.6
0.5
0.4
D/J = ∞
D/J = 20
D/J = 10
D/J = 2
D/J = 0
● – f.c.c.
▲ – b.c.c.
■ – s.c.
1/5
1/4
1/3
1/2
1/h

Figure 2.



$\frac{kT_c}{2zJ}$
1.0
0.9
0.8
0.7
0.6
0.5
0.4
10
20
30
50
100
D/J
MFA
● – f.c.c.
▲ – b.c.c.
■ – s.c.
S = 1



$\frac{T_c(D)}{T_c(0)}$
2.5
2.0
1.5
1.0
MFA
EXTRAP
MFA
EXTRAP.
S=5
MFA
EXTRAP
S=1.5
MFA
EXTRAP
S=1
5
10
20
30
50
100
D/J

Figure 3.

Figure 4.