THEORY OF TRANSITION TEMPERATURE FOR THE ISING MODEL IN d-DIMENSIONS

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ABSTRACT

THEORY OF TRANSITION TEMPERATURE FOR THE

ISING MODEL IN d-DIMENSIONS

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The critical temperatures K_c and the nearest-neighbour correlation functions U_c have been calculated for the d-dimensional hybercubic Ising ferromagnet for d = 4 to d = 30, by generalizing a recent theory reported for d = 3. The results are of relevance for Monte Carlo Renormalization Group work involving critical properties in random fields, which calls for a knowledge of K_c in the limit of zero field. As d becomes large K_c and U_c are found to approach the spherical model values. Polynomial expressions in 1/d are fitted to calculate values, using the analogous spherical model expressions as a guide. Comparison is made with the corresponding expressions of Fisher and Gaunt, those for the spherical model and for the Bethe approximation. An interesting thermodynamic ratio which should be unity in the present theory has been investigated for certain 2 - and 3 - dimensional lattices for which the critical temperatures and the relevant critical correlation functions are known, either exactly or from series analysis. Another ratio, $U_c / (1-K_c)$, which is independent of d for the spherical model, is investigated in the Ising case; it is seen to be approximately independent of lattice structure for d = 2 and also for d = 3. The decomposition method employed in an early work by Frank and Mitran has been re-investigated. Corrections have been made in some of their higher order correlation functions through use of a diagram technique, and an analytic method has been found as a check on these decompositions. The resulting K_c have been recalculated for the cubic lattices.

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INTRODUCTION

The Monte Carlo Renormalization Group (MCRG) method (Swendsen 1979) has recently been used (Rasmussen et al. 1982) to study the d-dimensional hypercubic Ising model in random magnetic fields ($\pm H$), for d = 2, 3 and 4. In this method, it is convenient (though not essential) to have a knowledge of accurate values of the critical temperature K_c (= T_c / T_c (Mean Field) = $4k_B T_c / JZ$, Z being the coordination number) at H = 0. Possible extension of the MCRG work to d > 4 suggests that it would be convenient to have at hand reasonably accurate values for K_c for all values of d, in the limit of zero random magnetic field.

There are several review articles on the Ising model (or more formally Lenz-Ising model). Of interest are Domb (1960) and Brush (1967).

Numerical estimates of K_c have indeed been made, by Fisher and Guant (1964) for d = 4, 5 and 6, by analysis of high-temperature series expansions of the susceptibility. They have, as well, produced (possibly asymptotic) expansions of K_c in powers of the inverse dimensionality, up to d^{-5}. It is not clear how to obtain numerical estimates of K_c from the expansion, especially as a similar expansion for the nearest-neighbour correlation function U_c at the critical temperature (so called because of its relation to the critical energy per spin: U_c = - 2 (energy)/ JNZ = $< S_i S_j >$, i and j being neighbouring sites) proves identical to that for the spherical model up to the term in d^{-5}, whereas the known respective values of U_c (= 0.0827 and 0.08513 respectively) differ by ~ 3%. The 1/d expansion for K_c has been calculated for the spherical model by Gerber and Fisher (1974). That for U_c

is easily derived from it through the spherical model formula $U_c = (1-K_c)^{-4}/4$. The exact Ising 1/d expansion of U_c is easily derived from the appropriate partition function double series of Fisher and Gaunt (1964), coupled with the K_c expansion referred to above.

A recent theory (Frank et al. 1982, to be referred to as FCM) for the Ising ferromagnet near critical point proving capable of predicting values of K_c, U_c and other correlation functions consistent to within 1% with the Monte Carlo data (FCM) for the three-dimensional cubic lattices, it was considered of interest to apply it to the d-dimensional hypercubic case for d = 4, 5,..., 30. In the expectation that this theory ("i - δ theory") would continue, for all values of d, to yield better than 1% accuracy, such a calculation would serve both to provide such values of K_c and U_c, and to check whether the terms up to d^{-5} in the expansion of K_c derived from high-temperature series do indeed give accurate results for d > 4.

In the process of understanding the higher order correlation functions, an early theory of Frank and Mitran (1977) (to be referred to as FM1) was investigated, certain mistakes were found, and corrections were made based on a diagram technique (Appendix E). An analytic method was also discovered which provides an exact check on the results. These correlation function values, though not used in the present work, are presented for the sake of completeness.

In order to organize the theoretically derived data, and for purposes of comparison, 1/d expansions are derived, as well, for K_c and U_c from the numerical results of the i-δ theory. It being considered too difficult to derive these expansions analytically from the theory, the

expansion coefficients are found essentially by fitting the expansion to the data for d = 20 - 30, using the principle that the coefficients must be non-zero rational fractions similar to those one finds in the spherical model expansions. The expansions thus derived are reported and compared with those from series analysis, the spherical model and the Bethe approximation.

In the development of the theory one reaches a point where "A" becomes 1 at critical temperature in zero external field (sec.1). The expression for "A" has indeed been worked out for certain 2 - and 3 - dimensional lattices for which the critical temperatures and the correlation functions required are either known exactly or known from the series analysis (sec.7). (This has been calculated by FCM too, using Monte Carlo techniques for the simple cubic lattice.) It is found that the value of "A" obtained is, to within about 1%, the value predicted by the present theory (except for the case of hydrogen peroxide lattice).

The function $U_c/(1-K_c)$ being exactly 1/4 and thus independent of d for the spherical model, one has also investigated its behavior with d. This behavior demonstrates a dependence on 1/d as strong as that of K_c alone, and so is not reported here. Of interest is that, for d = 3 and different lattice structures, the values of this expansion are clustered around 0.33, while for d = 2 they are clustered around 0.40.

Part of the present work has been presented in a poster session at the 3rd Joint Intermag Magnetism and Magnetic Materials held in Montréal in July, 1982 and published in Journal of Applied Physics (Nath and Frank 1982).

In this thesis the theory of FCM is outlined (sec. 1). Values are presented, in tabular form, for K_c and U_c, for d = 4 to 30 for the i - δ theory and the spherical model, and for d = 4, 5 and 6 from susceptibility series analysis of Fisher and Gaunt (1964) (sec. 1 & sec. 2). The method used for fitting the results of the i - δ theory to a 1/d formula extending to d^{-4} is reported, and the coefficients are presented in tabular form (sec. 4) along with the corresponding expansion coefficients, to d^{-5}, valid for the spherical (sec. 3) and Ising models (sec. 5) and, for comparison, the Bethe approximation (sec. 6). The value of "A" has been obtained in sec. 7 and presented in Table IV for different 2- and 3 - dimensional lattices along with the Monte Carlo results of FCM. In sec. 8 the behavior of $U_c/(1-K_c)$ has been investigated for various Ising lattices. Appendix E has been devoted to the correction of FMI and its extension. Finally a short discussion and the Fortran programme (Appendix F) to calculate K_c and U_c, are also given. The paper "Systematics of d-dimensional hypercubic spin-$\frac{1}{2}$ Ising ferromagnets: Critical temperature and critical energy" by K. Nath and B. Frank is included as Appendix G.

1. CRITICAL TEMPERATURE

THEORY:

The present theory for critical temperatures is essentially based on the i-δ theory proposed by Frank et al. (1982).

The system Hamiltonian considered for the spin - 1/2 Ising ferromagnet is

$$H = -1/2 \sum_i \sum_j J_{ij} S_i S_j - \sum_i h_i S_i \qquad (1)$$

where S_i is the z-component of the spin operator at the ith site of a d-dimensional hypercubic lattice with eigenvalues $\pm 1/2$, J_{ij} is the exchange integral which has the non-zero value, $J>0$, only if i and j are nearest neighbour, and h_i is the (generally non-uniform) external field in the z direction at site i.

The critical point of the 2nd order phase transition is located by the requirement that at $T = T_c$ the zero-field magnetic susceptibility χ approaches infinity

$$\chi \to \infty \qquad (2)$$

as $h_i \to 0$ for all i. An equivalent condition is (Brout 1965)

$$G(q \to 0) \to \infty \qquad (T = T_c) \qquad (3)$$

where G (q) is the Fourier transform of $\langle S_i S_j \rangle$:

$$G(q) = \sum_j \langle S_i S_j \rangle \, e^{i \vec{q} \cdot (\vec{R}_j - \vec{R}_i)} \qquad (4)$$

To find the critical temperature of the system we start by using the identity by Callen (1963) and Suzuki (1965) for the product of the spin operator at site i with any operator $\{ \bar{i} \}$ which is a combination of sums and products of operators that do not include the ith spin operator:

$$< S_i \{ \bar{i} \} > = 1/2 < \{ \bar{i} \} \tanh \frac{\beta(O_i + h_i)}{2} > \qquad (5)$$

where $\beta = \frac{1}{k_B T}$, k_B = Boltzmann constant, T = absolute temperature and $O_i = \sum_j J_{ij} S_j$.

With the choice $\{ \bar{i} \} = S_j$, and $h_k = 0$ for all k, the two-spin correlation function is given by

$$< S_i S_j > = \begin{cases} 1/2 < S_j \tanh \frac{\beta O_i}{2} > , & (j \neq i) \\ 1/4 , & (j = i) \end{cases} \qquad (6)$$

Using

$$< S_i \tanh \frac{\beta O_i}{2} > = 1/2 < \tanh^2 \frac{\beta O_i}{2} > \qquad (7)$$

which comes from (6) with $\{ \bar{i} \} = \tanh \frac{\beta O_i}{2}$,

one obtains, for all j, the exact equation (for $h_k = 0$, all k)

$$< S_i S_j > = 1/2 < S_j \tanh \frac{\beta O_i}{2} > + \delta_{ij} L \qquad (8)$$

where

$$L = 1/4 < \operatorname{sech}^2 \frac{\beta O_i}{2} > \qquad (9)$$

Also in the absence of an external field at $T = T_c$, all odd-order correlation functions vanish i.e.

$$< S_i S_j \; S_k \ldots \; > = 0 \; ; \; n = 0, 1, 2, \qquad (10)$$

$2n + 1$ operators

With the basic assumption (see, e.g. FM1) that

$$< O_i^{2n+1} > \text{ and } < O_i > \; (n = 1, 2, 3 \ldots)$$

approach zero in the same way for $T \to T_c^+, h_k \to 0$,

$$\frac{< S_j \, O_i^{2n+1} >}{< S_j \, O_i >} = R_n \qquad (11)$$

is independent of j (see FCM)

For convenience, one defines a quantity

$$A = \frac{1/2 < S_j \tanh \frac{\beta O_i}{2} >}{\frac{1}{J(o)} < S_j \, O_i >} \qquad (12)$$

which turns out to be site-independent due to the assumption just made, and where

$$J(q) = \sum_j J_{ij} \; e^{i \vec{q} . (\vec{R}_j - \vec{R}_i)} \qquad (13)$$

Putting i for j in (12), which gives better results for d = 3 (as pointed out by Girvin 1978), we get

$$A = \frac{1/2 < \tanh^2 \frac{1}{2}\beta O_i >}{\frac{1}{J(0)} < O_i \tanh \frac{1}{2}\beta O_i >} \tag{14}$$

Now equations (8) & (12) give

$$< S_i S_j > = \frac{A}{J(0)} < S_j O_i > + \delta_{ij} L \tag{15}$$

which from equation (4) turns out to be (see Appendix C)

$$G(q) = \frac{1/4}{\frac{1}{N}\sum_{q'} \left\{ \frac{1}{1 - A \frac{J(q')}{J(0)}} \right\}} \times \frac{1}{\left\{ 1 - A \frac{J(q)}{J(0)} \right\}} . \tag{16}$$

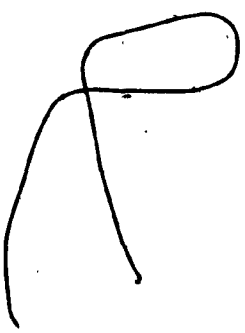
Applying the condition (3) we get at $T = T_c$ in zero external field

$$A = 1 \tag{17}$$

or, from (14),

$$\frac{1/2 < \tanh^2 \frac{1}{2}\beta O_i >}{\frac{1}{J(0)} < O_i \tanh \frac{\beta O_i}{2} >} = 1 \tag{18}$$

Now an attempt is made to find the critical temperature (in terms of a dimensionless quantity $\frac{4}{\beta_c J(0)} = K_c$



(K_c being defined in such a way as to give $K_c = 1$ as the prediction of mean field theory)) which satisfies equation (18).

We use a spin-operator reduction relation (Zhelifonov and Galiullin 1973). It is, for a given Z, an operator identity involving only the O_i and its powers. It expresses the fact that the eigenvalues of O_i/J are Z/2, Z/2-1, ...1,0,-1, ... -Z/2+1, -Z/2, which correspond to having all Z nearest neighbour spins of i pointing up, or Z-1 up and one down,... or Z pointing down. This identity may be written as

$$(O_i^2/J^2)(O_i^2/J^2 - 1^2)(O_i^2/J^2 - 2^2) \ldots (O_i^2/J^2 - Z^2/2^2) = 0 \qquad (19)$$

Due to this reduction relation we may write operator equations like

$$(O_i/J)^{Z+2n} = f_n\{(O_i/J)^Z, (O_i/J)^{Z-2}, \ldots (O_i/J)^2\}, \quad (n = 1,2\ldots) \qquad (20)$$

where f_n is a linear function of $(O_i/J)^Z$, $(O_i/J)^{Z-2}$ ...$(O_i/J)^2$.

Applying (20) to the numerator and denominator of (18), one obtains instead of (18),

$$\frac{A_2 \langle O_i^2/J^2(0)\rangle + A_4 \langle O_i^4/J^4(0)\rangle + \ldots + A_Z \langle O_i^Z/J^Z(0)\rangle}{B_2 \langle O_i^2/J^2(0)\rangle + B_4 \langle O_i^4/J^4(0)\rangle + \ldots \quad B_Z \langle O_i^Z/J^Z(0)\rangle} = 1 \qquad (21)$$

where A_{2n} and B_{2n} ($n = 1, 2, \ldots Z/2$) are explicit functions of β which are determined as follows. One puts $(0_i/J)^2$, in the equation

$$1/2 \tanh^2 \beta 0_i/2 = A_2 \; 0_i^2/J^2(0) + A_4 \; 0_i^4/J^4(0) + \ldots + A_Z \; 0_i^Z/J^Z(0) \tag{22a}$$

(e.g.) equal to its successive eigenvalues $0, 1^2, 2^2, \ldots (Z/2)^2$ and solves the resulting set of $Z/2$ simultaneous equations for A_2, A_4, ... and A_Z. (The eigenvalue zero does not give a non-trivial equation, so it is ignored.) A similar set of $Z/2$ simultaneous equations is used to find the values of B_2, B_4, ... and B_Z as functions of β from the equation.

$$1/J(0) \; 0_i \tanh \beta 0_i/2 = B_2 \; 0_i^2/J^2(0) + B_4 \; 0_i^4/J^4(0) + \ldots B_Z \; 0_i^Z/J^Z(0) \tag{22b}$$

Defining,

$$T_{2n} = \frac{< 0_i^{2n} >}{J^{2n}(0)} \tag{23}$$

allows equation (21) to be rewritten as

$$\frac{A_2T_2 + A_4T_4 + \ldots + A_ZT_Z}{B_2T_2 + B_4T_4 + \ldots + B_ZT_Z} = 1 \tag{24}$$

Now it remains to determine $T_2, T_4 \ldots T_Z$.

T_2 is known:

$$T_2 = < O_i^2 > / J^2(0) = 1/4 \sum_q J^2(q)\ G(q) \ / \ J^2(0) \qquad (25)$$

which becomes at $T = T_c$

$$T_2 = 1/4 \ (1 - 1/F(1)) \qquad (26)$$

(see Appendix B) where F(1), known in the literature as the Watson sum (Watson 1939), is defined by

$$F(1) = \frac{1}{N} \sum_q \frac{1}{1 - \frac{J(q)}{J(0)}} \qquad (27)$$

To find the values of $T_4, T_6 \ldots T_Z$, " i-δ " relations have been proposed by FCM. There one considers a specific chosen nearest neighbour of i. One forms the sum of spin operators at sites neighbouring on i, but excluding that at δ ; this sum may be written $(O_i/J - S_\delta)$. The assumption is now made that, at T_c, as the $h_j \to 0$,

$< (O_i/J - S_\delta)^{2n+1} >$, (n = 1, 2, .. Z/2 - 1) and $< O_i/J - S_\delta >$

approach zero in the same way (see FM1).

One can write then

$$< (O_i/J - S_\delta)^{2n+1} > = Q_n < O_i/J - S_\delta > \qquad (28)$$

Differentiating w.r.t. h_i then let h's $\to$ 0,

one gets

$$Q_n = \frac{<(O_i/J - S_\delta)^{2n+1} S_i>}{<(O_i/J - S_\delta) S_i>} \qquad (29a)$$

Again differentiating w.r.t. h_δ and let h's $\to$ 0,

one has

$$Q_n = \frac{< (O_i/J - S_\delta)^{2n+1} S_\delta>}{< (O_i/J - S_\delta) S_\delta >} \qquad (29b)$$

That uses the l'hopital rule, without saying so. Equations (29a) and (29b) lead to the i-δ relations

$$\frac{< (O_i/J - S_\delta)^{2n+1} S_i >}{< (O_i/J - S_\delta) S_i>} = \frac{< (O_i/J - S_\delta)^{2n+1} S_\delta >}{< (O_i/J - S_\delta) S_\delta>} \quad , n = 1,2,\ldots Z/2 - 1 \qquad (30)$$

The left-hand side of the above equation, when expanded, contains terms like

$$< O_i^{2n+1} S_i > = J^{2m+1}(0)\, U_{2m+2} \tag{31a}$$

and $$< O_i^{2m} S_\delta S_i > = J^{2m}(0)\, U_{2m+2}, \tag{31b}$$

where $0 \leq m$ (integer) $\leq (Z/2 - 1)$, and the U_{2n} have been defined as

$$U_{2n} = \frac{< O_i^{2n-1} S_i >}{J^{2n-1}(0)} \quad , (n = 1, 2, \dots) \tag{32}$$

Use of $S_\delta^2 = I$ has been made, as well as the use of symmetry. The right-hand side of (30) contains terms like

$$< O_i^{2m+1} S_\delta > = J^{2m+1}(0)\, T_{2m+2} \tag{33a}$$

and $$< O_i^{2m} > = J^{2m}(0)\, T_{2m} \tag{33b}$$

Equations (30) then connect successive higher-order correlation functions with lower-order ones. For example, for $n = 1$, (30) connects T_4 & U_4 with T_2 & U_2. For $n = 2$, (30) connects T_6 & U_6 with T_4, U_4, T_2 & U_2. For $n > (Z/2 - 1)$, nothing new is obtained (for then certain spin-operator reduction relations become operative):

At $T = T_c$, it may be shown that

$$U_{2n+2} = T_{2n+2} \quad , \quad (n = 0,1,2, \ldots) \tag{34}$$

(see Appendix D). So in reality, for $n = 1$ equation (30) connects T_4 with T_2, for $n = 2$ equation (30) connects T_6 with T_4 and T_2; etc. Thus one obtains a general expression for T_{2n+2} in terms of T_{2n}, T_{2n-2}, $\cdots$ T_4, T_2 (T_2 being known, all higher-order correlation functions up to T_Z are thus determined). The general relation is found to be:

$$T_{2n+2} = a_n(2Z)^{-(2n+1)} + \sum_{r=1}^{n} \left(a_n \, {}^{2n+1}D_{2r-1} + b_n \, {}^{2n+1}D_{2r} \right) T_{2n+2-2r} \tag{35}$$

where,

$$a_n = \tfrac{1}{2} \left\{ 1 - \left(1 - \frac{2n+1}{Z}\right) \left(1 - \frac{1}{4ZT_2}\right) \left(1 - \frac{1}{Z}\right)^{-1} \right\}^{-1} \tag{36}$$

$$b_n = 2\left(1 - \frac{1}{4ZT_2}\right)\left(1 - \frac{1}{Z}\right)^{-1} a_n \qquad (37)$$

and $^{2n+1}D_r$ is given in terms of the binomial coefficients, $^{n}C_r$ as

$$^{2n+1}D_r = \left(^{2n+1}C_r - {}^{2n+1}C_{r+1}/Z\right)(2Z)^{-r} \qquad (38)$$

Thus from equation (24) (or essentially equation (17)) the critical temperature ($K_c = \frac{4}{\beta_c J(0)}$) may be obtained for any lattice structure and for any spatial dimension, given the value of F(1) (which of course depends on structure and on dimension).

The theory as presented thus far is a recapitulation of the work of FCM, where the calculations were carried out for d = 3 only, for the cubic lattices. For the 3-dimensional cubic lattices (s.c., b.c.c. and f.c.c.) the F(1)'s are known exactly (Watson 1939).

In this thesis, the above theory is applied to the calculation of K_c for the hypercubic lattices for different values of d, from 4 to 30, for which the F(1) (for different values of d) are available (see Appendix C). The values thus obtained for K_c are listed in Table I.

They have been compared with the K_c values for the spherical model and, where possible, with those calculated from high and low-temperature series.

Table I. Values of K_c for the hypercubic Ising lattices for $4 \leq d \leq 30$

d	K_c [i-δ]	K_c (sph.)	$\hat{K}_c$(series)
4	0.84371559	0.80679833	0.83401
5	0.88419452	0.86482139	0.87694
6	0.90737533	0.89528450	0.90227
7	0.92249907	0.91415507	
8	0.93322581	0.92708735	
9	0.94127183	0.93655225	
10	0.94755067	0.94380246	
11	0.95259678	0.94954484	
12	0.95674577	0.95421088	
13	0.96022002	0.95808010	
14	0.96317327	0.96134212	
15	0.96571543	0.96413038	
16	0.96792731	0.96654164	
17	0.96986969	0.96864786	
18	0.97158923	0.97050371	
19	0.97312237	0.97215148	
20	0.97449796	0.97362440	
21	0.97573918	0.97494898	
22	0.97686486	0.97614660	
23	0.97789045	0.97723472	
24	0.97882878	0.97822773	
25	0.97969053	0.97913760	
26	0.98048475	0.97997436	
27	0.98121908	0.98074650	
28	0.98190007	0.98146124	
29	0.98253332	0.98212475	
30	0.98312370	0.98274236	

2. CRITICAL ENERGY

The dimensionless critical energy per spin is defined as

$$U_c = - \frac{\text{critical energy}}{JNZ/2} \tag{39}$$

where N is the total number of sites.

$$U_c = - \frac{\langle H \rangle}{JNZ/2} = \frac{\langle \frac{1}{2} \sum_{ij} J_{ij} S_i S_j \rangle}{JNZ/2}$$

$$\text{or, } U_c = \frac{\langle \sigma_i S_i \rangle}{J(0)} \tag{40}$$

since $J(0) = ZJ$ (from equation (13))

Using the identity(5) we have

$$U_c = \frac{\frac{1}{2} \langle \sigma_i \tanh \frac{1}{2} \beta \sigma_i \rangle}{J(0)} \tag{41}$$

The critical energy U_c at the critical temperature

($K_c = \frac{4}{\beta_c J(0)}$) being the thermal average of (22b),

has already been found. The values are listed in Table II along with those from the spherical model. In order to compare with the spherical model, the relevant spherical model formulas are given in the next section.

In figure 1, K_c and U_c from the present theory have been plotted.

Table II. Values of U_c for the hypercubic Ising lattices for $4 \leq d \leq 30$

d	U_c (i-δ)	U_c (sph.)
4	0.047800991	0.048300418
5	0.033572955	0.033794652
6	0.026060705	0.026178874
7	0.021390376	0.021461234
8	0.018182152	0.018228162
9	0.015830301	0.015861937
10	0.014026669	0.014049384
11	0.012596918	0.012613790
12	0.011434399	0.011447280
13	0.010469914	0.010479974
14	0.0096564603	0.0096644693
15	0.0089609251	0.0089674058
16	0.0083592725	0.0083645911
17	0.0078336161	0.0078380351
18	0.0073703605	0.0073740723
19	0.0069589827	0.0069621306
20	0.0065912068	0.0065938997
21	0.0062604334	0.0062627549
22	0.0059613338	0.0059633493
23	0.0056895580	0.0056913191
24	0.0054415191	0.0054430669
25	0.0052142327	0.0052156003
26	0.0050051955	0.0050064098
27	0.0048122915	0.0048133748
28	0.0046337205	0.0046346908
29	0.0044679405	0.0044688131
30	0.0043136234	0.0043144109

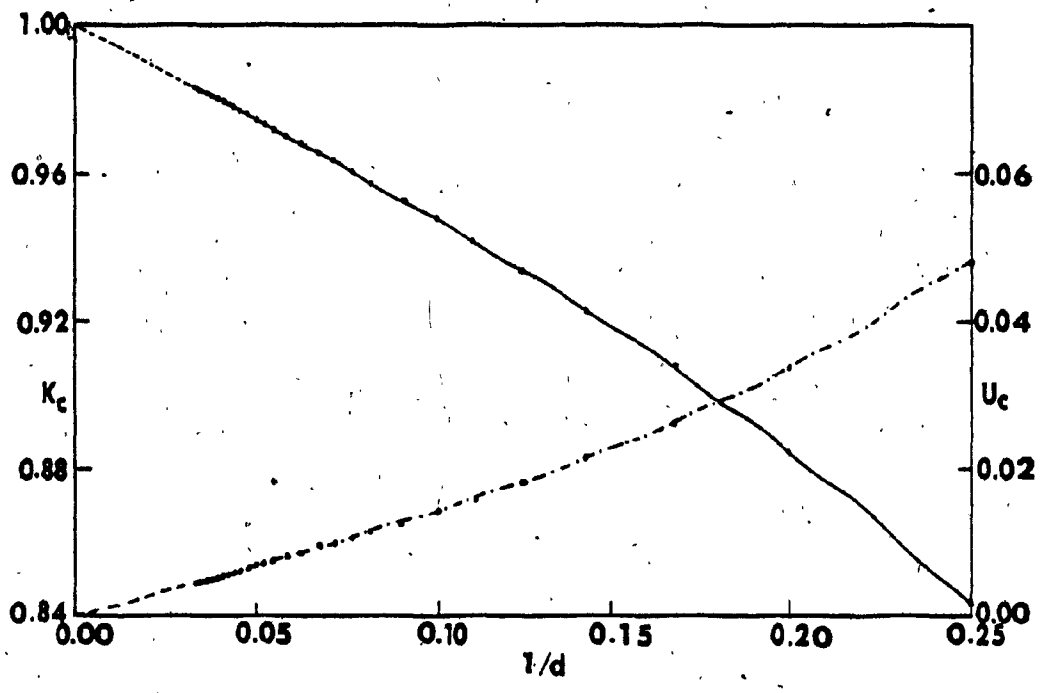


Fig. 1. K_c (——) and U_c (-·-·-)
for the i- δ theory using the
values from Table I and Table II

3. CRITICAL TEMPERATURE AND CRITICAL ENERGY FOR THE SPHERICAL MODEL

In the Berlin-Kac spherical model (Berlin and Kac 1952) one considers a d-dimensional lattice of N interacting "spins" which are allowed to take all values $-\infty < S_i < \infty$, subject to the constraint

$$\sum_i S_i^2 = N/4 \tag{42a}$$

(see Stanley 1971, Joyce 1972, Stanley 1974). That is the spin-dimensionality is considered infinite (where as it is unity for the Ising case).

The critical temperature for the spherical model is given as (Joyce 1972, Barber and Fisher 1973)

$$K_c\,(\text{sph.}) = \frac{1}{F(1)} \tag{42b}$$

where F (1) is the Watson sum (Watson 1939).

For a d-dimensional simple (hyper-) cubic lattice it can be expressed in powers of 1/d (see Appendix C);

$$K_c(\text{sph.}) = \left(1 + \frac{1}{2d} + \frac{3}{(2d)^2} + \frac{12}{(2d)^3} + \frac{60}{(2d)^4} + \ldots\right)^{-1}$$

$$\text{or, } K_c(\text{sph.}) = 1 - \frac{1}{2d} - \frac{1}{2d^2} - \frac{7}{8d^3} - \frac{35}{16d^4} - \frac{215}{32d^5} - \ldots \qquad (43)$$

The critical energy at the critical temperature in zero external field is related to the critical temperature as (Joyce 1972)

$$U_c(\text{sph.}) = \frac{1 - K_c(\text{sph.})}{4} \qquad (44)$$

and for a d-dimensional simple (hyper-) cubic lattice may be expressed in powers of 1/d,

$$U_c(\text{sph.}) = \frac{1}{8d} + \frac{1}{8d^2} + \frac{21}{96d^3} + \frac{105}{192d^4} + \frac{215}{128d^5} \qquad (45)$$

4. ORGANIZATION AND 1/d EXPANSIONS FOR THE VALUES OF K_c and U_c FROM THE PRESENT THEORY

Looking at Tables I and II it appears that the values of K_c and U_c (from "i-δ" theory) approach those for the spherical model in the large d limit. From Figure 1 it appears that U_c approaches zero and K_c approaches 1, the mean field values, as $1/d \to 0$. In order to organize the theoretical data, and for purposes of comparison, one is then led to express K_c and U_c (obtained from the numerical results of the "i-δ" theory) as power series in 1/d. In the process, one must find the coefficients $A_1, A_2, \ldots A_n$ in the series

$$1 - \frac{A_1}{d} - \frac{A_2}{d^2} - \frac{A_3}{d^3} \ldots . \tag{46}$$

for K_c (i-δ), or

$$\frac{A_1}{d} + \frac{A_2}{d^2} + \frac{A_3}{d^3} + \cdots \tag{47}$$

for U_c (i-δ). Attempts were made firstly with help of least-squares technique and secondly by solving 3 or 4 simultaneous equations of the type

$$1 - K_c^{(i-\delta)}\Big|_{d=d_1} = \frac{A_1}{d_1} + \frac{A_2}{d_1^2} + \frac{A_3}{d_1^3} \tag{48a}$$

$$1 - K_c^{(i-\delta)} \Big|_{d=d_2} = \frac{A_1}{d_2} + \frac{A_2}{d_2^2} + \frac{A_3}{d_2^3} \qquad (48b)$$

$$1 - K_c^{(i-\delta)} \Big|_{d=d_3} = \frac{A_1}{d_3} + \frac{A_2}{d_3^2} + \frac{A_3}{d_3^3} \qquad (48c)$$

with different combinations of values for d_1, d_2 and d_3. These attempts failed to provide consistent values for A_j ($j = 1, 2, \ldots$).

To take proper account of the asymptotic nature of the expansion, it is found preferable to adopt the following procedure (illustrated here for the K_c data):

(i) One forms the equation

$$\ln(1-K_c) \simeq \ln A_n - n \ln d \quad , \text{ (large d)} \qquad (49)$$

considering A_n and n as unknowns.

(ii) One chooses a pair of neighbouring d-values (d = 10 and 11, say) and the corresponding pair of K_c - values and solves equation (49) for A_n and n.

(iii) One repeats procedure (ii) for all neighbouring pairs d and d + 1 up to d = 29.

(iv) One plots the resulting A_n and n vs. 1/d.

(v) One extrapolates these curves to 1/d = 0. n will extrapolate to a value very close to 1, and is to be taken as 1. A_n will extrapolate to a value A_1^G which is to be guessed at, initially.

(vi) One forms the equation

$$\ell n \left(1-K_c - \frac{A_1^G}{d^1}\right) \simeq \ell n\, A_n - n\, \ell n\, d \qquad (50)$$

(vii) One proceeds as in procedures (ii) through (iv), using equation (50) now, to construct the curves for the new A_n and n, both vs. 1/d.

(viii) One extrapolates these curves to 1/d = 0. If A_1^G has not been guessed properly, n will extrapolate to a value which is either not an integer, or which is an integer $n \neq 2$. It turns out that the value of the extrapolated n is extremely sensitive to the value of A_1^G (a typical illustration is given in Figure 2). Using the spherical model expansion (given in section (3)) as a guide, one tries to find A_1^G as a simple rational fraction, now called A_1 , which allows for n to extrapolate to a value very close to 2.

(ix) One guesses a value for the extrapolated A_n, now called A_2^G , and proceeds from (vii), mutatis mutandis.

(x) One eventually reaches a value $N_{max} \equiv M$ such that when the equation

$$\ell n \left[1 - K_c - \sum_{j=1}^{M} \frac{A_j}{d^j} - \frac{A^G_{M+1}}{d^{M+1}} \right] = \ell n\, A_n - n\, \ell n d \qquad (51)$$

is formed, the curve of n vs. 1/d fluctuates in such a way (it does so because one retains data accurate to a limited number of significant figures, depending upon the computer time available) that extrapolation is completely unreliable for all reasonable A^G_{M+1}.
In our particular case of equation (46) (or equation (47), we find that M = 4. A knowledge of K_c to a greater number of significant figures would probably lead to an increase in the value of M.

In Table III are presented the results of this procedure for K_c and U_c , along with the respective coefficients for the spherical model (sec. 3), the series values for the Ising model (sec. 5) and those from the Bethe approximation (sec. 6).

Table III. Values of A_n in the expansion $\sum_{j=0} a_j\, d^{-j}$ of K_c and U_c

n	0	1	2	3	4	5
K_c (series)	1	$-\frac{1}{2}$	$-\frac{1}{3}$	$-\frac{13}{24}$	$-\frac{979}{720}$	$-\frac{2009}{480}$
K_c(sph.)	1	$-\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{7}{8}$	$-\frac{35}{16}$	$-\frac{215}{32}$
K_c (i-δ)	1	$-\frac{1}{2}$	$-\frac{1}{6}$	$-\frac{5}{8}$	$-\frac{83}{96}$	---
K_c (Bethe)	1	$-\frac{1}{2}$	$-\frac{1}{12}$	$-\frac{1}{24}$	$-\frac{19}{720}$	$-\frac{89}{480}$
U_c(series)	0	$\frac{1}{8}$	$\frac{1}{8}$	$\frac{21}{96}$	$\frac{105}{192}$	$\frac{215}{128}$
U_c(sph.)	0	$\frac{1}{8}$	$\frac{1}{8}$	$\frac{21}{96}$	$\frac{105}{192}$	$\frac{215}{128}$
U_c(i-δ)	0	$\frac{1}{8}$	$\frac{1}{8}$	$\frac{19}{96}$	$\frac{103}{192}$	---
U_c (Bethe)	0	$\frac{1}{8}$	$\frac{1}{16}$	$\frac{1}{32}$	$\frac{1}{64}$	$\frac{1}{128}$

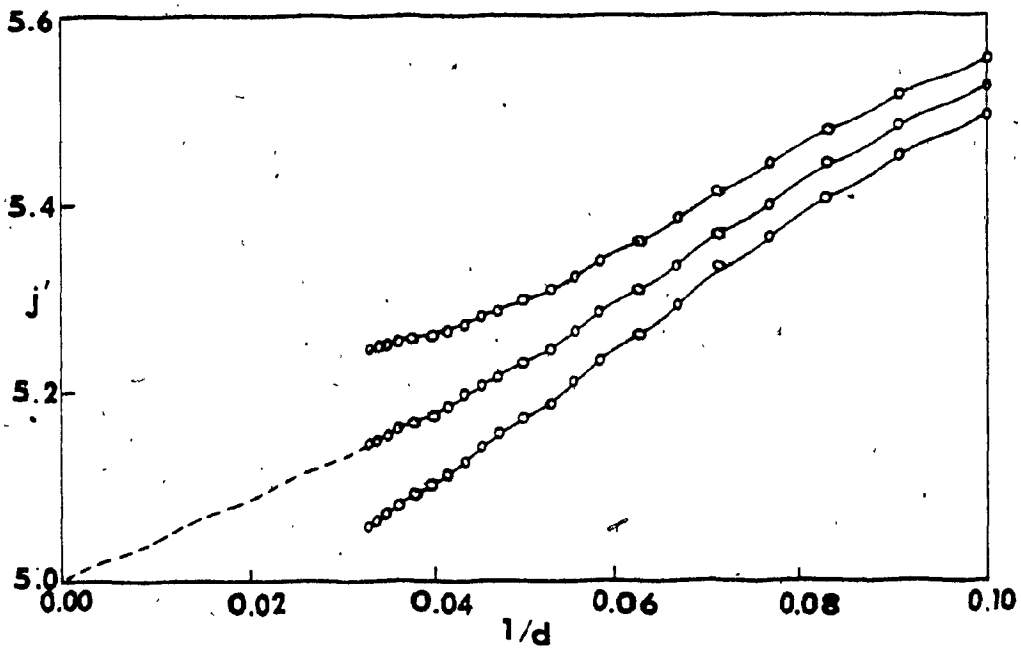


Fig. 2. Sensitivity of the extrapolated value of n to various guessed values of A_j^G (j is integer). Here, j = 4. A_j^G = 52/96, 51.5/96, and 51/96 for the upper, middle and lower curves respectively from the data for U_c (i-δ).

5. SERIES EXPANSIONS FOR THE CRITICAL TEMPERATURE AND THE CRITICAL ENERGY FOR THE ISING MODEL

The critical temperature $K_c \left\{ = \frac{4}{\beta_c J(0)} \right\}$ has been given as (Fisher and Gaunt 1964)

$$K_c(\text{series}) = 1 - \frac{1}{2d} - \frac{1}{3d^2} - \frac{13}{24d^3} - \frac{979}{720d^4} - \frac{2009}{480d^5} \qquad (52)$$

The partition function Z is given by (Fisher and Gaunt 1964)

$$\ell nZ = \ell n2 + \frac{1}{4q} K^{-2} + \frac{1}{8q^2} K^{-4} + \frac{1}{q^3}\left(-\frac{7}{24} K^{-4} + \frac{1}{3} K^{-6} \right)$$

$$+ \frac{1}{q^4}\left(-\frac{23}{12} K^{-6} + \frac{27K^{-8}}{16} \right) + \frac{1}{q^5}\left(\frac{113K^{-6}}{45} - \frac{415}{24} K^{-8} + \frac{62K^{-10}}{5} \right) + \ldots \qquad (53)$$

where $K = \frac{4}{\beta J(0)} = \frac{4}{\beta J q}$ and $q = 2d$.

Now it is easy for one to obtain the critical energy per spin U_c (defined in equation (39)), from equation (53):

$$U_c = \frac{1}{dJ} \frac{\partial}{\partial \beta} (\ell nZ)\Big|_{K=K_c} \qquad (54)$$

$$\text{or, } U_c = \frac{1}{8d} + \frac{1}{8d^2} + \frac{7}{64d^3} + \frac{35}{64d^4} + \frac{215}{128d^5} \qquad (55)$$

6. BETHE APPROXIMATION FOR THE CRITICAL TEMPERATURE AND THE CRITICAL ENERGY FOR THE ISING MODEL

The Bethe approximation (Bethe 1935) is a first-order approximation (or a "closed form" approximation). It takes exact account of the interaction of a given spin with its nearest neighbours, but uses a "mean field" to take account of the interactions of these neighbours with other spins of the lattice (Domb 1960, Burley 1972).

The critical temperature K_c ($= 4/\beta_c J(0)$) from the Bethe approximation is given by (Domb 1960)

$$K_c(\text{Bethe}) = \frac{-2/q}{\ln\left(1 - \frac{2}{q}\right)}, \quad (q > 2) \tag{56}$$

where q is the coordination number, equal to 2d for the d-dimensional (hyper-) cubic lattices. After proper expansion of the logarithmic term and taking its reciprocal, it turns out that

$$K_c(\text{Bethe}) = 1 - \frac{1}{2d} - \frac{1}{12d^2} - \frac{1}{24d^3} - \frac{19}{720d^4} - \frac{89}{480d^5} \cdots \tag{57}$$

The critical energy per spin U_c (defined in equation (39)) is given as (Domb 1960)

$$U_c\ (\text{Bethe}) = -\{1/(NJd)\}\{-NqJ/(8(q-1))\} \tag{58}$$

$$\text{or, } U_c\ (\text{Bethe}) = \frac{1}{8d} + \frac{1}{16d^2} + \frac{1}{32d^3} + \frac{1}{64d^4} + \frac{1}{128d^5} + \frac{1}{256d^6} + \cdots \tag{59}$$

7. THE VALUE OF "A" AT CRITICAL TEMPERATURE IN ZERO EXTERNAL FIELD FROM EXACT CALCULATION FOR CERTAIN 2-DIMENSIONAL LATTICES, AND FROM SERIES FOR THE HYDROGEN PEROXIDE LATTICE

We have the equation (17)

$$A = 1 \tag{17}$$

at critical temperature in zero external field. In the present theory for the critical temperature, one has used the expansion (14) for A;

$$A = \frac{\frac{1}{2}\langle S_i \tanh\frac{1}{2}\beta O_i \rangle}{1/J(0)\langle S_i O_i \rangle} = \frac{\frac{1}{2}\langle \tanh^2 \frac{1}{2}\beta O_i \rangle}{1/J(0)\langle O_i \tanh\frac{1}{2}\beta O_i \rangle} \tag{14}$$

which comes from the equation (12). Changing A to A' for the present purpose one can re-write (12) with the choice j = a neighbour of i, as

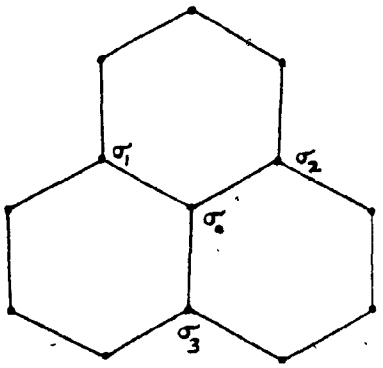
$$A' = \frac{\frac{1}{2}\langle S_j \tanh\frac{1}{2}\beta O_i \rangle}{1/J(0)\langle S_j O_i \rangle} = \frac{\frac{1}{2}\langle O_i \tanh\frac{1}{2}\beta O_i \rangle}{1/J(0)\langle O_i^2 \rangle} \tag{12a}$$

The values of A and A' computed, using the Monte Carlo techniques (FCM) for the 3-dimensional simple cubic lattice are approximately 1% off the theoretically predicted value of 1 for both cases.

Another check on equation (17) is provided by the availability of exact values for the critical temperature and certain correlation functions for some two-dimensional lattices. This is of interest even though the FCM theory, as it stands, is not applicable to the two-dimensional lattices. A still further check may be provided by the 3-dimensional hydrogen peroxide lattice, for which K_c and U_c are known from series (Leu et al. 1969 and Domb 1974) and the correlation functions going into (17) may be calculated exactly from theory.

The values of A and A' are here calculated for the honeycomb, simple quadratic and plane triangular 2-dimensional lattices and for the hydrogen peroxide 3-dimensional lattice.

(i) The honeycomb lattice (Z = 3):



$$\frac{O_i}{J(0)} = \frac{J(S_1+S_2+S_3)}{ZJ} = \frac{J(\sigma_1+\sigma_2+\sigma_3)}{2ZJ} \qquad (60)$$

Where sites 1, 2, and 3 are nearest neighbours to site 0 (one takes site i to be identical with site 0). Here the σ's have eigenvalues +1 and -1. Defining ϑ_i as the sum of σ-operators neighbouring site i,

$$\theta_i = \sigma_1 + \sigma_2 + \sigma_3 \tag{61}$$

one can write

$$\frac{O_i}{J(0)} = \frac{\theta_i}{2Z} \tag{62}$$

or,

$$\frac{O_i}{J(0)} = \frac{\theta_i}{6} \tag{63}$$

Due to the spin-operator reduction relation (cf. Sec.1),

$$(\theta_i^2 - 3^2)(\theta_i^2 - 1^2) = 0 \tag{64}$$

one can write (14) as

$$A = \frac{(1/2) < \tanh^2 [(\beta J(0)/12)\ \theta_i] >}{<(\theta_i/6)\ \tanh[(\beta J(0)/12)\theta_i] >} = \frac{x_1 < \theta_i^2 > + y_1}{x_2 < \theta_i^2 > + y_2} \tag{65}$$

the x_1, y_1, etc. being functions of β to be determined. The procedure is the same as the one outlined in section 1. One solves the following four equations (two for the numerator and two for the denominator of equation (65)),

$$(1/2)\ \tanh^2 [(\beta J(0)/12) \times 1\ ] = x_1 + y_1\ , \tag{66a}$$

$$(1/2)\ \tanh^2 [(\beta J(0)/12) \times 3\ ] = 9x_1 + y_1\ , \tag{66b}$$

$$(1/6)\ \tanh\left[(\beta J(0)/12) \times 1\right] = x_2 + y_2 \qquad (66c)$$

and $$(3/6)\ \tanh\left[(\beta J(0)/12) \times 3\right] = 9\,x_2 + y_2 \qquad (66d)$$

to get

$$\left.\begin{aligned} x_1 &= 1/27 \\ y_1 &= 7/54 \\ x_2 &= y_2 = 1/(12\sqrt{3}) \end{aligned}\right\} \qquad (67)$$

where use has been made of (Domb 1974)

$$\tanh(\beta J(0)/12) = 1/(\sqrt{3}) \qquad (68)$$

Using the identity (cf. sec. 1)

$$\langle \sigma_i \{ \bar{i} \} \rangle = \langle \{ \bar{i} \} \tanh[\beta J(0)/12)\ \theta_i] \rangle \qquad (69)$$

and putting θ_i for $\{ \bar{i} \}$, one gets

$$\langle \sigma_i \theta_i \rangle = \langle \theta_i \tanh[(\beta J(0)/12)\ \theta_i] \rangle \qquad (70)$$

or, $$3 \langle \sigma_o \sigma_1 \rangle = 6 \left[x_2 \langle \theta_i^2 \rangle + y_2 \right] \qquad (71)$$

using the denominator of equation (65).

Since, (see Syozi 1972)

$$\langle \sigma_o \sigma_1 \rangle = 4/(3\sqrt{3}) \qquad (72)$$

(71) leads to

$$< \theta_i^2 > \; = 7 \tag{73}$$

Substituting (73) into (65), one has the value for A:

$$A = 7/(4\sqrt{3}) = 1.01036 \text{ (H.C. lattice)} \tag{74}$$

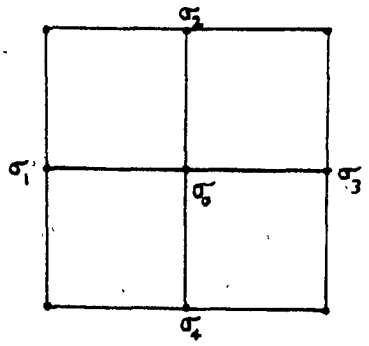
A′ can be obtained in a similar fashion,

$$A' = \frac{(1/2)<(\theta_i/6) \tanh [(\beta J(0)/12)\ \theta_i]>}{(1/6^2) < \theta_i^2>} \tag{75}$$

$$\text{or } A' = \frac{4\sqrt{3}}{7} = 0.98974 \tag{76}$$

Note that A A′ = 1 for this case.

(ii) The simple quadratic lattice:



Here Z = 4, so the equation (62) becomes

$$O_i/J(0) = \theta_i/(2Z) = \theta_i/8 \tag{77}$$

and the spin-operator reduction relation takes the form

$$(\theta_i^2 - 4^2) (\theta_i^2 - 2^2) = 0 \tag{78}$$

So one can write for A

$$A = \frac{(1/2) < \tanh^2 [(\beta J(0)/16)\theta_i] >}{<(\theta_i/8) \tanh[(\beta J(0)/16)\theta_i] >} = \frac{x_1 < \theta_i^4 > + y_1 < \theta_i^2 >}{x_2 < \theta_i^4 > + y_2 < \theta_i^2 >} \qquad (79)$$

One has (Domb 1974)

$$\tanh [\beta J(0)/16] = 1/(1+\sqrt{2}) \qquad (80)$$

from which one gets

$$\left.\begin{aligned} x_1 &= -5/(192 \times 9) \\ y_1 &= 2/27 \\ x_2 &= -1/(8 \times 72\sqrt{2}) \\ y_2 &= 5/(8 \times 9\sqrt{2}) \end{aligned}\right\} \qquad (81)$$

The two and four spin correlation functions are given as (Fisher 1963)

$$\left.\begin{aligned} <\sigma_0 \sigma_1> &= 1/\sqrt{2} \\ <\sigma_1 \sigma_2> &= 2/\Pi \\ <\sigma_1 \sigma_3> &= 1 - 4/\Pi^2 \\ <\sigma_1 \sigma_2 \sigma_3 \sigma_4> &= (4/\Pi)^2 (\Pi - 1) - 3 \end{aligned}\right\} \qquad (82)$$

So,

$$< \theta_i^2 > = <(\sigma_1+\sigma_2+\sigma_3+\sigma_4)^2 >$$

$$= 4< \sigma_1^2 > + 8 < \sigma_1\sigma_2> + 4 < \sigma_1\sigma_3 >$$

Or $< \theta_i^2 > = 11.47181924 \qquad (83)$

and $< \theta_i^4 > = 40 + 128 < \sigma_1\sigma_2> + 64 < \sigma_1\sigma_3> + 24 < \sigma_1\sigma_2\sigma_3\sigma_4> = 170.8727696$ (84)

Finally one gets the value of A as (from equation (79))

$$A = 0.355340865/0353553391 = 1.0050557 \quad (85)$$

[The denominator of A can be found in a different way also, giving the same result.

$$< \sigma_1\theta_i > = < \theta_i \tanh((\beta J(0)/16)\theta_i)>$$

or, $4 < \sigma_0\sigma_1 > = 8 \times A_D$, (A_D = denominator of A)

or, $A_D = 1/(2\sqrt{2}) = 0.3535533391$ (86)]

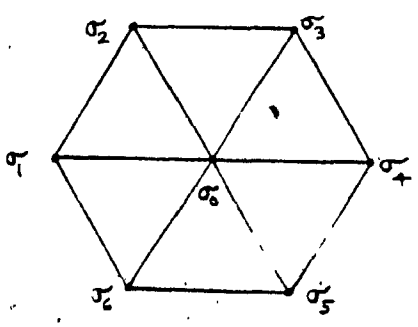
Now,

$$A = \frac{(1/2) <(O_i/J(0)) \tanh (\beta O_i/2)>}{<(O_i/J(0))^2>}$$

$$= \frac{(1/2) <(\theta_i/8) \tanh[(\beta J(0)/16)\theta_i]>}{(1/64)<\theta_i^2>} \quad (87)$$

so that $A = (1/2) \times 0.353553391/((1/64) \times 11.47181924) = 0.9862175$ (88)

(iii) The plane triangular lattice:



Here Z = 6 so that one has from equation (62)

$$O_i/J(0) = \theta_i/(2Z) = \theta_i/12 \tag{89}$$

From Stephenson (1964) we have

$$\left.\begin{aligned} &\langle \sigma_0\sigma_1 \rangle = \langle \sigma_1\sigma_2 \rangle = 2/3 \\ &\langle \sigma_1\sigma_3 \rangle = 0.5813215 \\ &\langle \sigma_1\sigma_4 \rangle = 0.56192357 \\ &\langle \sigma_1\sigma_2\sigma_3\sigma_4 \rangle = -0.48763512 \\ &\langle \sigma_1\sigma_2\sigma_3\sigma_5 \rangle = -0.45641434 \\ &\langle \sigma_1\sigma_2\sigma_4\sigma_5 \rangle = 0.47425596 \\ &\langle \sigma_1\sigma_2\sigma_3\sigma_4\sigma_5\sigma_6 \rangle = 0.39315517 \end{aligned}\right\} \tag{90}$$

and $\tanh(\beta J(0)/24) = 2 - \sqrt{3}$ (91)

Due to the spin-operator reduction relation

$$(\theta_i^2 - 6^2)(\theta_i^2 - 4^2)(\theta_i^2 - 2^2) = 0 \tag{92}$$

one can write

$$A = \frac{(1/2)\langle \tanh^2[(\beta J(0)/24)\theta_i] \rangle}{\langle (\theta_i/12) \tanh[(\beta J(0)/24)\theta_i] \rangle} \tag{93}$$

$$= \frac{x_1\langle \theta_i^6 \rangle + x_2\langle \theta_i^4 \rangle + x_3\langle \theta_i^2 \rangle}{(1/12)\langle \theta_i \tanh[(\beta J(0)/24)\theta_i] \rangle} \tag{94}$$

wherin

$$\left.\begin{aligned} x_1 &= 1.6758787 \times 10^{-5} \\ x_2 &= -1.2726757 \times 10^{-3} \\ x_3 &= 3.6072562 \times 10^{-2} \end{aligned}\right\} \tag{95}$$

One also gets

$$\langle \theta_i^2 \rangle = 6 + 2[\, 6 \langle \sigma_1\sigma_2 \rangle + 6 \langle \sigma_1\sigma_3 \rangle + 3 \langle \sigma_1\sigma_4 \rangle] = 24.347399, \quad (96)$$

$$\langle \theta_i^4 \rangle = 96 + 56\,[\, 6 \langle \sigma_1\sigma_2 \rangle + 6 \langle \sigma_1\sigma_3 \rangle + 3 \langle \sigma_1\sigma_4 \rangle]$$

$$+ 24\,[\, 6 \langle \sigma_1\sigma_2\sigma_3\sigma_4 \rangle + 6 \langle \sigma_1\sigma_2\sigma_3\sigma_5 \rangle + 3 \langle \sigma_1\sigma_2\sigma_4\sigma_5 \rangle]$$

$$= 779.81673 \quad (97)$$

$$\text{and } \langle \theta_i^6 \rangle = 2256 + 1712\,[\, 6 \langle \sigma_1\sigma_2 \rangle + 6 \langle \sigma_1\sigma_3 \rangle + 3 \langle \sigma_1\sigma_4 \rangle]$$

$$+ 1200\,[\, 6 \langle \sigma_1\sigma_2\sigma_3\sigma_4 \rangle + 6 \langle \sigma_1\sigma_2\sigma_3\sigma_5 \rangle + 3 \langle \sigma_1\sigma_2\sigma_4\sigma_5 \rangle]$$

$$+ 720 \langle \sigma_1\sigma_2\sigma_3\sigma_4\sigma_5\sigma_6 \rangle$$

$$= 26748.923 \quad (98)$$

thereby having the value of the numerator of A,

$$A_n = 0.33409876 \quad (99)$$

The denominator of A is obtained very easily;

$$\langle \sigma_i\theta_i \rangle = \langle \theta_i \tanh[(\beta J(0)/24)\theta_i] \rangle \quad (70)$$

or, $6 \langle \sigma_0\sigma_1 \rangle = 12\, A_D$

or, using (90), $A_D = (6/12)\times(2/3) = 0.3333$

giving

$$A = 1.002296 \quad (100)$$

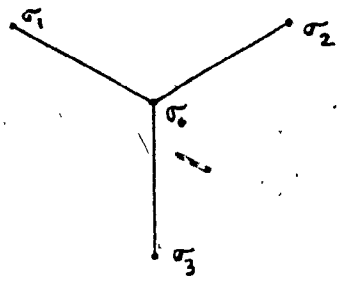
Now,

$$A' = \frac{(1/2) \langle (\theta_i/12) \tanh[(\beta J(0)/24)\theta_i] \rangle}{(1/144) \langle \theta_i^2 \rangle} \quad (101)$$

$$\text{or, } A = \frac{(1/2) \times (1/3)}{(1/144) \times 24.347397} = 0.9857315 \qquad (102)$$

(iv) The hydrogen peroxide lattice:

The hydrogen peroxide lattice is a 3-dimensional lattice with the coordination number equal to 3. The site under consideration and all the three nearest neighbours are in the same plane.



Here,

$$\theta_i/J(0) = \theta_i/(2Z) = \theta_i/6 \qquad (103)$$

One has from a series calculation (Leu et al. 1969 and Domb 1974)

$$\tanh(\beta J(0)/12) = 0.51814 \qquad (104)$$

and $$\langle \sigma_0\sigma_1 \rangle = 0.55769 \qquad (105)$$

Due to the spin operator reduction relation, one has

$$A = \frac{\langle (1/2) \tanh^2[(\beta J(0)/12)\ \theta_i] \rangle}{\langle (\theta_i/6) \tanh[(\beta J(0)/12)\ \theta_i] \rangle} = \frac{x_1 \langle \theta_i^2 \rangle + y_1}{x_2 \langle \theta_i^2 \rangle + y_2} \qquad (106)$$

and finds

$$\left.\begin{aligned} x_1 &= 0.038214 \\ y_1 &= 0.047832 \\ x_2 &= 0.09602 \\ y_2 &= 0.038524 \end{aligned}\right\} \qquad (107)$$

Also, the identity

$$< \sigma_i \theta_i > \; = < \theta_i \tanh [(\beta J(0)/12)\ \theta_i] > \qquad (70)$$

leads to

$$3 < \sigma_0 \sigma_1 > \; = 6 \; [\; x_2 < \theta_i^{\,2} > + y_2 \;] \qquad (108)$$

So that,

$$< \theta_i^{\,2} > \; = 5.0243 \qquad (109)$$

Thus

$$A = 0.28802/0.27885 \; = \; 1.033 \qquad (110)$$

and

$$A' = \frac{(1/2) < (\theta_i/6) \tanh [(\beta J(0)/12)\ \theta_i] >}{(1/36) \;\; < \theta_i^{\,2} >} \qquad (111)$$

$$\text{or,} \quad A' = 18 \; \times 0.27885/\; 5.0243 \; = 0.999 \qquad (112)$$

The values of A and A' have been written down in Table IV (Monte Carlo values have been estimated from the graph of FCM).

Looking at Table IV one finds that the values of A for different

lattices are closer to 1 than those of A′ except for the hydrogen peroxide lattice, where the reverse is true. But then those for the hydrogen peroxide are based on the series values so that firm conclusions can not yet be reached. For the case of the honeycomb lattice one finds that the product of A and A′ is exactly 1.

It is hoped that, since the A = 1 aspect of the FCM theory holds for the 2-dimensional lattices, the theory may yet be generalized to cover the 2-dimensional case.

Table IV. Values A and A′ for the simple cubic (SC), honycomb (HC), simple quadratic (SQ), plane triangular (PT) and hydrogen peroxide (HP) lattices, as given in section 7.

Lattices	A	A′
SC	1.007±0.003	0.990±0.003
HC	1.01036	0.98974
SQ	1.00506	0.98622
PT	1.0023	0.98573
HP	1.033	0.999

8. INVESTIGATION OF THE FUNCTION $U_c/(1-K_c)$ FOR VARIOUS ISING LATTICES.

From the equation (44) it is obvious that

$$\frac{U_c}{1-K_c} = 1/4 \qquad (44a)$$

for the spherical model, independent of the dimensionality d.

It is considered worth investigating the behaviour of this function for certain chosen 2- and 3-dimensional lattices for which K_c and U_c are known. In Table V are presented values of K_c, U_c and $U_c/(1-K_c)$, constructed from Syozi (1972) and Domb (1974), for various lattices. The values of $U_c/(1-K_c)$ appear to be clustered about 0.33 and about 0.40 for d = 3 and d = 2 lattices respectively.

Table V K_c, U_c and $U_c/(1-K_c)$ for the honeycomb (HC), simple quadratic (SQ), plane triangular (PT), Kagomé (K), diced (D), simple cubic (SC), body-centered cubic (BCC), face-centered cubic (FCC), diamond (DIA), hydrogen peroxide (HP) and hyper-triangular (HTr) lattices.

Lattices	d	Z	K_c	U_c	$U_c/(1-K_c)$
HC	2	3	0.50622	0.19245	0.3897
SQ	2	4	0.5673	0.17678	0.4085
PT	2	6	0.60683	0.16667	0.4239
K	2	4	0.53583	0.186	0.4007
D	2	4**	0.6014	0.16708	0.4191
SC	3	6	0.7518	0.082698	0.3332
BCC	3	8	0.79416	0.068298	0.3318
FCC	3	12	0.81627	0.061873	0.3368
DIA	3	4	0.6761	0.10919	0.3371
HP	3	3	0.58093	0.13942	0.3327
HTr	3	6	0.73795	0.084127	0.3210
SC(i-δ)*	3	6	0.7564	0.08368	0.3436
BCC(i-δ)*	3	8	0.7926	0.06958	0.3355
FCC(i-δ)*	3	12	0.8121	0.06334	0.3371

* Values have been taken from FCM.

** The diced lattice has average coordination number four.

DISCUSSION

It is seen from Tables I, II, and III that (i) the coefficients in the U_c (series) and U_c (spherical) expansions (Table III) are equal; nevertheless, the value of U_c (i-δ) is closer to U_c (series) than is U_c (spherical) for d=3 (FCM); (ii) the coefficients in the i-δ and series expansions in Table III do not greatly differ as the power of 1/d continues to increase; this is reminiscent of diagram expansions wherin certain classes of diagrams are neglected (Burley 1972); (iii) the i-δ theory values of K_c and U_c are consistent with the series values to within 1% for $4 \leq d \leq 6$; (iv) K_c(spherical) and K_c (i-δ) approach each other much faster than either one approaches the Mean Field Value, as $d \to \infty$; (v) for all entries, $U_c \to 0$ as $d \to \infty$; this is so for different reasons than for Mean Field theory, since the system energy per spin → 0 in Mean Field theory, while here it acquires an extra factor d (see Table III); (vi) the series formula gives values, $d \geq 6$, consistent with i-δ theory to within 0.5%; (vii) the value of A is closer to 1 for certain chosen 2-and 3-dimensional lattices (Table IV) when one puts S_i itself for S_j in equation (12) as pointed out by Girvin (1978) than the choice of S_j as a neighbour spin of i, except for the case of hydrogen peroxide lattice, where the reverse is true (the values for hydrogen peroxide are based on the series values so that firm conclusions cannot yet be reached).

The motivation behind the present work is its relevance to MCRG calculations. Apart from that, however, the work shows to what extent the i-δ theory is a "high-density" theory, and demonstrates the need for any theory, however consistent with the best available estimates for small d, to be studied at high d. It also demonstrates how such a theory may be

analyzed for its "1/d expansion" from the generated numerical data. This expansion should be regarded rather as a formula to which values for high d may be fitted. For example, in the case of K_c, the discrepancy for $d > 7$ is $\leq 0.053\%$ between the formula and the calculated values.

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APPENDIX A

We have equation (15)

$$< S_i S_j > = (A/J(0)) < S_j O_i > + \delta_{ij} L \qquad (15)$$

The Fourier transforms of $< S_i S_j >$ is by definition

$$G(q) = \sum_j < S_i S_j > \exp \{ i\vec{q}. (\vec{R}_j - \vec{R}_i) \} \qquad (4)$$

Substituting from (15),

$$G(q) = \sum_j (A/J(0)) < O_i S_j > \exp \{i\vec{q}.(\vec{R}_j - \vec{R}_i)\} + \sum_j \delta_{ij} L \exp \{ i\vec{q}.(\vec{R}_j - \vec{R}_i)\}$$

$$= L + \sum_{j,l} (A/J(0)) J_{il} < S_l S_j > \exp \{i\vec{q}.(\vec{R}_j - \vec{R}_l)\} \exp\{i\vec{q}.(\vec{R}_l - \vec{R}_i)\}$$

$$= L + A/J(0) \sum_l J_{il} \exp \{i\vec{q}. (\vec{R}_l - \vec{R}_i) \sum_j < S_l S_j > \exp \{i\vec{q}.(\vec{R}_j - \vec{R}_l)\}$$

or,

$$G(q) = L + (A/J(0)) J(q)\ G(q) \qquad (A\ 1)$$

J (q) has been defined in equation (13). Rewriting the above equation,

$$G(q) = L/\{1 - AJ(q)/J(0)\} \qquad (A\ 2)$$

From (A 2),

$$\sum_q G(q) = L \sum_q 1/\{1 - AJ(q)/J(0)\} \qquad (A\ 3)$$

Now, from the definition (4) of G(q),

$$(1/N) \sum_q G(q) = < S_i^2 > = 1/4 \qquad (A\ 4)$$

for the spin - 1/2 system. Thus we have for L

$$L = (1/4) \; / \; [\; (1/N) \sum_{q'} 1/\{1 - A\, J(q')/J(0)\} \;] \qquad (A\ 5)$$

Thus equation (A 2)is

$$G(q) = \frac{1/4}{(1/N) \sum_{q'} 1/\{1 - AJ(q')/J(0)\}} \times \frac{1}{\{1 - AJ(q)/J(0)\}} \qquad (16)$$

APPENDIX B

By definition

$$T_2 = \frac{\langle O_i^2 \rangle}{J^2(0)} \tag{23}$$

$$= \frac{1}{J^2(0)} \sum_{k,l} J_{ik} J_{il} \langle S_k S_l \rangle$$

$$= \frac{1}{J^2(0)} \frac{1}{N} \sum_{i} \sum_{k,l} J_{ik} J_{il} \langle S_k S_l \rangle$$

$$= 1/J^2(0) \quad 1/N \sum_{i,k,l} 1/N \sum_{q} J(q) \exp\{-i (\vec{R}_k - \vec{R}_i) \cdot \vec{q}\} \times$$

$$1/N \sum_{q'} J(q') \exp\{ i (\vec{R}_l - \vec{R}_i) \cdot \vec{q}'\} \langle S_k S_l \rangle \tag{B1}$$

Because by definition

$$J(q) = \sum_{j} J_{ij} \exp \{ i \vec{q} \cdot (\vec{R}_j - \vec{R}_i)\} \tag{13}$$

giving,

$$J_{ij} = 1/N \sum_{q} J(q) \exp \{ -i \vec{q} \cdot (\vec{R}_j - \vec{R}_i)\} \tag{B2}$$

Thus

$$T_2 = 1/J^2(0) \quad 1/N^3 \sum_{i,k,l,q,q'} J(q) J(q') \langle S_k S_l \rangle \exp \{i (\vec{R}_l \cdot \vec{q}' - \vec{R}_k \cdot \vec{q})\}$$

$$\times \exp \{i \vec{R}_i \cdot (\vec{q} - \vec{q}')\}$$

or, $$T_2 = 1/J^2(0) \quad 1/N^2 \sum_{k,l,q} J^2(q) \langle S_k S_l \rangle \exp \{i (\vec{R}_l - \vec{R}_k) \cdot \vec{q}\} \tag{B3}$$

where use was made of

$$\sum_{i} \exp \{ i \vec{R}_i \cdot (\vec{q} - \vec{q}')\} = N \delta_{qq'} \tag{B4}$$

Thus

$$T_2 = 1/J^2(0) \quad 1/N^2 \sum_{q,1} J^2(q)\ G(q)$$

or,

$$T_2 = 1/N \sum_q J^2(q)\ G(q)/J^2(0) \tag{25}$$

$$= \frac{1}{N} \sum_q \frac{J^2(q)}{J^2(0)} \times \frac{1/4}{F(1)} \times \frac{1}{\left(1 - \frac{J(q)}{J(0)}\right)}$$

$$= \frac{1}{4NF(1)} \sum_q \frac{\left(\frac{J^2(q)}{J^2(0)}\right)}{\left(1 - \frac{J(q)}{J(0)}\right)}$$

$$= \frac{1}{4F(1)} \left[-\frac{1}{N} \sum_q \left(\frac{J(q)}{J(0)} + 1 \right) + \frac{1}{N} \sum_q \frac{1}{1 - \frac{J(q)}{J(0)}} \right]$$

$$= \frac{1}{4F(1)} \left[-\frac{1}{N} \sum_q 1 + F(1) \right] \tag{B5}$$

where use was made of

$$\sum_q J(q) = \sum_q \sum_j J_{ij} \exp \{ i \vec{q} . (\vec{R}_j - \vec{R}_i) \}$$

$$= \sum_j J_{ij} \sum_q \exp \{ i \vec{q} . (\vec{R}_j - \vec{R}_i) \}$$

$$= \sum_j J_{ij}\ N\delta_{ij}$$

$$= NJ_{ii}$$

$$\text{or, } \sum_q J(q) = 0 \tag{B6}$$

from the definition of the exchange integral J_{ii}. Thus

$$T_2 = 1/4 \ (1- 1/F(1)) \qquad (26)$$

APPENDIX C

The Watson sum

$$F_d(1) = \frac{1}{N} \sum_q \frac{1}{1 - J(q)/J(0)} \tag{27}$$

may be expressed for the d-dimensional (hyper-) cubic lattice, as (Barber and Fisher 1973)

$$F_d(1) = d \int_0^\infty \{ e^{-x} I_0(x) \}^d \, dx \tag{C1}$$

where $I_0(x)$ is the modified Bessel function of the first kind of order zero. The above expression has closed forms for d = 1 and 2 (Barber and Fisher 1973) and for d = 3 (Watson 1939)

However $F_d(1)$ can be obtained for $d \geq 4$ by two methods. Firstly, by the numerical integration of the integrand of (C1) from zero to a very high number; and secondly, by expressing the integral in terms of a power series in $\frac{1}{d}$ (Gerber and Fisher 1974):

$$F_d(1) = 1 + \frac{1}{2d} + \frac{3}{(2d)^2} + \frac{12}{(2d)^3} + \frac{60}{(2d)^4} + \ldots - \ldots + \tag{C2}$$

[Since,

$$d \int_0^\infty \{e^{-x} I_0(x)\}^d dx$$

$$= d \int_0^\infty e^{-dx} \{ 1 + \frac{x^2}{2^2} + \frac{x^4}{2^2.4^2} + \frac{x^6}{2^2.4^2.6^2} + \ldots \}^d \, dx$$

$$= d \cdot \{ \int_0^\infty e^{-y} \frac{dy}{d} + \int_0^\infty e^{-y} \frac{y^2}{d^2} \left(\frac{d}{4}\right) \frac{dy}{d} + \ldots \}$$

putting $d.x = y$. Thus

$$F_d(1) = d \{ \frac{1}{d} \Gamma(1) + \frac{d}{4d^3} \Gamma(3) + \ldots \}$$

leading to the equation (C2)

In the present work $F_d(1)$ was calculated using (C1), intergrating from $x = 0$ to $x = 10^8$, and also from (C2) using the series up to the term containing $1/d^{13}$.

The second method (C2) does not give reasonable values for smaller d's whereas the numerical integration gives the exact value (Barber and Fisher 1973) for $d = 4$ up to at least six significant figures. For $d = 3$, this method gives $F_3(1)$ correct to 5 significant figures, beyond which the truncation errors in the numerical integration start to take effect (the calculated value was 1.516348 versus the exact value of 1.516386). The truncation error is much smaller for $d \geq 4$. For $d = 4$, the series up to d^{-13} gives $F_4(1)$ about 2% off the exact value. For $d = 3$, this series is of no use, since $F_3(1)$ thus obtained is - 0.00347 which is plainly meaningless.

For numerical integration the IMSLIB library function MMBSI0 was used. The value of the function $e^{-x} I_0(x)$ obtained from IMSLIB library function DCADRE was found correct up to at least 9 decimal places for two values of x chosen randomly (Abramowitz and Stegun 1965).

APPENDIX D

We have equation (15)

$$< S_i S_j > = A/J(0) \quad < S_j O_i > + \delta_{ij} L \qquad (15)$$

which reduces to

$$<S_i S_j> = < O_i S_j > /J(0) + \delta_{ij} L \qquad (D1)$$

at $T = T_c$ and in zero external field, since

$$A = 1 \qquad (17)$$

Multiplying (D1) by J_{ij} and summing over j one gets

$$< S_i O_i> = < O_i^2 > / J(O) + 0 \qquad (D2)$$

giving

$$U_2 = T_2 \qquad (D3)$$

In the present theory

$$< O_i^{2n+1} S_j > / < O_i S_j > = R_n, \text{ independent of } j \qquad (11)$$

So one can write, for all j,

$$< O_i^{2n+1} S_j > / < O_i S_j > = < O_i^{2n+1} S_i > / < O_i S_i > \qquad (D4)$$

or, from (32), $< O_i^{2n+1} S_j > = \dfrac{U_{2n+2}\, J^{2n+1}(0)}{U_2 J(0)} < O_i S_j >$ (D5)

Again multiplying (D5) by J_{ij} and summing over j, one gets

$$T_{2n+2} = (U_{2n+2} / U_2) T_2$$

or, from (D3), $T_{2n+2} = U_{2n+2}$ $(n = 0, 1, \ldots)$ (34)

APPENDIX E

Correction and extension of the Appendix of FM1 with the help of a diagram technique, an analytical check and recalculation of critical temperatures for 3-dimensional lattices using higher order correlation functions thus obtained:

The T_{2n} have been defined by equation (23)

$$T_{2n} = \langle O_i^{2n} \rangle / J^{2n}(0) \quad , n=1,2 \ldots Z/2 \tag{23}$$

To evaluate them, FM1 has prescribed a method. Say one wants to find T_4 (n being 2 in equation (23)) for example:

$$T_4 = 1/(Z^4 J^4) \sum_{j,k,l,m}^{Z} J_{ij} J_{ik} J_{il} J_{im} \langle S_j S_k S_l S_m \rangle \tag{E1}$$

where the indices j,k,l and m all represent nearest neighbours of the spin i, ($J_{ij} = J_{ik} = J_{il} = J_{im} = J$). The right hand side of (E1) contains all possible combinations of S_j, S_k, S_l and S_m, sometimes two of them being the same, sometimes three and sometimes all. According to the prescription of FM1, the square of any spin operator is replaced by 1/4. Then one is left with the combination of terms containing products of an even number of spin operators at different sites. Each pair average is approximated by its contribution $\bar{p}$ to T_2 on the assumption that all such pairs contribute equally. $\bar{p}$ has been given there as

$$\bar{p} = (T_2 - 1/4Z)/(1-1/z) \tag{E2}$$

Thus higher order correlation functions T_4, T_6 etc. can be obtained in terms of T_2 as is obvious for the example for T_4:

$$Z^4 T_4 = \sum_{j\neq k\neq l\neq m} \langle S_j S_k S_l S_m \rangle + \sum_{j=k\neq l\neq m} 1/4 \langle S_l S_m \rangle$$

$$+ \sum_{j=k=l\neq m} 1/4 \langle S_l S_m \rangle + \sum_{j=k\neq l=m} 1/16 + \sum_{j=k=l=m} 1/16 \qquad (E3)$$

or,

$$Z^4 T_4 = Z(Z-1)(Z-2)(Z-3)\,\bar{p}^2 + {}^4C_2\, Z(Z-1)(Z-2)\,\bar{p}/4$$

$$+ {}^4C_3\, Z(Z-1)\bar{p}/4 + (1/2!)\,{}^4C_2\,{}^2C_2\, Z(Z-1)/16 + {}^4C_4\, Z/16 \qquad (E4)$$

As n increases in equation (23), it becomes more and more complicated to keep track of the neighbouring equal and unequal indices and their possible contributions. The calculation is then vulnerable to error; this led to an incorrect calculation in FM1 for T_8 and T_{10}.

One proposes then a diagram technique which simplifies the bookkeeping. The rules to construct such diagrams, in the process of finding T_{2n}, are as follows:

(i) One prints out all the 2n vertices of a polygon (square corresponsing T_4, hexagon corresponding to T_6, etc.) with no vertices joined with a straight line. This corresponds to the contribution due to the term on the right-hand side of equation (23) where no two of the indices are equal. The contribution is (note that $2n \leq Z$)

$$Z(Z-1)(Z-2)\ldots\ldots(Z-2n+1)\,\bar{P}^n, \qquad (E5)$$

since the first of the unequal indices can take Z values, the next one

(Z-1) values, etc.

(ii) One then joins any two of the vertices of a similar diagram by a straight line, corresponding to the contribution where two indices are equal, the rest being unequal. For simplicity, only consecutive vertices have been joined in such a diagram and a factor of $^{2n}C_2$ takes care of the possibility of having any two indices equal. The corresponding contribution is

$$^{2n}C_2\ Z(Z-1)\ \ldots\ldots(Z - 2n + 1 + n_s)\ \bar{p}^{n-1}\ (1/4),\ (n_s = 1) \qquad \text{(E6)}$$

where the factor 1/4 has been introduced to take care of the square of the two spin-operators at the same site. n_s is defined as the number of straight lines present in such a diagram ($0 \leq n_s \leq 2n - 1$).

(iii) One then constructs the diagram with three of the consecutive vertices joined by two straight lines, representing three indices being identical. The contribution is

$$^{2n}C_3\ \ Z(Z-1)\ \ \ldots\ (Z - 2n + 1 + n_s)\ \bar{p}^{n-1}\ \ (1/4),\ (n_s=2) \qquad \text{(E7)}$$

(iv) Next, one joins two different pairs of consecutive vertices (the pairs not having any vertex in common) with two different straight lines, each representing the equality of two indices. The corresponding contribution is

$$(1/2!)\ \ ^{2n}C_2\ \ ^{2n-2}C_2\ \ Z(Z-1)\ldots\ (Z-2n+1+n_s)\bar{p}^{n-2}\ \ (1/4^2),\ (n_s = 2) \qquad \text{(E8)}$$

Factorial 2 in the denominator eliminates multiple counting of sets of identical indices.

(v) One then proceeds to the diagrams where three straight lines join (a) four consecutive vertices, (b) three consecutive vertices and two other consecutive vertices and (c) three different sets of two consecutive vertices each. The respective contributing terms are

$$^{2n}C_4 \; Z(Z-1) \; \ldots \; (Z-2n+1+n_s) \; \bar{p}^{n-2} \; (1/4^2) \quad , \tag{E9}$$

$$^{2n}C_3 \; ^{2n-3}C_2 \; Z(Z-1) \; \ldots \; (Z-2n+1+n_s) \; \bar{p}^{n-2} \; (1/4^2) \tag{E10}$$

$$\text{and } (1/3!) \; ^{2n}C_2 \; ^{2n-2}C_2 \; ^{2n-4}C_2 \; Z(Z-1) \; \ldots (Z-2n+1+n_s) \bar{p}^{n-3} \; (1/4^3) \tag{E11}$$

where $n_s = 3$ for all the above expressions.

(vi) One proceeds in the same way to construct diagrams where now n_s is increased by one. One takes account of all the different combinations of positions of straight lines in the polygons as exemplified in the previous paragraph.

(vii) One keeps on increasing n_s by one each time until finally one reaches the point where all the 2n indices are the same; in that case only (2n - 1) straight lines are needed to construct a diagram to represent this possibility. So n_s for that case is (2n - 1). However this diagram should not be distinguished from the one where all the sides of the

polygon are connected. The corresponding contribution is

$$C_{2n}^{2n} Z \; 1/4^n \qquad \text{(E12)}$$

(the alternative way to define n_s is 2n minus number of topologically discrete objects in the diagram. Thus for the last case n_s is equal to (2n-1) for both equivalent diagrams according to this alternative definition.)

As an example the diagrams for T_6 (n=3) are recorded in Table EI.

Applying this technique one can find higher order correlation functions. We quote here the expressions for T_8, T_{10} and T_{12}.

$$\begin{aligned}\frac{Z^8 T_8}{Z!} &= \bar{p}^4/(Z-8)! + (\bar{p}^3/4)\{28/(Z-7)! + 56/(Z-6)!\} \\ &+ (\bar{p}^2/16)\{210/(Z-6)! + 630/(Z-5)! \\ &+ 336/(Z-4)!\} + (\bar{p}/64)\{420/(Z-5)! \\ &+ 1260/(Z-4)! + 756/(Z-3)! + 64/(Z-2)!\} \\ &+ (1/256)\{105/(Z-4)! + 210/(Z-3)! \\ &+ 63/(Z-2)! + 1/(Z-1)!\}\end{aligned} \qquad \text{(E13)}$$

$$\begin{aligned}\frac{Z^{10} T_{10}}{Z!} &= \bar{p}^5/(Z-10)! + (\bar{p}^4/4)\{45/(Z-9)! + 120/(Z-8)!\} \\ &+ (\bar{p}^3/16)\{630/(Z-8)! + 2730/(Z-7)! \\ &+ 2352/(Z-6)!\} + (\bar{p}^2/64)\{3150/(Z-7)!\end{aligned}$$

$$+ \quad 15750/(Z-6)! + 19530/(Z-5)!$$

$$+ \quad 5540/(Z-4)! \; \} + (\bar{p}/256) \; \{4725/(Z-6)!$$

$$+ \quad 22050/(Z-5)! + 25515/(Z-4)!$$

$$+ \quad 7125/(Z-3)! + 256/(Z-2)! \}$$

$$+ \; (1/1024) \; \{945/(Z-5)! + 3150/(Z-4)!$$

$$+ \quad 2205/(Z-3)! + 255/(Z-2)! + 1/(Z-1)! \; \} \qquad \text{(E14)}$$

$$\frac{Z^{12}T_{12}}{Z!} = \bar{p}^6/(Z-12)! + (\bar{p}^5/4) \; \{ \; 66/(Z-11)! + 220/(Z-10)! \; \}$$

$$+ \; (\bar{p}^4/16) \; \{1485/(Z-10)! + 8415/(Z-9)!$$

$$+ \quad 10032/(Z-8)! \; \} + (\bar{p}^3/64) \; \{13860/(Z-9)!$$

$$+ \quad 97020/(Z-8)! + 183876/(Z-7)!$$

$$+ \quad 90112/(Z-6)! \; \} + (\bar{p}^2/256) \; \{ \; 51975/(Z-8)! \; \}$$

$$+ \quad 381150/(Z-7)! + 807345/(Z-6)!$$

$$+ \quad 544335/(Z-5)! + 87296/(Z-4)! \; \}$$

$$+ \quad (p/1024) \{ \; 62370/(Z-7)! + 415800/(Z-6)!$$

$$+ \quad 783090/(Z-5)! + 458370/(Z-4)!$$

$$+ \quad 65406/(Z-3)! + 1024/(Z-2)! \; \}$$

$$+ \ (1/4096)\ \{10395/(Z-6)! + 51975/(Z-5)!$$

$$+ \ 65835/(Z-4)! + 21120/(Z-3)!$$

$$+ \ 1023/(Z-2)! + 1/(Z-1)!\ \} \qquad \text{(E15)}$$

The expressions for T_8 and T_{10} are correct while those of FM1 are not. It was thought worthwhile to express T_{12} as well (not done in FM1), noting that Z is equal to 12 for the FCC lattice.

Analytic check on values thus obtained:

The i-δ relations are

$$\frac{\langle (O_i/J - S_\delta)^{2n+1} S_i \rangle}{\langle (O_i/J - S_\delta) S_i \rangle} = \frac{\langle (O_i/J - S_\delta)^{2n+1} S_\delta \rangle}{\langle (O_i/J - S_\delta) S_\delta \rangle} \ , \ (n = 1,2,.. \ \frac{Z}{2} - 1) \qquad (30)$$

Using the definitions of T_{2n} and U_{2n} (equations (23) and (32) respectively), one can easily write (30) in the form

$$T_{2n+2} = (1/Z^{2n+1}) \Big[\sum_{q=1}^{n} (1/2)^{2q} \ T_{2n+2-2q} \ Z^{2n+2-2q} \ ({}^{2n+1}C_{2q-1} - \frac{1}{Z} {}^{2n+1}C_{2q})$$

$$+ (1/2)^{2n+2} + (T_2 Z - 1/4) \{ U_{2n+2} \ (Z^{2n+1} - (2n+1) \ Z^{2n})$$

$$+ \sum_{q=1}^{n} Z^{2n-2q} \ U_{2n+2-2q} \ (1/2)^{2q} \ (Z^{2n+1} \ {}^{2n+1}C_{2q} - {}^{2n+1}C_{2q+1}) \} / U_2 (Z-1) \Big]$$

(E16)

By substituting $n = 1,2 \ldots Z/2 - 1$ respectively into the above equation (E16) it can be seen that each of $T_4, T_6, \ldots T_Z$ can be expressed in terms of lower-order T's and U's.

$U_2, U_4, \ldots U_Z$ can be written as

$$U_2 = C_{22} T_2 + C_{24} T_4 + \ldots + C_{2Z} T_Z$$

$$U_4 = C_{42} T_2 + C_{44} T_4 + \ldots + C_{4Z} T_Z$$

$$U_Z = C_{Z2} T_2 + C_{Z4} T_4 + \ldots + C_{ZZ} T_Z \qquad \text{(E17)}$$

where the coefficients C_{mn} can be obtained by the procedure outlined in Sec. 1 (equations (22a) and (22b)) for a given β. Thus we have (Z-1) linearly independent simultaneous equations to solve for (Z-1) unknowns $T_4, T_6, \cdots, T_Z, U_2, U_4, \ldots, U_Z$. (The assumption is not made here that $U_{2n} = T_{2n}$.)

It is found that the T's obtained thus are identical to the ones obtained by FM1 provided one uses the β given by

$$\bar{p} = (1/4) \tanh^2 (\beta J/4) \qquad \text{(E18)}$$

or, using equation (E2) for $\bar{p}$

$$(T_2 - 1/4Z) / (1-1/Z) = (1/4) \tanh^2 (\beta J/2) \qquad \text{(E19)}$$

(For the present case the method of successive approximation was used to find the values of T_4, T_6 ... T_Z and U_2, U_4 ... U_Z.) The rationale for this remarkable coincidence, is not given in this thesis.

In Table EII are presented the values of the critical temperature and the critical energy for the SC, BCC and FCC lattices using the T's obtained thus, together with (18), using the method of solution of Sec.1. For the purposes of comparison, the values of K_c and U_c have also been included from FCM, FM1 and series analysis (Sykes et al. 1972).

Table EI: Contributions to Z^6T_6 based on the FM1 prescription with the help of the diagram technique. n_s is the number of straight lines present in such a diagram.

n_s	Simplest possible diagram	Contribution to Z^6T_6 from such diagrams
0		$Z(Z-1)(Z-2)(Z-3)(Z-4)(Z-5)\ \bar{p}^{\,3}$
1		${}^6C_2\ Z(Z-1)(Z-2)(Z-3)(Z-4)\ \bar{p}^{\,2}/4$
2		${}^6C_3\ Z(Z-1)(Z-2)(Z-3)\ \bar{p}^{\,2}/4$
		$(1/2!)\ {}^6C_2\ {}^4C_2\ Z(Z-1)(Z-2)(Z-3)\ \bar{p}/4^2$
3		${}^6C_4\ Z(Z-1)(Z-2)\ \bar{p}/4^2$
		${}^6C_3\ {}^3C_2\ Z(Z-1)(Z-2)\ \bar{p}/4^2$
		$(1/3!)\ {}^6C_2\ {}^4C_2\ {}^2C_2\ Z(Z-1)(Z-2)/4^3$
4		${}^6C_5\ Z(Z-1)\ \bar{p}/4^4$
		${}^6C_4\ {}^4C_2\ Z(Z-1)/4^3$
		$(1/2!)\ {}^6C_3\ {}^3C_3\ Z(Z-1)\ \bar{p}/4^2$
5		${}^6C_6 Z/4^3$

Table E II. The values of K_c ($= \frac{4}{\beta_c J(0)}$) and the nearest neighbour correlation function U_c ($= \frac{\langle H \rangle}{JNZ/2}$) for the SC, BCC and FCC 3-dimensional lattices, based on the T's obtained using the FM1 prescription, and from FCM, FM1, and from series analysis.

		SC	BCC	FCC
K_c	present method	0.7724	0.8124	0.8437
	FCM	0.7564	0.7926	0.8121
	FM1	0.738[a]	---[b]	---[c]
	series analysis	0.7517	0.7938	0.8162
U_c	present method	0.08384	0.06978	0.06361
	FCM	0.08368	0.06958	0.06334
	series analysis	0.0827	0.0683	0.0619

a - correct T_{2n}'s, but approximate cumulant expansion used.

b - not reported as incorrect T_8 was used.

c - not reported as incorrect T_8 and T_{10} were used.

APPENDIX F

THE FORTRAN PROGRAMME TO CALCULATE K_c AND U_c.

```
      PROGRAM IDELTA (INPUT,OUTPUT)
C
C   TO FIND CRITICAL TEMPERATURE AND CRITICAL ENERGY FOR
C   THREE DIMENSIONAL LATTICES AND D-DIMENSIONAL
C   HYPERCUBIC LATTICES WITH NUMBER OF NEAREST
C   NEIGHBOURS = 2*D (FIXED POINT OR INTEGRAL VALUE)
C
      DIMENSION U(100),COL(100)
      DIMENSION UC(100)
C   UC(2) IS THE CRITICAL ENERGY
      COMMON N,Z,T2,IOPTA,T(100)
      COMMON/UUU/IOPTION
      CALL UERSET(0,LEVOLD)
C           TO GET RID OF ERROR MESSAGE
  101 PRINT*,"ENTER NUMBER OF NEAREST NEIGHBOURS AND GUESSED CRITEMP"
      READ*,N,XX
      Z=FLOAT(N)
      X=2./(Z*XX)
      ND=N/2
C     IF(N-4)2,14,16
C    14 T2=.25
C       GO TO 9
   16 IF(N-6)2,3,4
    3 T2=.0851343323821
C           THIS T2 IS FOR 3-DIMENSION I.E. WHEN Z=6
      GO TO 9
    4 IF (N-8) 2,5,6
    5 PRINT*,"ENTER 3 FOR BCC OR 4 FOR 4-DIMENSIONAL HYPERCUBIC"
      READ*,NDIM
      IF (NDIM-3) 2,32,33
   32 T2=.07055749724031
C           THIS IS FOR Z=8 (IN 3-DIMENSION, I.E. BCC LATTICE)
      GO TO 9
   33 IF (NDIM-4) 2,34,2
   34 CALL INTBES(ND,T2)
      GO TO 9
    6 IF (N-10) 2,7,8
    7 CALL INTBES(ND,T2)
      GO TO 9
    8 IF (N-12) 2,1,15
    1 PRINT*,"ENTER 3 FOR FCC OR 6 FOR 6-DIMENSIONAL HYPERCUBIC"
      READ*,NDIM
      IF (NDIM-3) 2,42,43
   42 T2=.06407955913098
C           THIS IS FOR Z=12 (IN 3-DIMENSION, I.E. FCC LATTICE)
      GO TO 9
   43 IF (NDIM-6) 2,44,2
   44 CALL INTBES(ND,T2)
      GO TO 9
   15 CALL INTBES(ND,T2)
    9 CONTINUE
      PBAR=(T2-.25/Z)/(1.-1./Z)
      XY=2.*ATANH(SQRT(4.*PBAR))
```

```
      PRINT*,"ENTER IOPTION"
      PRINT*,"1 FOR I-DELTA, 2 FOR FM1(MAX Z=12), 3 FOR ITERATION"
      READ*,IOPTION
      PRINT*,"ENTER IOPTA  1 FOR A=1, 2 FOR A'=1"
      READ*,IOPTA
      IF(IOPTION.EQ.1)CALL T2N(T2,N T)
      IF(IOPTION.EQ.2)CALL T2NFM1(PBAR,N,T)
      IF(IOPTION.EQ.3)CALL T2NIT(T2,N,T,U,XY)
      IF(IOPTION.EQ.2)GO TO 91
      GO TO 92
   91 IF(N.GT.12) GO TO 2
   92 CONTINUE
      CALL NR1VAR(X)
      XX=2./(X*Z)
C            XX=4./(BETA(C)*J(0))
      PRINT*,"CRITEMP=",XX
      Y=X
      PRINT* "T2N="
      PRINT100,(T(K),K=2,N,2)
      IF(IOPTION.EQ.1)CALL U2N(T2,U,N,Y)
      IF(IOPTION.EQ.2)CALL U2NFM1(PBAR,U,N,XY)
      PRINT*,"U2N="
      PRINT 100,(U(K),K=2,N,2)
      CALL U2N(T2,UC,N,Y)
      PRINT*,"UC2N="
      PRINT 100,(UC(K),K=2,N,2)
      CALL COLSOL(Y,COL,1,ND,ND+1,7)
      PRINT*,"A2N="
      PRINT100,(COL(K),K=1,ND)
      PRINT*,"CRITENERGY = ",UC(2)
  100 FORMAT (1P5E22.10/)
    2 GO TO 101
      STOP
      END
C
C-------------------------------------------------------
C
      FUNCTION FUN(YY)
C   THIS IS FOR A=1
      DIMENSION COL(50),DOL(50)
      COMMON N,Z,T2,IOPTA,T(100)
      N1=N/2
      IF(IOPTA.EQ.1)CALL COLSOL(YY,COL,1,N1,N1+1,7)
      IF(IOPTA.EQ.2)CALL COLSOL(YY,COL,1,N1,N1+1,8)
      CALL COLSOL(YY,DOL,1,N1,N1+1,2)
      SUM=0.
      DO 70 I=2,N,2
      J=I/2
      SUM=SUM+(T(I)*COL(J))
   70 CONTINUE
      AN=SUM
      ASU=0.
      DO 80 I=2,N,2
```

```
      J=I/2
      ASU=ASU+(T(I)*DOL(J))
   80 CONTINUE
      U2=ASU
      IF(IOPTA.EQ.1)FUN=(AN/(4.*U2))-1.
      IF(IOPTA.EQ.2)FUN=U2/AN-1.
      RETURN
      END
C
C-- ----------------------------------------------------
C
      SUBROUTINE LEQSOL(D,COL,ND,NP)
C   FROM FORTRAN IV - PROGRAMMING AND COMPUTING BY J.T.GOLDEN
C   THIS SOLVES SIMULTANIOUS LINEARLY INDEPENDENT EQUATIONS.
      DIMENSION D(100,101) COL(ND),LOC(100),CK(100)
      NP=ND+1
      DO 1 I=1,ND
    1 CK(I)=0.
      DO 100 I=1,ND
      IP=I+1
      AMAX=0.
      DO 2 K=1,ND
      IF(AMAX-ABS(D(K,I))) 3,2,2
    3 IF(CK(K))4,4,2
    4 LOC(I)=K
      AMAX=ABS(D(K,I))
    2 CONTINUE
      IF(ABS(AMAX).LE.10.E-19) GO TO 99
    5 L=LOC(I)
      CK(L)=1.
      DO 49 J=1,ND
      IF(L-J)6,49,6
    6 F=-D(J,I)/D(L,I)
      DO 39 K=IP,NP
   39 D(J,K)=D(J,K)+F*D(L,K)
   49 CONTINUE
  100 CONTINUE
      DO 200 I=1,ND
      L=LOC(I)
  200 COL(I)=D(L,NP)/D(L,I)
      GO TO 103
   99 PRINT*,"NO UNIQUE SOLUTION FROM LEQSOL"
  103 RETURN
      END
C
C-------------------------------------------------------
C
      SUBROUTINE T2N(T2,N,T)
C   THIS GIVES T'S BASED ON I-DELTA EQUATIONS
C   WHERE T2N=U2N
      DIMENSION T(N)
      Z=FLOAT(N)
      T(2)=T2
```

```
      NN=N-2
      DO 16 I=2,NN,2
      M=I/2
      SUM=COEFA(Z,T2,M)*(2.*Z)**(-(2*M+1))
      ASUM=0.
      DO14 J=1,M
      ASUM=ASUM+(COEFA(Z,T2,M)*DDJ(Z,2*M+1,2*J-1)+
     1  COEFB(Z,T2,M)*DDJ(Z,2*M+1,2*J))*T(2*M+2-2*J)
   14 CONTINUE
      K=I+2
      T(K)=SUM+ASUM
   16 CONTINUE
      RETURN
      END
C
C-----------------------------------------------------
C
      FUNCTION DDJ(Z,M,J)
      DDJ=(BIN(M,J)-BIN(M,J+1)/Z)*(2.*Z)**(-J)
      RETURN
      END
C
C-----------------------------------------------------
C
      FUNCTION BIN(K,L)
      BIN=1.
      IF(L.EQ.0)GO TO 19
      DO 18 I=1,L
      AL=FLOAT(L)
      AI=FLOAT(I)
      AK=FLOAT(K)
      TERM=(AK-AL+AI)/AI
      BIN=BIN*TERM
   18 CONTINUE
   19 CONTINUE
      RETURN
      END
C
C-- ----------------------------------------------------
C
      FUNCTION COEFB(Z,T2,L)
      ZI=1./(1.-1./Z)
      ZT2=1.-1./(4.*Z*T2)
      COEFB=2.*ZT2*ZI*COEFA(Z,T2,L)
      RETURN
      END
C
C-----------------------------------------------------
C
      FUNCTION COEFA(Z,T2,L)
      ZI=1./(1.-1./Z)
      ZT2=1.-1./(4.*Z*T2)
      AL=FLOAT(L)
```

```
      COEFA=.5/(1.-(1. (2.*AL+1.)/Z)*ZI*ZT2)
      RETURN
      END
C
C-----------------------------------------------
C
      SUBROUTINE COLSOL(YY,COL,NB,ND,NP,IOP)
C   CONTAINS MATRIX TO BE SOLVED WITH HELP OF LEQSOL
      DIMENSION D(100 101),COL(ND)
      N=2*ND
      Z=FLOAT(N)
      DO 40 I=1,ND
      DO 30 J=1,ND
      AI=FLOAT(I)
      D(I,J)=AI**(2*J)*Z**(N-2*J)
   30 CONTINUE
   40 CONTINUE
      IF(IOP.EQ.7)GO TO 45
      IF(IOP.EQ.2)GO TO 55
      IF(IOP.EQ.5)GO TO 65
      IF(IOP.EQ.6)GO TO 75
      IF(IOP.EQ.8)GO TO 85
   45 DO 46  I=1,ND
      BI=FLOAT(I)
      D(I,NP)=Z**N*(TANH(BI*YY))**2
   46 CONTINUE
      GO TO 95
   55 DO 56 I=1,ND
      AI=FLOAT(I)
      D(I,NP)=Z**N/2.*(AI/Z)**(2*NB-1)*TANH(AI*YY)
   56 CONTINUE
      GO TO 95
   65 DO 66 I=1,ND
      AI=FLOAT(I)
      D(I,NP)=Z**N*(TANH(AI*YY))**4
   66 CONTINUE
      GO TO 95
   75 DO 76 I=1,ND
      AI=FLOAT(I)
      D(I,NP)=Z**N/4.*((AI/Z)**(2*NB-1)*TANH(AI*YY))**2
   76 CONTINUE
      GO TO 95
   85 DO 86 I=1,ND
      AI=FLOAT(I)
      D(I,NP)=Z**N*(AI/Z)**2
   86 CONTINUE
      GO TO 95
   95 CALL LEQSOL(D,COL,ND,NP)
      RETURN
      END
C
C-----------------------------------------------
C
```

```
      FUNCTION FAC(L)
      IFAC=1
      IF(L.EQ.0)GO TO 56
      DO 55 I=1,L
      IFAC=IFAC*I
   55 CONTINUE
   56 CONTINUE
      FAC=FLOAT(IFAC)
      RETURN
      END
C
C-----------------------------------------------------
C
      FUNCTION SIG(K)
      SIG=0.
      DO 56 I=1,K
      SIG=SIG+1.
   56 CONTINUE
      RETURN
      END
C
C-----------------------------------------------------
C
      SUBROUTINE DIF(X,FPRIM)
C   FOR DIFFERENTIATING THE FUNCTION FUN
      H=.001
      DO 12 I=1,50
      A=X+2.*H
      D=X+H
      Y2=X-H
      Z1=X-2.*H
      F1=FUN(Y2)
      F2=FUN(Z1)
      F4=FUN(A)
      F5=FUN(D)
      F3=FPRIM
      FPRIM=(F2-8.*F1+8.*F5-F4)/(12.*H)
      ERR=ABS(F3-FPRIM)
      IF(ERR .LE. 1.E-10) GO TO 24
      H=H/2.
   12 CONTINUE
   24 RETURN
      END
C
C-----------------------------------------------------
C
      SUBROUTINE U2N(T2,U,N,Y)
C   THIS FINDS U'S BASED ON SUZUKI IDENTITY (EXACT)
      DIMENSION DOL(100),U(N),T(100)
      COMMON/UUU/IOPTION
      Z=N
      PBAR=(T2-.25/Z)/(1.-1./Z)
      XY=2.*ATANH(SQRT(4.*PBAR))
```

```
      ND=N/2
      IF(IOPTION.EQ.1)CALL T2N(T2,N,T)
      IF(IOPTION.EQ.2)CALL T2NFM1(PBAR,N,T)
      IF(IOPTION.EQ.3)CALL T2NIT(T2,N,T,U,XY)
      DO 86 L1=2,N,2
      L1H=L1/2
      CALL COLSOL(Y,DOL,L1H,ND,ND+1,2)
      ASU=0.
      DO 81 II=2,N,2
      J=II/2
      ASU=ASU+(T(II)*DOL(J))
   81 CONTINUE
      U(L1)=ASU
   86 CONTINUE
      RETURN
      END
C
C-------------------------------------------------------
C
      SUBROUTINE T2NFM1(P,N,TPP)
C    CALCULATES T'S BASED ON FM1
C    P=.25*(TANH(BETA*J/4))**2=.25*(TANH(.5*X))**2 FOR S.G.
      DIMENSION TPP(100)
      Z=FLOAT(N)
      TPP(2)=(.25+(Z-1.)*P)/Z
      TPP(4)=FAC(N)/Z**4*(P**2/FAC(N-4)+P*(1.5/FAC(N-3)+
     1 1./FAC(N-2))+(3./FAC(N-2)+1./FAC(N-1))/16.)
      TPP(6)=FAC(N)/Z**6*(P**3/FAC(N-6)+P**2*(15./FAC(N-5)+
     1 20./FAC(N-4))/4.+P*(45./FAC(N-4)+75./FAC(N-3)+16./FAC(N
     2 -2))/16.+(1./FAC(N-1)+15./FAC(N-2)+15./FAC(N-3))/64.)
      TPP(8)=FAC(N)/Z**8*(P**4/FAC(N-8)+P**3*(14./FAC(N-6)+
     1 7./FAC(N-7))+P**2*(168./FAC(N-4)+315./FAC(N-5)+105./FAC(
     2 N-6))/8.+P*(16./FAC(N-2)+189./FAC(N-3)+315./FAC(N-4)+
     3 105./FAC(N-5))/16.+(1./FAC(N-1)+63./FAC(N-2)+210./FAC(N
     4 -3)+105./FAC(N-4))/256.)
      TPP(10)=FAC(N)/Z**10*(P**5/FAC(N-10)+P**4*(120./FAC(N-8)
     1 +45./FAC(N-9))/4.+P**3*(1176./FAC(N-6)+1365./FAC(N-7)+
     2 315./FAC(N-8))/8.+P**2*(2720./FAC(N-4)+9765./FAC(N-5)+
     3 7875./FAC(N-6)+1575./FAC(N-7))/32.+P*(256./FAC(N-2)+
     4 7125./FAC(N-3)+25515./FAC(N-4)+22050./FAC(N-5)+4725./FAC
     5 (N-6))/256.+(1./FAC(N-1)+255./FAC(N-2)+2205./FAC(N-3)+
     6 3150./FAC(N-4)+945./FAC(N-5))/1024.)
      TPP(12)=FAC(N)/Z**12*(P**6/FAC(N-12)+P**5/4.*(66./FAC(
     1 N-11)+220./FAC(N-10))+P**4/16.*(1485./FAC(N-10)+8415./
     2 FAC(N-9)+10032./FAC(N-8))+P**3/64.*(13860./FAC(N-9)+
     3 97020./FAC(N-8)+183876./FAC(N-7)+90112./FAC(N-6))+P**
     4 2/256.*(51975./FAC(N-8)+381150./FAC(N-7)+807345./FAC(
     5 N-6)+544335./FAC(N-5)+87296./FAC(N-4))+P/1024.*(62370.
     6 /FAC(N-7)+415800./FAC(N-6)+783090./FAC(N-5)+458370./
     7 FAC(N-4)+65406./FAC(N-3)+1024./FAC(N-2))+1./4096.*(
     8 10395./FAC(N-6)+51975./FAC(N-5)+65835./FAC(N-4)+21120.
     9 /FAC(N-3)+1023./FAC(N-2)+1./FAC(N-1)))
      RETURN
```

```
      END
C
C-----------------------------------------------------------
C
      SUBROUTINE T2NIT(T2,N,TIT,UN,X)
C   CALCULATES T'S AND U'S USING METHOD OF SUCCESSIVE
C   APPROXIMATION (HERE T2N ARE NOT EQUAL TO U2N)
C   X=BETA*J/2=2*ATANH(SQRT(4*P))
      DIMENSION TT(100),TIT(100),UN(100),DOL(100)
      ND=N/2
      Z=FLOAT(N)
      CALL T2N(T2,N,TT)
      DO 201 I=2,N,2
      TIT(I)=TT(I)
  201 CONTINUE
      DO 203 IJ2=1,100
      TIT1=TIT(4)
C  MERGE THE PROGRAM FOR U2N
      DO 86 L1=2,N,2
      L1H=L1/2
      CALL COLSOL(X,DOL,L1H,ND,ND+1,2)
      ASU=0.
      DO 81 II=2,N,2
      J=II/2
      ASU=ASU+(TIT(II)*DOL(J))
   81 CONTINUE
      UN(L1)=ASU
   86 CONTINUE
C  MERGE PROGRAM TITP TO CALCULATE T6,T8,ETC.
      NN=N-2
      DO 50 I=2,NN,2
      FACT1=Z**(-(I+1))
      M=I/2
      SUM1=.5**(I+2)
      FACT2=(T2*Z-.25)/(UN(2)*(Z-1.))
      ASUM1=0.
      DO 30 J=1,M
      IIJ2=I+2-2*J
      XY=(2.*Z)**(2*J-1)
      ASUM1=ASUM1+(.5**(2*J))*TIT(IIJ2)*(Z**IIJ2)*XY*DDJ(Z,I+1,2*J-1)
   30 CONTINUE
      II2=I+2
      SUM2=UN(II2)*(Z**(I+1)-(I+1)*Z**I)
      ASUM2=0.
      DO 40 J=1,M
      IIJ1=I+1-2*J
      IIJ2=IIJ1+1
      XZ=(2.*Z)**(2*J)
      ASUM2=ASUM2+(Z**IIJ1)*UN(IIJ2)*( 5**(2*J))*XZ*DDJ(Z,I+1,2*J)
   40 CONTINUE
      K=I+2
      TIT(K)=FACT1*(SUM1+ASUM1+FACT2*(SUM2+ASUM2))
   50 CONTINUE
```

```
      ERR1=ABS(TIT1-TIT(4))
      IF (ERR1 .LE. 1.E-10) GO TO 204
  203 CONTINUE
  204 RETURN
      END
C
C-----------------------------------------------------
C
      SUBROUTINE U2NFM1(P,U,N,Y)
C   CALCULATES U'S BASED ON FM1 AT A TEMPERARURE (Y=BETA*J/2)
      DIMENSION DOL(100),U(N),T(100)
      ND=N/2
      CALL T2NFM1(P,N,T)
      DO 86 L1=2,N,2
      L1H=L1/2
      CALL COLSOL(Y,DOL,L1H,ND,ND+1,2)
      ASU=0.
      DO 81 II=2,N,2
      J=II/2
      ASU=ASU+(T(II)*DOL(J))
   81 CONTINUE
      U(L1)=ASU
   86 CONTINUE
      RETURN
      END
C
C-----------------------------------------------------
C
      SUBROUTINE INTBES(ND,T2)
C           FOR INTEGRATION OF BESSSEL FUNCTION
      COMMON/IBESS/ND1
      INTEGER IER
      REAL DCADRE,FBESS,A,B,AERR,RERR,ERROR,C
      EXTERNAL FBESS
      ND1=ND
      A=0.
      B=100000000.
      AERR=.0000000001
      RERR=.0000000001
      C=DCADRE(FBESS,A,B,AERR,RERR,ERROR,IER)
      CC=C/4.
      F1=FLOAT(ND)*C
      FF1=1./F1
C           FF1=4./(BETA(C)*J(0)) FOR SPHERICAL MODEL
      T2=.25*(1.-1./F1)
      PRINT*,"    INTDECA=",C,"     CRITFIS=",CC
      PRINT*,"    F(1)    =",F1,"     CRITOUR=",FF1
C   CRITOUR IS CRITICAL TEMPERATURE IN OUR SCALE (4/(BETA*J(0)))
      PRINT* "    T2      =",T2,"     IER    =",IER
      RETURN
      END
C
C-----------------------------------------------------
```

```
C
      REAL FUNCTION FBESS(X)
C           MODIFIED BESSSEL FUNCTION OF THE FIRST KIND OF ORDER ZERO
      COMMON/IBESS/ND1
      INTEGER IOPT,IER
      REAL MMBSI0,ARG,Y,X
      ND=ND1
      IOPT=2
      ARG=X
      Y=MMBSI0(IOPT,ARG,IER)
      ZZ=Y**ND
      FBESS=ZZ
      RETURN
      END
C
C-------------------------------------------------------
C
      FUNCTION FOF1(ND)
C   ANOTHER METHOD TO CALCULATE F(1)
C   NOT GOOD FOR SMALL D'S
      N=2*ND
      Z=FLOAT(N)
      FOF1=1.+1./Z+3./Z**2+12./Z**3+60./Z**4+355./Z**5+2380./Z**6
     1 +17430./Z**7+134190./Z**8+1027656./Z**9+6922146./Z**10+
     2 21248073./Z**11-601744143./Z**12-20802115620/Z**13
      RETURN
      END
C
C-------------------------------------------------------
C
      SUBROUTINE NR1VAR(X)
C   NEWTON-RAPHSON METHOD TO FIND SOLUTION OF ONE VARIABLE
      DO 10 J=1,50
      X1=X
      CALL DIF(X,FPRIM)
      X=X-FUN(X)/FPRIM
C           NEWTON-RAPHSON METHOD
      ERROR=ABS(X1-X)
      IF (ERROR .LE. 1.E-10) GO TO 11
   10 CONTINUE
   11 RETURN
      END
```

APPENDIX G

This Appendix consists of the paper by Nath and Frank (1982), first presented in a poster session at the 3rd Joint Intermag Magnetism and Magnetic Materials, Montréal, July 1982.

Systematics of d-dimensional hypercubic spin-1/2 Ising ferromagnets: Critical temperature and critical energy[a)]

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The critical temperatures K_c and the nearest-neighbour correlation functions U_c have been calculated for the d-dimensional hypercubic Ising ferromagnet for d = 4 to d = 30, by generalizing a recent theory reported for d = 3. The results are of relevance for Monte Carlo Renormalization Group work involving critical properties in random fields, which calls for a knowledge of K_c in the limit of zero field. As d becomes large, K_c and U_c are found to approach the spherical model values. Polynomial expressions in 1/d are fitted to the calculated values, using the analogous spherical model expressions as guide. Comparison is made with the corresponding expressions of Fisher and Gaunt. $U_c/(1 - K_c)$, independent of d for the spherical model, is investigated; it is seen to be approximately independent of lattice structure for d = 2 and for d = 3.

PACS numbers: 75.10.Hk, 05.50. + q, 64.60. — i

INTRODUCTION

The Monte Carlo Renormalization Group (MCRG) method [1] has recently been used [2] to study the d-dimensional hypercubic Ising model in random magnetic fields ($\pm H$), for d=2,3 and 4. In this method, it is convenient (though not essential) to have a knowledge of accurate values of the critical temperature K_c ($=T_c/T_c(\text{Mean Field})=2k_BT_c/Jd$) at H=0. Possible extension of the MCRG work to d>4 suggests that it would be convenient to have at hand reasonably accurate values for K_c for all values of d, in the limit of zero random magnetic field.

Numerical estimates of K_c have indeed been made, by Fisher and Gaunt [3] for d=4,5 and 6, by analysis of high-temperature series expansions of the susceptibility. They have, as well, produced (possibly asymptotic) expansions of K_c in powers of the inverse dimensionality, up to d^{-5}. It is not clear how to obtain numerical estimates of K_c from this expansion, especially as a similar expansion for the nearest-neighbour correlation function U_c at the critical temperature (so called because of its relation to the critical energy per spin: $U_c=-(\text{energy})/JNd$) proves identical to that for the spherical model up to the term in d^{-5}, whereas the known respective values of U_c differ by ~3%. The 1/d expansion for K_c has been calculated for the spherical model by Gerber and Fisher [4]. That for U_c is easily derived from it through the spherical model formula $U_c=(1-K_c)/4$. The exact Ising 1/d expansion of U_c is easily derived from the appropriate partition function double series of Fisher and Gaunt [3], coupled with the K_c expansion referred to above.

A recent theory [5] for the Ising ferromagnet near the critical point proving capable of predicting values of K_c, U_c and other correlation functions consistent to within 1% with the Monte Carlo data [5] for the three-dimensional cubic lattices, it was considered of interest to apply it to the d-dimensional hypercubic case for d=4, 5,...,30. In the expectation that this theory ("i-δ theory") would continue, for all values of d, to yield better than 1% accuracy, such a calculation would serve both to provide such values of K_c and U_c, and to check whether the terms up to d^{-5} in the expansion of K_c derived from high-temperature series do indeed give accurate results for d>4.

In order to organize the theoretically-derived data, and for purposes of comparison, 1/d expansions are derived, as well, for K_c and U_c from the numerical results of the i-δ theory. It being too difficult to derive these expansions analytically, the expansion coefficients are found essentially by fitting the expansion to the data for d=20-30, using the principle that the coefficients must be non-zero rational fractions similar to those one finds in the spherical model expansions.

The expansions thus derived are reported and compared. The function $U_c/(1-K_c)$ being exactly 1/4 and thus independent of d for the spherical model, we have also investigated its behavior with d. This behavior demonstrates a dependence on 1/d as strong as that of K_c alone, and so is not reported here. Of interest is that, for d=3 and different lattice structures, the values of this expression are clustered around 0.33, while for d=2 they are clustered around 0.40.

In this paper values are presented, in tabular form, for K_c and U_c, for d=4 to 30 for the i-δ theory and the spherical model, and for d=4, 5 and 6 from susceptibility series analysis [3]. The method used for fitting the results of the i-δ theory to a 1/d formula extending to d^{-4} is reported, and the coefficients are presented in tabular form along with the corresponding expansion coefficients, to d^{-5}, valid for the spherical and Ising models and, for comparison, the Bethe approximation [6].

THEORY

The system Hamiltonian considered is

$$H=-(1/2)\Sigma_i\Sigma_j J_{ij}S_iS_j - \Sigma_i h_iS_i \qquad (1)$$

where S_i are the Ising spins ($S_i=\pm 1$) placed on d-dimensional hypercubic lattices; $J_{ij}=J$ if i and j are nearest neighbours and zero otherwise; and h_i is the (generally non-uniform) external field at site i. The basic approximation of the i-δ theory is that odd correlation functions involving spins localized around site i, all go to zero in the same way as the

h_j tend to zero, at $T=T_c$. This leads to a set of equations to be solved for K_c and certain second- and higher-order correlation functions, among them U_c. The details are exactly as in Frank et al. [5], the coordination number z now being $2d$; it remains only to calculate the Watson sum $F_d(1)$ for the d-dimensional hypercubic lattice. This is accomplished by numerical integration from the formula given, e.g., in Barber et al. [7]:

$$F_d(1)=d\int_0^\infty \{e^{-x}I_0(x)\}^d\,dx\ , \qquad (2)$$

where $I_0(x)$ is the modified Bessel function of the first kind of order zero.

Values of $K_c(i\text{-}\delta)$, $K_c(\text{spherical})=1/F_d(1)$, and $K_c(\text{series})$ (available best numerical estimates [3]) for selected values of d are presented in Table I, as well as values of $U_c(i\text{-}\delta)$ and $U_c(\text{spherical})$. These values are given here to 5 significant figures; they are available, however, to 8 significant figures, and for all values of $d\leq 30$. While the accuracy of the theory by no means justifies the retention of such a large number of significant figures, we find that this is necessary for our derivation of the 1/d expansions to order d^{-4}. In Figure 1 we plot K_c and U_c for the i-δ theory using the values from Table I.

Table I. Values of K_c and U_c for the hypercubic Ising lattices for selected values of $d\leq 30$.

d	$K_c(i\text{-}\delta)$	$K_c(\text{sph.})$	$K_c(\text{series})$	$U_c(i\text{-}\delta)$	$U_c(\text{sph.})$
4	0.84372	0.80680	0.83401	0.047801	0.048300
5	0.88419	0.86482	0.87694	0.033573	0.033795
6	0.90738	0.89528	0.90227	0.026061	0.026179
7	0.92250	0.91416		0.021390	0.021461
8	0.93323	0.92709		0.018182	0.018228
9	0.94127	0.93655		0.015830	0.015862
10	0.94755	0.94380		0.014027	0.014049
15	0.96572	0.96413		0.0089609	0.0089674
20	0.97450	0.97362		0.0065912	0.0065939
25	0.97969	0.97914		0.0052142	0.0052156
30	0.98312	0.98274		0.0043136	0.0043144

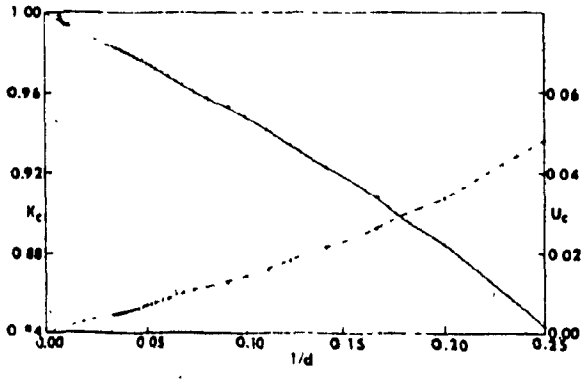

Fig. 1. K_c (——) and U_c (-.-.-) for i-δ theory using the values from Table I.

EXPANSION METHOD

In the attempt to find an expansion in powers of 1/d for $K_c(i\text{-}\delta)$ of the form $1-\sum_{n=1}^{M}A_n/d^n$ (3) from the data, it is found that the conventional least-squares technique is of little use. To take proper account of the asymptotic nature of the expansion, it is found preferable to adopt the following procedure. Assuming one has all the A_n of (3) exactly up to and including $n=j-1$, and approximately for $n=j$, one attempts to fit the natural logarithm of $1-K_c(i\text{-}\delta)-\sum_{m=1}^{j}A_m/d^m$, regarded as our data points, to the one term $\ln(A_{j+1}/d^{j'})$ asymptotically in the limit of large d. In doing so, A_{j+1} and j' are regarded as unknowns to be evaluated as functions of 1/d using the data for neighboring pairs d and d+1. The value of A_j is adjusted until j' extrapolates (for $1/d\to 0$) to $j+1$, this adjustment following the principle of analogy with the spherical model coefficients. One then accepts the corresponding value of A_{j+1} as approximate. One eventually reaches a value of j such that the extrapolation of j' (d large) is unreliable. Then $j=M+1$ defines M in (3). As we have found $M=4$, we report only up to d^{-4} in Table II. A knowledge of K_c to a greater number of significant figures would presumably lead to a greater value for M.

The extrapolated value of j' is very sensitive to the various adjusted values of A_j; this is illustrated in Figure 2.

In Table II are presented the results of this procedure for K_c and U_c, along with the respective coefficients found in the literature for the spherical model [4], the Ising model [3], and the Bethe approximation [6].

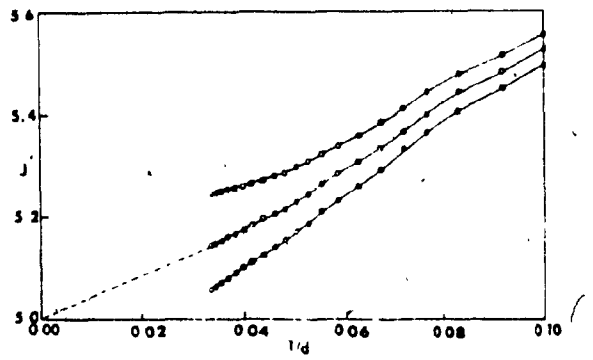

Fig. 2. Sensitivity of the extrapolated value of j' to various adjusted values of A_j. Here, $j=4$. $A_j=52/96$, 51.5/96, and 51/96 for the upper, middle and lower curves respectively.

Table II. Values of a_n in the expansion $\sum_{j=0}^{n}a_j d^{-j}$ of K_c and of U_c.

n	0	1	2	3	4	5
$K_c(\text{series})$	1	-1/2	-1/3	-13/24	-979/720	-2009/480
$K_c(\text{sph.})$	1	-1/2	-1/2	-7/8	-35/16	-215/32
$K_c(i\text{-}\delta)$	1	-1/2	-1/6	-5/8	-83/96	---
$K_c(\text{Bethe})$	1	-1/2	-1/12	-1/24	-19/720	-89/480
$U_c(\text{series})$	0	1/8	1/8	21/96	105/192	215/128
$U_c(\text{sph.})$	0	1/8	1/8	21/96	105/192	215/128
$U_c(i\text{-}\delta)$	0	1/8	1/8	19/96	103/192	---
$U_c(\text{Bethe})$	0	1/8	1/16	1/32	1/64	1/128

Finally, in Tables III and IV are presented values of $U_c/(1-K_c)$, constructed from Ref. 8, for some three- and two-dimensional lattices. These values appear to be clustered about 0.33 and about 0.40 for the d=3 and d=2 lattices respectively.

Table III. $U_c/(1-K_c)$ for the simple cubic (SC), body-centered cubic (BCC), face-centered cubic (FCC), diamond (DIA), hydrogen peroxide (HP), and hypertriangular (HTr) d=3 lattices. Values for U_c and K_c are taken from Domb [8].

SC	BCC	FCC	DIA	HP	HTr
.3332	.3318	.3368	.3371	.3327	.3210

Table IV. $U_c/(1-K_c)$ for the honeycomb (HC), simple quadratic(SQ), plane triangular (PT), kagomé (K) and diced (D) d=2 lattices. Values for U_c and K_c are taken from Domb [8] and Syozi [9].

HC	SQ	PT	K	D
.3897	.4085	.4239	.4007	.4191

DISCUSSION

It is seen from Tables I and II that (i) the coefficients in the U_c(series) and U_c(spherical) expansions (Table II) are equal; nevertheless, the value of U_c(i-δ) is closer to U_c(series) than is U_c(spherical) for d=3 (Ref. 5); (ii) the coefficients in the i-δ and series expansions in Table II do not greatly differ as the power of 1/d continues to increase; this is reminiscent of diagram expansions wherein certain classes of diagrams are neglected [10]; (iii) the i-δ theory values of K_c and U_c are consistent with the series values to within 1% for $4 \leq d \leq 6$; (iv) K_c(spherical) and K_c(i-δ) approach each other much faster than either one approaches the Mean Field value, as $d \to \infty$; (v) for all entries, $U_c \to 0$ as $d \to \infty$; this is so for different reasons than for Mean Field theory, since the system energy per spin $\to 0$ in Mean Field theory, while here it acquires an extra factor d (see Table II); (vi) the series formula gives values, for d>6, consistent with i-δ theory to within 0.5%.

The motivation behind the present work is its relevance to MCRG calculations. Apart from that, however, this work shows to what extent the i-δ theory is a "high-density" theory, and demonstrates the need for any theory, however consistent with the best available estimates for small d, to be studied at high d. It also demonstrates how such a theory may be analyzed for its "1/d expansion" from the generated numerical data. This expansion should be regarded rather as a formula to which values for high d may be fitted. For example, in the case of K_c, the discrepancy for d>7 is <0.053% between the formula and the calculated values.

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