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

Kashi Nath

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ABSTRACT

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ISING MODEL IN d-DIMENSIONS

Kashi Nath

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 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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TABLE OF CONTENTS

ABSTRACT
i
ACKNOWLEDGMENTS
ii
TABLE OF CONTENTS
iii
LIST OF FIGURES
v
LIST OF TABLES
vi
INTRODUCTION
vii
SECTION 1. Critical Temperature
1
SECTION 2. Critical Energy
14
SECTION 3. Critical Temperature and Critical Energy for the Spherical Model
18
SECTION 4. Organization and l/d Expansions for the Values of $K_c$ and $U_c$ from the Present Theory
20
SECTION 5. Series Expansions for the Critical Temperature and the Critical Energy for the Ising Model
26
SECTION 6. Bethe Approximation for the Critical Temperature and the Critical Energy for the Ising Model
27
SECTION 7. The Value of an Interesting Thermodynamic Ratio for Various Lattices
28
SECTION 8. Investigation of the Function $U_c/(1 - K_c)$ for Various Ising Lattices
41
DISCUSSION
43
REFERENCES
45
APPENDIX A
A1
APPENDIX B
A3
APPENDIC C
A6
<table>
<thead>
<tr>
<th>TABLE OF CONTENTS</th>
</tr>
</thead>
<tbody>
<tr>
<td>APPENDIX D</td>
</tr>
<tr>
<td>A8</td>
</tr>
<tr>
<td>APPENDIX E</td>
</tr>
<tr>
<td>A9</td>
</tr>
<tr>
<td>APPENDIX F</td>
</tr>
<tr>
<td>A20</td>
</tr>
<tr>
<td>APPENDIX G</td>
</tr>
<tr>
<td>A31</td>
</tr>
</tbody>
</table>
LIST OF FIGURES

Figure | Page
--- | ---
1. Plot of $K_C$ and $U_C$ as functions of $1/d$ | 17
2. A sensitivity curve to find a coefficient in the $1/d$ expansion | 25
**LIST OF TABLES**

<table>
<thead>
<tr>
<th>Table</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>Values of $K_c$ for the hypercubic Ising lattices for $4 \leq d \leq 30$</td>
<td>13</td>
</tr>
<tr>
<td>II</td>
<td>Values of $\mu_c$ for the hypercubic Ising lattices for $4 \leq d \leq 30$</td>
<td>16</td>
</tr>
<tr>
<td>III</td>
<td>Values of coefficients in the $1/d$ expansions of $K_c$ and $\mu_c$</td>
<td>24</td>
</tr>
<tr>
<td>IV</td>
<td>Values of certain thermodynamic ratios for certain lattices</td>
<td>40</td>
</tr>
<tr>
<td>V</td>
<td>Values of $K_c$, $\mu_c$ and $\mu_c/(1-K_c)$ for various Ising lattices</td>
<td>42</td>
</tr>
<tr>
<td>E I</td>
<td>Contributions with help of a diagram technique for multi-spin correlation functions</td>
<td>A18</td>
</tr>
<tr>
<td>E II</td>
<td>Values of $K_c$ and $\mu_c$ for 3-dimensional lattices</td>
<td>A19</td>
</tr>
</tbody>
</table>
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 $K_C (= T_C / T_C (\text{Mean Field}) = 4k_B T_C / JZ^2, Z$ 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: $U_C = -2 \langle \text{energy} \rangle / J N Z = \langle S_i S_j \rangle$, $i$ 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 $\sim 3\%$. 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

\[ U_c = \frac{(1-K_c)}{4}. \]

The exact Ising 1/d expansion of \( U_c \) is easily derived from the appropriate partition function double series of Fisher and Gaunt (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 three-dimensional cubic lattices, it was considered of interest to apply it to the d-dimensional hypercubic case for \( d = 4, 5, \ldots, 30 \). In the expectation that this theory ('i-5 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 FMI) 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-5 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 Internmag 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 \( i - 8 \) 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 \( i - 8 \) 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

\[ H = -1/2 \sum_{i,j} J_{ij} S_i S_j - \sum_i h_i S_i \]  \hspace{1cm} (1)

where \( S_i \) is the \( z \)-component of the spin operator at the \( i \)th 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 \( \chi \) approaches infinity

\[ \chi \rightarrow \infty \]  \hspace{1cm} (2)

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

\[ G(q \rightarrow 0) \rightarrow \infty \]  \hspace{1cm} \( (T = T_c) \)  \hspace{1cm} (3)

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

\[ G(q) = \sum_j \langle S_i S_j \rangle e^{i \mathbf{q} \cdot (\mathbf{R}_j - \mathbf{R}_i)} \]  \hspace{1cm} (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 $\{ i \}$ which is a combination of sums and products of operators that do not include the $i$th spin operator:

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

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

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

Using

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

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

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

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

where

$$L = \frac{1}{4} < \text{sech} \frac{\beta O_i}{2} > \quad (9)$$
Also in the absence of an external field at $T = T_c$, all odd-order correlation functions vanish i.e.

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

2n + 1 operators

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

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

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

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

is independent of $j$ (see FCM)

For convenience, one defines a quantity

$$A = \frac{1}{2} \frac{1}{J(o)} \frac{1}{\tanh \frac{80_i}{2}} \ (12)$$

$$< S_j O_i >$$

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

$$J(q) = \sum_j J_{ij} e^{i q \cdot (R_j - R_i)} \ (13)$$
Putting $i$ for $j$ in (12), which gives better results for $d = 3$ (as pointed out by Girvin 1978), we get

$$A = \frac{1/2 < \tanh^2 \frac{z}{2} S_0 >}{\frac{1}{J(0)} < 0_1 \tanh \frac{z}{2} S_0 >}$$

(14)

Now equations (8) & (12) give

$$< S_i S_j > = \frac{A}{J(0)} < S_i 0_1 > + \delta_{ij} L$$

(15)

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

$$G(q) = \frac{1/4}{\frac{1}{N q'} \left( \frac{1}{1 - A \frac{J(q)}{J(0)}} \right)} \times \frac{1}{\left[ 1 - A \frac{J(q)}{J(0)} \right]}$$

(16)

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

$$A = 1$$

(17)

or, from (14),

$$\frac{1/2 < \tanh^2 \frac{z}{2} S_0 >}{\frac{1}{J(0)} < 0_1 \tanh \frac{z}{2} S_0 >} = 1$$

(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 \( Z/2, Z/2 - 1, \ldots, 1, 0, -1, \ldots, -Z/2 + 1, -Z/2 \), which correspond to having all \( Z \) nearest neighbour spins of \( i \) pointing up, or \( Z - 1 \) up and one down, \ldots or \( Z \) pointing down. This identity may be written as

\[
(O_i \, \frac{Z}{J}) (O_i \, \frac{Z}{J} - 1) (O_i \, \frac{Z}{J} - 2^2) \ldots (O_i \, \frac{Z}{J} - Z^2 / 4^2) = 0
\]

(19)

Due to this reduction relation we may write operator equations like

\[
(O_i \, \frac{Z}{J})^{n+2n} = f_n \left( \frac{O_i \, \frac{Z}{J}}, (O_i \, \frac{Z}{J}), \ldots (O_i \, \frac{Z}{J}) \right), \quad (n = 1, 2, \ldots)
\]

(20)

where \( f_n \) is a linear function of \( (O_i \, \frac{Z}{J}), (O_i \, \frac{Z}{J}), \ldots (O_i \, \frac{Z}{J}) \).

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

\[
\frac{A_2 \, <O_i \, \frac{Z}{J}^2(0)> + A_4 \, <O_i \, \frac{Z}{J}^4(0)> + \cdots + A_{Z} \, <O_i \, \frac{Z}{J}^Z(0)>}{B_2 \, <O_i \, \frac{Z}{J}^2(0)> + B_4 \, <O_i \, \frac{Z}{J}^4(0)> + \cdots + B_{Z} \, <O_i \, \frac{Z}{J}^Z(0)>} = 1
\]

(21)
where $A_{2n}$ and $B_{2n}$ ($n = 1, 2, \ldots, Z/2$) are explicit functions of $\beta$
which are determined as follows. One puts $(O_1/J)^2$, in the equation
\[ 1/2 \tanh^2 \beta O_1/2 = A_2 O_2^2/J^2(O) + A_4 O_4^4/J^4(O) + \ldots + A_Z O_Z^Z/J^Z(O) \]  
(22a)

(e.g.) equal to its successive eigenvalues $0^2, 1^2, 2^2, \ldots, (Z/2)^2$
and solves the resulting set of $Z/2$ simultaneous equations for $A_2$, $A_4$, \ldots 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 $B_2$, $B_4$, \ldots and $B_Z$ as functions of $\beta$ from the equation.

\[ 1/J(O) O_1 \tanh \beta O_1/2 = B_2 O_2^2/J^2(O) + B_4 O_4^4/J^4(O) + \ldots + B_Z O_Z^Z/J^Z(O) \]  
(22b)

Defining,

\[ T_{2n} = \frac{<O_1^{2n}>}{J^{2n}(O)} \]  
(23)

allows equation (21) to be rewritten as

\[ \frac{A_2 T_2 + A_4 T_4 + \ldots + A_Z T_Z}{B_2 T_2 + B_4 T_4 + \ldots + B_Z T_Z} = 1 \]  
(24)
Now it remains to determine $T_2, T_4, \ldots, T_n$.

$T_2$ is known:

$$T_2 = \langle 0_1^2 \rangle \frac{J^2(0)}{\langle J^2 \rangle} = 1/4 \sum_q \frac{J^2(q)}{G(q)} \frac{J^2(0)}{J^2(0)} \quad (25)$$

which becomes at $T = T_C$

$$T_2 = \frac{1}{4} \left( 1 - \frac{1}{F(1)} \right) \quad (26)$$

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

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

To find the values of $T_4, T_6, \ldots, T_n$, "\( i-\delta \)" 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 \( \delta \); this sum may be written \( (0_1/J - S_\delta) \). The assumption is now made that, at $T_C$, as the $h_j \to 0$,

$$\langle 0_1/J - S_\delta \rangle^{2n+1}, \quad (n = 1, 2, \ldots, 2/2 + 1) \quad \text{and} \quad \langle 0_1/J - S_\delta \rangle$$

approach zero in the same way (see FM1).
One can write then

\[ \langle (O_1/J - S_\delta)^{2n+1} \rangle = Q_n \langle O_1/J - S_\delta \rangle \]  \hspace{1cm} (28)

Differentiating w.r.t. \( h_1 \) then let \( h's \to 0 \), one gets

\[ Q_n = \frac{\langle (O_1/J - S_\delta)^{2n+1} S_1 \rangle}{\langle (O_1/J - S_\delta) S_1 \rangle} \] \hspace{1cm} (29a)

Again differentiating w.r.t. \( h_\delta \) and let \( h's \to 0 \), one has

\[ Q_n = \frac{\langle (O_1/J - S_\delta)^{2n+1} S_\delta \rangle}{\langle (O_1/J - S_\delta) S_\delta \rangle} \] \hspace{1cm} (29b)

That uses the l'hoptial rule, without saying so. Equations (29a) and (29b) lead to the \( 1-\delta \) relations

\[ \frac{\langle (O_1/J - S_\delta)^{2n+1} S_1 \rangle}{\langle (O_1/J - S_\delta) S_1 \rangle} = \frac{\langle (O_1/J - S_\delta)^{2n+1} S_\delta \rangle}{\langle (O_1/J - S_\delta) S_\delta \rangle}, \hspace{0.5cm} n = 1, 2, \ldots, Z/2 - 1 \] \hspace{1cm} (30)
The left-hand side of the above equation, when expanded, contains terms like

\[ \langle 0_i 2^{m+1} S_i \rangle = J^{2^{m+1}} (0) U_{2m+2} \]  \hspace{1cm} (31a)

and

\[ \langle 0_i 2^{m} S_\delta S_i \rangle = J^{2^{m}} (0) U_{2m+2} \] \hspace{1cm} (31b)

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

\[ U_{2n} = \frac{\langle 0_i 2^{2n-1} S_i \rangle}{J^{2^{n-1}} (0)} , \quad (n = 1, 2, \ldots) \] \hspace{1cm} (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

\[ \langle 0_i 2^{m+1} S_\delta \rangle = J^{2^{m+1}} (0) T_{2m+2} \] \hspace{1cm} (33a)

and

\[ \langle 0_i 2^{m} \rangle = J^{2^{m}} (0) T_{2m} \] \hspace{1cm} (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 \( n > (2/2 - 1) \), nothing new is obtained (for then certain spin-operator reduction relations become operative).

At \( T = T_C \), it may be shown that

\[
U_{2n+2} = T_{2n+2}, \quad (n = 0, 1, 2, \ldots)
\]  

(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 \( T_{2n'} \), \( T_{2n'-2} \), \ldots, \( T_4 \), \( T_2 \) (\( T_2 \) being known, all higher-order correlation functions up to \( T_x \) are thus determined). The general relation is found to be:

\[
T_{2n+2} = a_n (22)^{(2n+1)} + \sum_{r=1}^{n} \left( a_n \frac{2n+1}{2r-1} + b_n \frac{2n+1}{2r} \right) T_{2n+2-2r},
\]  

(35)

where,

\[
a_n = \frac{1}{2} \left( 1 - \left( \frac{2n+1}{2} \right) \left( 1 - \frac{1}{2} \right) \left( 1 - \frac{1}{2} \right)^{-1} \right)^{-1}
\]  

(36)
\[ b_n = 2(1 - \frac{1}{4Z^2}) (1 - \frac{1}{Z})^{-1} a_n \tag{37} \]

and \( \frac{2^{n+1} \Delta}{\tau} \) is given in terms of the binomial coefficients, \( \binom{n}{r} \), as

\[ \frac{2^{n+1} \Delta}{\tau} = \binom{2^{n+1}}{\tau} \binom{2^{n+1}}{\tau + 1/Z} \tag{38} \]

Thus from equation (24) (or essentially equation (17)) the critical temperature \( K_c = \frac{4}{E_c J(0)} \) 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 $4 \leq d \leq 50$

<table>
<thead>
<tr>
<th>$d$</th>
<th>$k_c$ (i-$\delta$)</th>
<th>$k_c$ (sph.)</th>
<th>$k_c$ (series)</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>0.84371559</td>
<td>0.80679833</td>
<td>0.83401</td>
</tr>
<tr>
<td>5</td>
<td>0.88419452</td>
<td>0.86482139</td>
<td>0.87694</td>
</tr>
<tr>
<td>6</td>
<td>0.90737533</td>
<td>0.89528450</td>
<td>0.90227</td>
</tr>
<tr>
<td>7</td>
<td>0.92249907</td>
<td>0.91415507</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>0.93322581</td>
<td>0.92708735</td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>0.94127183</td>
<td>0.93655225</td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>0.94755067</td>
<td>0.94380246</td>
<td></td>
</tr>
<tr>
<td>11</td>
<td>0.95259678</td>
<td>0.94954484</td>
<td></td>
</tr>
<tr>
<td>12</td>
<td>0.95674577</td>
<td>0.95421088</td>
<td></td>
</tr>
<tr>
<td>13</td>
<td>0.96022002</td>
<td>0.95808010</td>
<td></td>
</tr>
<tr>
<td>14</td>
<td>0.96317327</td>
<td>0.96134212</td>
<td></td>
</tr>
<tr>
<td>15</td>
<td>0.96571543</td>
<td>0.9613038</td>
<td></td>
</tr>
<tr>
<td>16</td>
<td>0.96792731</td>
<td>0.96654164</td>
<td></td>
</tr>
<tr>
<td>17</td>
<td>0.96986969</td>
<td>0.96864786</td>
<td></td>
</tr>
<tr>
<td>18</td>
<td>0.97158923</td>
<td>0.97050371</td>
<td></td>
</tr>
<tr>
<td>19</td>
<td>0.97312237</td>
<td>0.97215148</td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>0.97449796</td>
<td>0.97362440</td>
<td></td>
</tr>
<tr>
<td>21</td>
<td>0.97573918</td>
<td>0.97494898</td>
<td></td>
</tr>
<tr>
<td>22</td>
<td>0.97686486</td>
<td>0.97614660</td>
<td></td>
</tr>
<tr>
<td>23</td>
<td>0.97789045</td>
<td>0.97723472</td>
<td></td>
</tr>
<tr>
<td>24</td>
<td>0.97882878</td>
<td>0.97822773</td>
<td></td>
</tr>
<tr>
<td>25</td>
<td>0.97969053</td>
<td>0.97913760</td>
<td></td>
</tr>
<tr>
<td>26</td>
<td>0.98048475</td>
<td>0.97997436</td>
<td></td>
</tr>
<tr>
<td>27</td>
<td>0.98121908</td>
<td>0.98074650</td>
<td></td>
</tr>
<tr>
<td>28</td>
<td>0.98190007</td>
<td>0.98146124</td>
<td></td>
</tr>
<tr>
<td>29</td>
<td>0.98253332</td>
<td>0.98212475</td>
<td></td>
</tr>
<tr>
<td>30</td>
<td>0.98312370</td>
<td>0.98274236</td>
<td></td>
</tr>
</tbody>
</table>
2. CRITICAL ENERGY

The dimensionless critical energy per spin is defined as

\[ U_c = \frac{\text{critical energy}}{J/NZ/2} \]  

(39)

where \( N \) is the total number of sites.

\[ U_c = \frac{\langle H \rangle}{J/NZ/2} = \frac{\langle \sum_i \sum_j J_{ij} S_i S_j \rangle}{J/NZ/2} \]

or, \( U_c = \frac{\langle 0, S_i, S_j \rangle}{J(0)} \)  

(40)

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

Using the identity (5) we have

\[ U_c = \frac{\langle 0, \tan h^{-1} \theta \rangle}{J(0)} \]

(41)

The critical energy \( U_c \) at the critical temperature

\[ \left( k_c = \frac{4}{c J(0)} \right) \]  

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 $4 \leq d \leq 30$

<table>
<thead>
<tr>
<th>$d$</th>
<th>$U_c$ (i-δ)</th>
<th>$U_c$ (sph.)</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>0.047800991</td>
<td>0.048300418</td>
</tr>
<tr>
<td>5</td>
<td>0.033572955</td>
<td>0.033794652</td>
</tr>
<tr>
<td>6</td>
<td>0.026060705</td>
<td>0.026178874</td>
</tr>
<tr>
<td>7</td>
<td>0.021390376</td>
<td>0.021461234</td>
</tr>
<tr>
<td>8</td>
<td>0.018182152</td>
<td>0.018228162</td>
</tr>
<tr>
<td>9</td>
<td>0.015830301</td>
<td>0.015861937</td>
</tr>
<tr>
<td>10</td>
<td>0.014026669</td>
<td>0.014049384</td>
</tr>
<tr>
<td>11</td>
<td>0.012596918</td>
<td>0.012613790</td>
</tr>
<tr>
<td>12</td>
<td>0.011434399</td>
<td>0.011447280</td>
</tr>
<tr>
<td>13</td>
<td>0.010469914</td>
<td>0.010479974</td>
</tr>
<tr>
<td>14</td>
<td>0.0096564603</td>
<td>0.0096644693</td>
</tr>
<tr>
<td>15</td>
<td>0.0089609251</td>
<td>0.0089674058</td>
</tr>
<tr>
<td>16</td>
<td>0.0083592725</td>
<td>0.0083645911</td>
</tr>
<tr>
<td>17</td>
<td>0.0073536161</td>
<td>0.0078380351</td>
</tr>
<tr>
<td>18</td>
<td>0.0073703605</td>
<td>0.0073740723</td>
</tr>
<tr>
<td>19</td>
<td>0.0069589827</td>
<td>0.0069621306</td>
</tr>
<tr>
<td>20</td>
<td>0.0065912068</td>
<td>0.0065938997</td>
</tr>
<tr>
<td>21</td>
<td>0.0062604334</td>
<td>0.0062627549</td>
</tr>
<tr>
<td>22</td>
<td>0.0059613338</td>
<td>0.0059633493</td>
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<tr>
<td>23</td>
<td>0.0056895580</td>
<td>0.0056913191</td>
</tr>
<tr>
<td>24</td>
<td>0.0054415191</td>
<td>0.0054430669</td>
</tr>
<tr>
<td>25</td>
<td>0.0052142327</td>
<td>0.0052156003</td>
</tr>
<tr>
<td>26</td>
<td>0.0050051955</td>
<td>0.0050064098</td>
</tr>
<tr>
<td>27</td>
<td>0.0048122915</td>
<td>0.0048133748</td>
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<td>0.0046337205</td>
<td>0.0046346908</td>
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<td>29</td>
<td>0.0044679405</td>
<td>0.004468131</td>
</tr>
<tr>
<td>30</td>
<td>0.0043136234</td>
<td>0.0043144109</td>
</tr>
</tbody>
</table>
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:

$$\sum_i S_i^2 = N/4 \quad (42a)$$

(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)

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

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).
\begin{align*}
K_c(\text{sph.}) &= (1 + \frac{1}{2d} + \frac{3}{(2d)^2} + \frac{12}{(2d)^3} + \frac{60}{(2d)^4} + \ldots)^{-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 \tag{43}
\end{align*}

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

\begin{align*}
U_c(\text{sph.}) &= \frac{1 - K_c(\text{sph.})}{4} \tag{44}
\end{align*}

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

\begin{align*}
U_c(\text{sph.}) &= \frac{1}{8d} + \frac{1}{8d^2} + \frac{21}{96d^3} + \frac{105}{192d^4} + \frac{215}{128d^5} \tag{45}
\end{align*}
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

$$\frac{1}{d} - \frac{A_1}{d^2} - \frac{A_2}{d^3} + \ldots$$

(46)

for $K_c$ (i-δ), or

$$\frac{A_1}{d} + \frac{A_2}{d^2} + \frac{A_3}{d^3} + \ldots$$

(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

$$1 - K_c(i-δ) = \frac{A_1}{d_1} + \frac{A_2}{d_1^2} + \frac{A_3}{d_1^3}$$

(48a)
\[ 1 - K_c \frac{(i-\delta)}{d=d_2} = \frac{A_1}{d_2} + \frac{A_2}{d_2^2} + \frac{A_3}{d_2^3} \]  
(48b)

\[ 1 - K_c \frac{(i-\delta)}{d=d_3} = \frac{A_1}{d_3} + \frac{A_2}{d_3^2} + \frac{A_3}{d_3^3} \]  
(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

\[ \ln(1-K_c) = \ln A_n - n \ln d, \text{ (large } d) \]  
(49)

considering \(A_n\) and \(n\) as unknowns.

(ii) One chooses a pair of neighbouring \(d\)-values \((d = 10 \text{ and } 11, \text{say})\) 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 \(d = 3\).
(iv) One plots the resulting $A_n$ and $n$ vs. $1/d$.

(v) One extrapolates these curves to $1/d \to 0$. $n$ 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

$$\ln \left( 1 - K_c \frac{A_1^G}{d^1} \right) = \ln A_n - n \ln d$$

(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 $1/d \to 0$. 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 $\Lambda_{\text{max}} \equiv M$ such that when the equation
\[ \ln \left( \prod_{j=1}^{M} K_c - \frac{A_j}{d^j} - \frac{A_{G+1}}{d^{G+1}} \right) = \ln A_n - n \ln d \]  

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 \( A_M + 1 \).

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 $\sum_{j=0}^{\infty} a_j d^{-j}$ of $K_c$ and $U_c$

<table>
<thead>
<tr>
<th>n</th>
<th>0</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
</tr>
</thead>
<tbody>
<tr>
<td>$K_c$ (series)</td>
<td>1</td>
<td>-1/2</td>
<td>-1/3</td>
<td>-13/24</td>
<td>-979/720</td>
<td>-2009/480</td>
</tr>
<tr>
<td>$K_c$ (sph.)</td>
<td>1</td>
<td>-1/2</td>
<td>-1/2</td>
<td>-7/8</td>
<td>-35/16</td>
<td>-215/32</td>
</tr>
<tr>
<td>$K_c$ (i-δ)</td>
<td>1</td>
<td>-1/2</td>
<td>-1/6</td>
<td>-5/8</td>
<td>-83/96</td>
<td>---</td>
</tr>
<tr>
<td>$K_c$ (Bethe)</td>
<td>1</td>
<td>-1/2</td>
<td>-1/12</td>
<td>-1/24</td>
<td>-19/720</td>
<td>-89/480</td>
</tr>
<tr>
<td>$U_c$ (series)</td>
<td>0</td>
<td>1/8</td>
<td>1/8</td>
<td>21/96</td>
<td>105/192</td>
<td>215/128</td>
</tr>
<tr>
<td>$U_c$ (sph.)</td>
<td>0</td>
<td>1/8</td>
<td>1/8</td>
<td>21/96</td>
<td>105/192</td>
<td>215/128</td>
</tr>
<tr>
<td>$U_c$ (i-δ)</td>
<td>0</td>
<td>1/8</td>
<td>1/8</td>
<td>19/96</td>
<td>103/192</td>
<td>---</td>
</tr>
<tr>
<td>$U_c$ (Bethe)</td>
<td>0</td>
<td>1/8</td>
<td>1/16</td>
<td>1/32</td>
<td>1/64</td>
<td>1/128</td>
</tr>
</tbody>
</table>
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)

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

(52)

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

\[
\ln Z = \ln 2 + \frac{1}{4q} K^{-2} + \frac{1}{8q} K^{-4} + \frac{1}{q^3} \left[ -\frac{7}{24} K^{-4} + \frac{1}{3} K^{-6} \right] + \frac{1}{q^4} \left[ \frac{23}{12} K^{-6} + \frac{27}{16} K^{-8} \right] + \frac{1}{q^5} \left[ \frac{113}{45} K^{-6} - \frac{415}{24} K^{-8} + \frac{62}{5} K^{-10} \right] + \ldots
\]  

(53)

where \( K = \frac{4}{\beta J(0)} = \frac{4}{\beta q} \) 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):

\[
U_c = \frac{1}{3q} \left( \frac{\partial \ln Z}{\partial \beta} \right)_{K = K_c}
\]  

(54)

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

(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 \( K_c(=4/\beta_cJ(0)) \) from the Bethe approximation is given by (Domb 1960)

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

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

\[
K_c(\text{Bethe}) = 1 - \frac{1}{2d} - \frac{1}{12d^2} - \frac{1}{24d^3} - \frac{19}{720d^4} - \frac{89}{480d^5} \quad \ldots \quad (57)
\]

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

\[
U_c(\text{Bethe}) = -\left\{1/(N\beta d)\right\} - NqJ/(8(q-1)) \quad (58)
\]

or,

\[
U_c(\text{Bethe}) = \frac{1}{8d} + \frac{1}{16d^2} + \frac{1}{32d^3} + \frac{1}{64d^4} + \frac{1}{128d^5} + \frac{1}{256d^6} + \ldots \quad (59)
\]
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)

\[
A = 1 
\]

(17)

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

\[
\frac{1}{\langle S_i \tanh S_0 \rangle} \frac{1}{\langle \tanh S_0 \rangle} = \frac{1}{1/J(0) < S_i S_i >} \frac{1}{1/J(0) < O_i \tanh S_0 >} 
\]

(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

\[
\frac{1}{\langle S_j \tanh S_0 \rangle} \frac{1}{\langle \tanh S_0 \rangle} = \frac{1}{1/J(0) < S_j S_i >} \frac{1}{1/J(0) < O_i ^2 >} 
\]

(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 (Lee 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 ($Z = 3$):

\[
\frac{O_i}{J(0)} = \frac{J(S_1 S_2 S_3)}{ZJ} = \frac{J(\sigma_1^x \sigma_2^x \sigma_3^x)}{2ZJ}
\]  

(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 $\sigma$'s have eigenvalues +1 and -1. Defining $\sigma_i$ as the sum of $\sigma$-operators neighbouring site $i$,
\[ \theta_i = \sigma_1 + \sigma_2 + \sigma_3 \]  

one can write

\[ \frac{O_i}{J(0)} = \frac{\theta_i}{2Z} \]  

or,

\[ \frac{O_i}{J(0)} = \frac{\theta_i}{6} \]  

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

\[ (\theta_i^2 - 3) (\theta_i^2 - 1^2) = 0 \]  

one can write (14) as

\[ A = \frac{(1/2) \left< \tanh^2 \left( \frac{\theta_i}{26} \right) \right>}{\left< \theta_i \right> \tanh \left( \frac{\theta_i}{26} \right)} = \frac{x_1 < \theta_i^2 > + y_1}{x_2 < \theta_i^2 > + y_2} \]  

the \( x_1, y_1 \), etc. being functions of \( \beta \) 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)),

\[ (1/2) \tanh^2 \left( \frac{\beta J(0)/12 \times 1}{2} \right) = x_1 + y_1 \]  

\[ (1/2) \tanh^2 \left( \frac{\beta J(0)/12 \times 3}{2} \right) = 9x_1 + y_1 \]
$$\frac{1}{6} \tanh \left[ \left( \frac{\beta J(0)}{12} \right) \times 1 \right] = x_2 + y_2 \quad (66c)$$

and

$$\frac{3}{6} \tanh \left[ \left( \frac{\beta J(0)}{12} \right) \times 3 \right] = 9 x_2 + y_2 \quad (66d)$$

to get

$$x_1 = \frac{1}{27}$$

$$y_1 = \frac{7}{54}$$

$$x_2 = y_2 = \frac{1}{12\sqrt{3}} \quad (67)$$

where use has been made of \((\text{Dom}b\ 1974)\)

$$\tanh \left( \frac{\beta J(0)}{12} \right) = \frac{1}{\sqrt{3}} \quad (68)$$

Using the identity (cf. sec. 1)

$$\langle \sigma_1 \sigma_i \rangle = \langle \sigma_i \rangle \tanh \left( \frac{\beta J(0)}{12} \theta_i \right) \quad (69)$$

and putting \(\theta_i\) for \(\sigma_i\), one gets

$$\langle \sigma_1 \theta_i \rangle = \langle \theta_i \rangle \tanh \left( \frac{\beta J(0)}{12} \theta_i \right) \quad (70)$$

or,

$$3 \langle \sigma_0 \sigma_1 \rangle = 6 \left[ x_2 \langle \theta_1^2 \rangle + y_2 \right] \quad (71)$$

using the denominator of equation (65).

Since, (see Syozi 1972)

$$\langle \sigma_0 \sigma_1 \rangle = \frac{4}{3\sqrt{3}} \quad (72)$$

(71) leads to
\[
< q_i^2 > = 7
\]  \hspace{1cm} (73)

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

\[
A = \frac{7}{(4\sqrt{3})} = 1.01036 \text{ (H.C. lattice)}
\]  \hspace{1cm} (74)

A' can be obtained in a similar fashion,

\[
A' = \frac{(1/2) < q_i / 6 \tanh [(8J(0)/12) \theta_i] >}{(1/6^2) < \theta_i^2 >}
\]  \hspace{1cm} (75)

or \[
A' = \frac{4\sqrt{3}}{7} = 0.98974
\]  \hspace{1cm} (76)

Note that \( A A' = 1 \) for this case.

(ii) The simple quadratic lattice:

\[
\begin{array}{c}
\sigma_1 \\
\sigma_2 \\
\sigma_3 \\
\sigma_4
\end{array}
\]

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

\[
0_i/J(0) = q_i/(2Z) = q_i/8
\]  \hspace{1cm} (77)

and the spin-operator reduction relation takes the form

\[
\left( q_i^2 - 4 \right) \left( q_i^2 - 2 \right) = 0
\]  \hspace{1cm} (78)

So one can write for A
A = \frac{(1/2) \tanh^2 [(\beta J(0)/16)\theta_i]}{\langle (\theta_i/8) \tanh[(\beta J(0)/16)\theta_i]\rangle} = \frac{x_1 < \theta_i^4 > + y_1 < \theta_i^2 >}{x_2 < \theta_i^4 > + y_2 < \theta_i^2 >} \quad (79)

One has (Domb 1974)

\tanh \left[ \beta J(0)/16 \right] = 1/(1+\sqrt{2}) \quad (80)

from which one gets

\begin{align*}
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{align*} \quad (81)

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

\begin{align*}
\langle \sigma_0 \sigma_1 \rangle &= \frac{1}{\sqrt{2}} \\
\langle \sigma_1 \sigma_2 \rangle &= \frac{2}{\pi} \\
\langle \sigma_1 \sigma_3 \rangle &= 1 - \frac{4}{\pi}^2 \\
\langle \sigma_1 \sigma_2 \sigma_3 \sigma_4 \rangle &= (\frac{4}{\pi})^2 (\pi - 1) - 3
\end{align*} \quad (82)

So,

\begin{align*}
\langle \theta_i^2 \rangle &= \langle (\sigma_1 + \sigma_2 + \sigma_3 + \sigma_4)^2 \rangle \\
&= 4 < \sigma_1^2 > + 8 < \sigma_1 \sigma_2 > + 4 < \sigma_1 \sigma_3 >
\end{align*}

Or \( \langle \theta_i^2 \rangle = 11.47181924 \) \quad (83)
\[ \langle \sigma_i \rangle = 40 + 128 < \sigma_i \sigma_i > + 64 < \sigma_i \sigma_j > + 24 < \sigma_i \sigma_j \sigma_j \sigma_i > = 170.8727696 \]  
(84)

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

\[ A = 0.355340865/0353553391 = 1.0050557 \]  
(85)

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

\[ < \sigma_i \theta_i > = < \theta_i \tanh((\beta J(0)/16)\theta_i) > \]

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

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

Now,

\[ A' = \frac{(1/2) \langle (\sigma_i/J(0)) \tanh (\beta \sigma_i/2) \rangle}{\langle (\sigma_i/J(0))^2 \rangle} \]

\[ = \frac{(1/2) \langle \sigma_i \tanh((\beta J(0)/16)\sigma_i) \rangle}{(1/64)\langle \sigma_i^2 \rangle} \]  
(87)

so that \( A' = (1/2) \times 0.353553391/((1/64) \times 11.47181924) = 0.9862176 \)  
(88)

(iii) The plane triangular lattice:
Here $\mathcal{Z} = 6$ so that one has from equation (62)

$$O_1/J(0) = \phi_1^{(22)} = \phi_1/12$$

(89)

From Stephenson (1964) we have

$$< \sigma_1^{0} \sigma_1^{1} > = < \sigma_1^{2} \sigma_2^{2} > = 2/3$$

$$< \sigma_1^{1} \sigma_1^{2} > = 0.5813215$$

$$< \sigma_1^{1} \sigma_4^{1} > = 0.56192357$$

$$< \sigma_1^{2} \sigma_3^{4} \sigma_4^{2} > = -0.48763512$$

$$< \sigma_1^{2} \sigma_3^{4} \sigma_5^{2} > = -0.45641434$$

$$< \sigma_1^{2} \sigma_4^{4} \sigma_5^{2} > = 0.47425596$$

$$< \sigma_1^{2} \sigma_3^{4} \sigma_4^{6} \sigma_6^{2} > = 0.39315517$$

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

Due to the spin-operator reduction relation

$$\left(\phi_i^2 - 6^2\right) \left(\phi_i^2 - 4^2\right) \left(\phi_i^2 - 2^2\right) = 0$$

(92)

one can write

$$A = \frac{(1/2) \tanh^2 \left[\mathcal{B}J(0)/24 \phi_1\right]}{\left< (\phi_1^{1/2}) \tanh \left[\mathcal{B}J(0)/24 \phi_1\right]\right> \tanh \left[\mathcal{B}J(0)/24 \phi_1\right]}$$

(93)

$$= \frac{x_1 \phi_1^6 + x_2 \phi_1^4 + x_3 \phi_1^2}{(1/12) \phi_1 \tanh\left[\mathcal{B}J(0)/24 \phi_1\right]}$$

(94)

wherin

$$\begin{align*}
x_1 &= 1.6758787 \times 10^{-5} \\
x_2 &= -1.2726757 \times 10^{-3} \\
x_3 &= 3.6072562 \times 10^{-2}
\end{align*}$$

(95)
One also gets

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

$$ < \theta_i^4 > = 96 + 56 \left[ 6 < \sigma_1 \sigma_2 > + 6 < \sigma_1 \sigma_3 > + 3 < \sigma_1 \sigma_4 > \right] $$

$$ + 24 \left[ 6 < \sigma_1 \sigma_2 \sigma_3 \sigma_4 > + 6 < \sigma_1 \sigma_2 \sigma_3 \sigma_5 > + 3 < \sigma_1 \sigma_2 \sigma_4 \sigma_5 > \right] $$

$$ = 779.81673 \quad (97) $$

and

$$ < \theta_i^6 > = 2256 + 1712 \left[ 6 < \sigma_1 \sigma_2 > + 6 < \sigma_1 \sigma_3 > + 3 < \sigma_1 \sigma_4 > \right] $$

$$ + 1200 \left[ 6 < \sigma_1 \sigma_2 \sigma_3 \sigma_4 > + 6 < \sigma_1 \sigma_2 \sigma_3 \sigma_5 > + 3 < \sigma_1 \sigma_2 \sigma_4 \sigma_5 > \right] $$

$$ + 720 < \sigma_1 \sigma_2 \sigma_3 \sigma_4 \sigma_5 \sigma_6 > $$

$$ = 26748.923 \quad (98) $$

thereby having the value of the numerator of \( A \),

\[
A_n = 0.33409876 \quad (99)
\]

The denominator of \( A \) is obtained very easily;

\[
< \sigma_0 \theta_i > = < \theta_i \tanh[(8J(0)/24)\theta_i] > \quad (70)
\]

or, \( 6 < \sigma_0 \sigma_i > = 12 A_D \)

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

giving

\[
A = 1.002296 \quad (100)
\]

Now,

\[
A' = \frac{(1/2) < (\theta_i/12) \tanh[(8J(0)/24)\theta_i] >}{(1/144) < \theta_i^2 >} \quad (101)
\]
or, \[ A' = \frac{(1/2)}{(1/3)} = 0.9857315 \]
\[ (1/144) \times 24.347397 \]

(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.

\[ \begin{array}{c}
\sigma_1 \\
\sigma_2 \\
\sigma_3 \\
\end{array} \]

Here,
\[ \theta_i / J(0) = \theta_i (2Z) = \theta_i / 6 \]

(103)

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

\[ \tanh \left( \frac{\beta J(0)}{12} \right) = 0.51814 \]

(104)

and \[ \langle \sigma_0 \sigma_1 \rangle = 0.55769 \]

(105)

Due to the spin operator reduction relation, one has

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

(106)
and finds
\[
x_1 = 0.038214
\]
\[
y_1 = 0.047832
\]
\[
x_2 = 0.09602
\]
\[
y_2 = 0.038524
\]

Also, the identity
\[
< \sigma_1 \theta_i > = < \theta_i \tanh [(\beta J/12) \theta_i] >
\]

leads to
\[
3 < \sigma_0 \sigma_1 > = 6 [ x_2 \theta_i^2 ] + y_2
\]

So that,
\[
< \theta_i^2 > = 5.0243
\]

Thus
\[
A = \frac{0.28802}{0.27885} = 1.033
\]

and
\[
A' = \frac{(1/2) < \theta_i / 6 \tanh [(\beta J/12) \theta_i] >}{(1/36) < \theta_i^2 >}
\]

or, \( A' = 18 \times \frac{0.27885}{5.0243} = 0.999 \)

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 of $A$ and $A'$ for the simple cubic (SC), honeycomb (HC),
simple quadratic (SQ), plane triangular (PT) and
hydrogen peroxide (HP) lattices, as given in section 7.

<table>
<thead>
<tr>
<th>Lattices</th>
<th>$A$</th>
<th>$A'$</th>
</tr>
</thead>
<tbody>
<tr>
<td>SC</td>
<td>1.007±0.003</td>
<td>0.990±0.003</td>
</tr>
<tr>
<td>HC</td>
<td>1.01036</td>
<td>0.98974</td>
</tr>
<tr>
<td>SQ</td>
<td>1.00506</td>
<td>0.98622</td>
</tr>
<tr>
<td>PT</td>
<td>1.0023</td>
<td>0.98573</td>
</tr>
<tr>
<td>HP</td>
<td>1.033</td>
<td>0.999</td>
</tr>
</tbody>
</table>
8. INVESTIGATION OF THE FUNCTION \( \frac{U_c}{(1-K_c)} \) FOR VARIOUS ISING LATTICES.

From the equation (44) it is obvious that

\[
\frac{U_c}{1 - K_c} = \frac{1}{4}
\]

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 \( \frac{U_c}{(1-K_c)} \), constructed from Syozi (1972) and Domb (1974), for various lattices. The values of \( \frac{U_c}{(1-K_c)} \) 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 hypertriangular (HTr) lattices.

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

* Values have been taken from FGM.

** 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 wherein certain classes of diagrams are neglected (Burley 1972); (iii) the i-δ theory values of $K_h$ and $U_c$ are consistent with the series values to within 1% for $4<d<6$; (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 III); (vi) the series formula gives values, $d>6$, 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 MERV 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 Kc, the discrepancy for d > 7 is < 0.053% between the formula and the calculated values.
REFERENCES


REFERENCES


APPENDIX A

We have equation (15)

\[ \langle S_i S_j \rangle = (A/J(0)) \langle S_j O_i \rangle + \delta_{ij} L \]  

(15)

The Fourier transforms of \( \langle S_i S_j \rangle \) is by definition

\[ G(q) = \sum_j \langle S_i S_j \rangle \exp \left( iq \cdot (\mathbf{R}_j - \mathbf{R}_i) \right) \]  

(4)

Substituting from (15),

\[
G(q) = \sum_j (A/J(0)) \langle O_i S_j \rangle \exp \left( -iq \cdot (\mathbf{R}_j - \mathbf{R}_i) \right) + \sum_j \delta_{ij} L \exp \left( iq \cdot (\mathbf{R}_j - \mathbf{R}_i) \right)
\]

\[
= L + \sum_j (A/J(0)) \langle S_j S_j \rangle \exp \left( -iq \cdot (\mathbf{R}_j - \mathbf{R}_i) \right) \exp \left( iq \cdot (\mathbf{R}_j - \mathbf{R}_i) \right)
\]

\[
= L + A/J(0) \sum_i J_{ii} \exp \left( -iq \cdot (\mathbf{R}_j - \mathbf{R}_i) \right) \sum_j \langle S_i S_j \rangle \exp \left( iq \cdot (\mathbf{R}_j - \mathbf{R}_i) \right)
\]

or,

\[ G(q) = L + (A/J(0)) J(q) G(q) \]  

(A 1)

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

\[ G(q) = L/1 - A J(q)/J(0) \]  

(A 2)

From (A 2),

\[ q \rightarrow G(q) = L \sum_q \frac{1}{1 - A J(q)} / J(0) \]  

(A 3)

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

\[ \frac{1}{N} \sum_q G(q) = \langle S_i^2 \rangle = 1/4 \]  

(A 4)
for the spin - 1/2 system. Thus we have for \( L \)

\[
L = \frac{1}{4} \left/ \left( \frac{1}{N} \sum_{q^*} \frac{1}{1 - A J(q^*) / J(0)} \right) \right.
\]

\[ (A \, 5) \]

Thus equation (A 2) is

\[
G(q) = \frac{1/4}{(1/N) \sum_{q^*} 1/ \left( 1 - A J(q^*) / J(0) \right)} \times \frac{1}{(1 - A J(q) / J(0))}.
\]

\[ (16) \]
APPENDIX B

By definition

\[ T_2 = \frac{\langle O_i^2 \rangle}{J^2(0)} \]  

(23)

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

\[ = \frac{1}{J^2(0)} \sum_{i,k,l} \frac{1}{N} \sum_q J(q) \exp\left\{ -i \left( \hat{R}_k - \hat{R}_l \right) \cdot q \right\} \times \]

\[ \frac{1}{N} \sum_q J(q') \exp\left\{ i \left( \hat{R}_l - \hat{R}_k \right) \cdot q' \right\} \langle S_k S_l \rangle \]  

(B1)

Because by definition

\[ J(q) = \sum_j J_{ij} \exp\left\{ + i q \cdot (R_j - R_i) \right\} \]  

(13)

giving,

\[ J_{ij} = \frac{1}{N} \sum_q J(q) \exp\left\{ -i q \cdot (R_j - R_i) \right\} \]  

(B2)

Thus

\[ T_2 = \frac{1}{J^2(0)} \sum_{k,l,q,q'} J(q) J(q') \langle S_k S_l \rangle \exp\left\{ i \left( \hat{R}_k - \hat{R}_l \right) \cdot q \right\} \]

\[ \times \exp\left\{ i \hat{R}_i \cdot \left( q - q' \right) \right\} \]

or,

\[ T_2 = \frac{1}{J^2(0)} \sum_{k,l,q} J^2(q) \langle S_k S_l \rangle \exp\left\{ i \left( \hat{R}_l - \hat{R}_k \right) \cdot q \right\} \]  

(B3)

where use was made of

\[ \sum_i \exp\left\{ i \hat{R}_i \cdot (q - q') \right\} = N \delta_{qq'} \]  

(B4)
Thus

\[ T_2 = 1/J^2(0) \quad 1/N^2 \sum_q J^2(q) \quad G(q) \]

or,

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

\[ = \frac{1}{N} \sum_q \frac{J^2(q)}{J^2(0)} \times \frac{1}{4F(1)} \times \frac{1}{1-\frac{J(q)}{J(0)}} \]

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

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

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

where use was made of

\[ \sum_q J(q) = \sum_q \sum_j^i J_{ij} \exp \{ i q, \cdot (\mathbf{R}_j - \mathbf{R}_i) \} \]

\[ = \sum_j^{i} \sum_q J_{ij} \exp \{ i q, \cdot (\mathbf{R}_j - \mathbf{R}_i) \} \]

\[ = \sum_j^{i} N \delta_{ij} \]

\[ = N J_{ii} \]

or, \[ \sum_q J(q) = 0 \] \tag{B6}
from the definition of the exchange integral $J_{ii}$. Thus

$$T_2 = \frac{1}{4} \left( 1 - \frac{1}{F(1)} \right)$$

(26)
APPENDIX C

The Watson sum

\[ F_d(1) = \frac{1}{N} \sum_q \frac{1}{1 - J(q)/J(0)} \]  

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

\[ F_d(1) = d \int_0^\infty \{ e^{-x} I_0(x) \}^d \text{dx} \]  

(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 \( 1/d \) (Gerber and Fisher 1974):

\[ F_d(1) = 1 + \frac{1}{2d} + \frac{3}{(2d)^2} + \frac{12}{(2d)^3} + \frac{60}{(2d)^4} + \cdots + \cdots \]  

(C2)

Since,

\[ d \int_0^\infty \{ e^{-x} I_0(x) \}^d \text{dx} \]

\[ = d \int_0^\infty e^{-x} \left( 1 + \frac{x^2}{2^2} + \frac{x^4}{2^4.4^2} + \frac{x^6}{2^6.4^2.6^2} + \cdots \right)^d \text{dx} \]
\[ d \cdot \left\{ \int_{0}^{\infty} e^{-x} \frac{dy}{d} + \int_{0}^{\infty} e^{-x} \frac{y^2}{2} \left( \frac{d}{dy} \cdot \frac{dy}{d} + \ldots \right) \right\} \]

putting \( d \cdot x = y \). Thus

\[ F_d(1) = d \left\{ \frac{1}{d} \Gamma(1) + \frac{d}{4d^3} \Gamma(3) + \ldots \right\} \]

leading to the equation (C2)

In the present work \( F_d(1) \) was calculated using (C1), integrating 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 \( d > 4 \). 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 INSLIB library function MMBS10 was used.

The value of the function \( e^{-x} I_0(x) \) obtained from INSLIB library function DCA0RE was found correct up to at least 9 decimal places for two values of \( x \) chosen randomly (Abramowitz and Stegun 1965).
We have equation (15)

\[ \langle S_i S_j \rangle = A/J(0) \langle S_i^0 S_j^0 \rangle + \delta_{ij} L \]

which reduces to

\[ \langle S_i S_j \rangle = \langle O_i S_j \rangle / J(0) + \delta_{ij} L \]

at \( T = T_c \) and in zero external field, since

\[ A = 1 \]

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

\[ \langle S_i O_i \rangle = \langle O_i^2 \rangle / J(0) + 0 \]

giving

\[ U_2 = T_2 \]

In the present theory

\[ \langle O_i^{2n+1} S_j \rangle / \langle O_i S_j \rangle = R_n, \] independent of \( j \)

So one can write, for all \( j \),

\[ \langle O_i^{2n+1} S_j \rangle / \langle O_i S_j \rangle = \langle O_i^{2n+1} S_i \rangle / \langle O_i S_i \rangle \]

or, from (33),

\[ \langle O_i^{2n+1} S_j \rangle = \frac{U_{2n+2} J^{2n+1} (0)}{U_{2n} (0)} \langle O_i S_j \rangle \]

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

\[ T_{2n+2} = \left( \frac{U_{2n+2}}{U_2} \right) T_2 \]

or, from (D3),

\[ T_{2n+2} = U_{2n+2} \quad (n = 0, 1, \ldots) \]
APPENDIX E

Correction and extension of the Appendix of FMI 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):

$$T_{2n} = \langle 0_1^{2n} \rangle / J^{2n}(0), \quad n=1,2,..,Z/2$$

(23)

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

$$T_4 = \mathcal{M}^4 \sum_{j,k,l,m} J_{ij} J_{ik} J_{il} J_{im} \langle S_j S_k S_l S_m \rangle$$

(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 FMI, 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

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

(E2)

Thus higher order correlation functions $T_4, T_6, \ldots$ etc. can be obtained in terms of $T_2$ as is obvious for the example for $T_4$.
\[ Z^{4}T_{4} = \sum_{j \neq k \neq m}^{\infty} S_{j} S_{k} S_{l} S_{m} + \sum_{j = k \neq m}^{\infty} S_{j} = \frac{1}{4} S_{l} S_{m} \]

\[ + \sum_{j = k = l = m}^{\infty} \frac{1}{16} S_{j} = \frac{1}{16} S_{k} = \frac{1}{16} S_{l} = \frac{1}{16} S_{m} \]  

(E3)

or,

\[ Z^{4}T_{4} = Z(Z-1)(Z-2)(Z-3) \frac{2}{p} \frac{4}{C_2} Z(Z-1)(Z-2) \frac{p}{4} \]

\[ + \frac{4}{C_3} Z(Z-1)p/4 + (1/2!) \frac{4}{C_2} \frac{2}{C_2} Z(Z-1)/16 + \frac{4}{C_4} Z/16 \]  

(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 FML 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 corresponding to \( T_{4} \), 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 \( 2n \leq Z \))

\[ Z(Z-1)(Z-2) \ldots . (Z-2n+1) \frac{n}{p} \]  

(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 $2nC_2$ takes care of the possibility of having any two indices equal. The corresponding contribution is

$$2^nC_2 \quad Z(Z-1) \quad \ldots (Z - 2n + 1 + n_s) \quad \frac{n-1}{P} \quad (1/4), \quad (n_s = 1) \quad \text{(E6)}$$

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

$$2^nC_3 \quad Z(Z-1) \quad \ldots (Z - 2n + 1 + n_s) \quad \frac{n-1}{P} \quad (1/4), \quad (n_s = 2) \quad \text{(E7)}$$

(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

$$(1/2!) \quad 2nC_2 \quad 2n-2C_2 \quad Z(Z-1) \quad \ldots (Z - 2n +1 + n_s) \quad \frac{n-2}{P} \quad (1/4^2), \quad (n_s = 2) \quad \text{(E8)}$$
Factorial 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

\[ 2^{n} \binom{4}{n} (Z-1) \ldots (Z-2n + 1 + n_s) \frac{n-2}{p} \left(\frac{1}{4}\right)^2 \]  \hspace{1cm} (E9)

\[ 2^{n} \binom{5}{n} (Z-1) \ldots (Z-2n + 1 + n_s) \frac{n-2}{p} \left(\frac{1}{4}\right)^2 \]  \hspace{1cm} (E10)

\[ \frac{1}{3!} \frac{2^{n} \binom{2}{n} \binom{2}{n} \binom{2}{n} (Z-1) \ldots (Z-2n+1+n_s)}{p} \left(\frac{1}{4}\right)^3 \]  \hspace{1cm} (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
polygons are connected. The corresponding contribution is

\[ \frac{2n}{C_n Z} \frac{1}{4^n} \]  

(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 E1.

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

\[ \frac{Z^{8}, T_8}{Z!} = \frac{4}{\bar{p}}/(Z-8)! + \left( \frac{3}{\bar{p}}/4 \right) \left( \frac{28}{(Z-7)!} + \frac{56}{(Z-6)!} \right) \]

\[ + \left( \frac{2}{\bar{p}/16} \right) \left( \frac{210}{(Z-6)!} + \frac{630}{(Z-5)!} \right) \]

\[ + \frac{336}{(Z-4)!} + \left( \frac{\bar{p}/64}{420/(Z-5)!} \right) \]

\[ + \frac{1260}{(Z-4)!} + \frac{756}{(Z-3)!} + \frac{64}{(Z-2)!} \}

\[ + \left( 1/256 \right) \left( \frac{105}{(Z-4)!} + \frac{110}{(Z-3)!} \right) \]

\[ + \frac{63}{(Z-2)!} + \frac{1}{(Z-1)!} \} \]  

(E13)

\[ \frac{Z^{10}, T_{10}}{Z!} = \frac{5}{\bar{p}}/(Z-10)! + \left( \frac{4}{\bar{p}/4} \right) \left( \frac{45}{(Z-9)!} + \frac{120}{(Z-8)!} \right) \]

\[ + \left( \frac{3}{\bar{p}/16} \right) \left( \frac{630}{(Z-8)!} + \frac{270}{(Z-7)!} \right) \]

\[ + \frac{2552}{(Z-6)!} + \left( \frac{2}{\bar{p}/64} \right) \left( \frac{3150}{(Z-7)!} \right) \]
\[
\frac{Z^{12}}{12!} = \frac{\hat{p}^6}{(Z-12)!} \times \left\{ \frac{\hat{p}^5}{4} \left\{ 66/(Z-11)! + 220/(Z-10)! \right\} \right. \\
+ \left. \frac{\hat{p}^4}{16} \left\{ 1485/(Z-10)! + 8415/(Z-9)! \right\} \right. \\
+ \left. 10032/(Z-8)! \right\} \times \left\{ \frac{\hat{p}^3}{64} \left\{ 13860/(Z-9)! \right\} \right. \\
+ \left. 97020/(Z-8)! + 183876/(Z-7)! \right\} \\
+ \left. 90112/(Z-6)! \right\} \times \left\{ \frac{\hat{p}^2}{256} \left\{ 51975/(Z-8)! \right\} \right. \\
+ \left. 381150/(Z-7)! + 807345/(Z-6)! \right\} \\
+ \left. 544335/(Z-5)! + 87296/(Z-4)! \right\} \\
+ \left. (\hat{p}/1024) \left\{ 62370/(Z-7)! + 415800/(Z-6)! \right\} \right. \\
+ \left. 783090/(Z-5)! + 458370/(Z-4)! \right\} \\
+ \left. 65406/(Z-3)! + 1024/(Z-2)! \right\}
\]
\[ + \left( \frac{1}{4095} \right) \left( \frac{10395}{(Z-6)!} + \frac{51975}{(Z-5)!} \right) \]
\[ + \frac{65835}{(Z-4)!} + \frac{21120}{(Z-3)!} \]
\[ + \frac{1023}{(Z-2)!} + \frac{1}{(Z-1)!} \}
\]

\[ (E15) \]

The expressions for \( T_8 \) and \( T_{10} \) are correct while those of \( R1 \) are not. It was thought worthwhile to express \( T_{12} \) as well (not done in \( R1 \)), noting that \( Z \) is equal to 12 for the FCC lattice.

Analytic check on values thus obtained:

The 1-\( \delta \) relations are

\[
\frac{\langle O_1 / J - S_\delta \rangle^{2n+1}}{\langle O_1 / J - S_\delta \rangle^{2n+1}} S_1 = \frac{\langle O_1 / J - S_\delta \rangle^{2n+1}}{\langle O_1 / J - S_\delta \rangle^{2n+1}} S_\delta, \quad (n = 1, 2, \ldots, \frac{Z}{2} - 1)
\]

\[ (30) \]

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

\[
T_{2n+2} = \left( \frac{1}{Z} \right)^{2n+1} \sum_{q=1}^{n} \left( \frac{2q}{2} \right) T_{2n+2-2q} \left( \frac{2n+1}{C_{2q-1} - \frac{1}{2}} \right) C_{2q}
\]

\[ + \left( \frac{1}{Z} \right)^{2n+2} + \left( T_{Z-1}/4 \right) \sum_{q=1}^{n} \left( Z - \left( \frac{2n+1}{Z} \right) \right)
\]

\[ + \left( \frac{1}{Z} \right)^{2n-2q} U_{2n+2-2q, (1/2)} \left( \frac{2q}{Z} \right) \left( \frac{2n+1}{C_{2q} - C_{2q+1}} \right) / U_{2(Z-1)} \]

\[ (E16) \]
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

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

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

\[
U_Z = C_{Z2} T_2 + C_{Z4} T_4 + \ldots + C_{ZZ} T_Z
\]  \hspace{1cm} \text{(E17)}

where the coefficients \( C_{mn} \) can be obtained by the procedure outlined in Sec. 1 (equations (22a) and (22b)) for a given \( \beta \). Thus we have \((Z-1)\) linearly independent simultaneous equations to solve for \((Z-1)\) unknowns \( T_4, T_6, \ldots, T_Z, U_2, U_4, \ldots, U_Z \). (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 FMI provided one uses the \( \beta \) given by

\[
\bar{\beta} = \left(1/4\right) \tanh^2 (\beta J/4)
\]  \hspace{1cm} \text{(E18)}

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

\[
\left( T_2 - 1/4Z \right) / \left( 1-1/Z \right) = \left(1/4\right) \tanh^2 (\beta J/2)
\]  \hspace{1cm} \text{(E19)}
(For the present case the method of successive approximation was used to find the values of $T_4$, $T_6$, ..., $T_2$, and $U_2$, $U_4$, ..., $U_2$.) 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, FMI and series analysis (Sykes et al. 1972).
Table E1: Contributions to $z^6 T_6$ 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.

<table>
<thead>
<tr>
<th>$n_s$</th>
<th>Simplest possible diagram</th>
<th>Contribution to $z^6 T_6$ from such diagrams</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>...</td>
<td>$z(z-1)(z-2)(z-3)(z-4)(z-5) \bar{p}^3$</td>
</tr>
<tr>
<td>1</td>
<td>[ \cdots ]</td>
<td>$6C_2 z(z-1)(z-2)(z-3)(z-4) \bar{p}^2/4$</td>
</tr>
<tr>
<td>2</td>
<td>[ \cdots ]</td>
<td>$6C_3 z(z-1)(z-2)(z-3) \bar{p}^2/4$</td>
</tr>
<tr>
<td></td>
<td>[ \cdots ]</td>
<td>$\frac{1}{(2!)} 6C_2 C_2 z(z-1)(z-2)(z-3) \bar{p}/4^2$</td>
</tr>
<tr>
<td>3</td>
<td>[ \cdots ]</td>
<td>$6C_4 z(z-1)(z-2) \bar{p}/4^2$</td>
</tr>
<tr>
<td></td>
<td>[ \cdots ]</td>
<td>$6C_3 C_2 z(z-1)(z-2) \bar{p}/4^2$</td>
</tr>
<tr>
<td></td>
<td>[ \cdots ]</td>
<td>$\frac{1}{(3!)} 6C_2 C_2 z(z-1)(z-2)/4^3$</td>
</tr>
<tr>
<td>4</td>
<td>[ \cdots ]</td>
<td>$6C_5 z(z-1) \bar{p}/4^4$</td>
</tr>
<tr>
<td></td>
<td>[ \cdots ]</td>
<td>$6C_4 C_2 z(z-1)/4^3$</td>
</tr>
<tr>
<td></td>
<td>[ \cdots ]</td>
<td>$\frac{1}{(2!)} 6C_3 C_3 z(z-1) \bar{p}/4^2$</td>
</tr>
<tr>
<td>5</td>
<td>[ \cdots ]</td>
<td>$6C_6 z/4^3$</td>
</tr>
</tbody>
</table>
Table E II. The values of $K_c = \frac{4}{\beta \langle J(0) \rangle}$ and the nearest neighbour correlation function $U_c(= \frac{<H>}{JNZ/2})$ for the SC, BCC and FCC 3-dimensional lattices, based on the T's obtained using the FMI prescription, and from FCM, FMI, and from series analysis.

<table>
<thead>
<tr>
<th></th>
<th>SC</th>
<th>BCC</th>
<th>FCC</th>
</tr>
</thead>
<tbody>
<tr>
<td>$K_c$</td>
<td>present method</td>
<td>0.7724</td>
<td>0.8124</td>
</tr>
<tr>
<td></td>
<td>FCM</td>
<td>0.7564</td>
<td>0.7926</td>
</tr>
<tr>
<td></td>
<td>FMI</td>
<td>0.738^a</td>
<td>---^b</td>
</tr>
<tr>
<td></td>
<td>series analysis</td>
<td>0.7517</td>
<td>0.7938</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>SC</th>
<th>BCC</th>
<th>FCC</th>
</tr>
</thead>
<tbody>
<tr>
<td>$U_c$</td>
<td>present method</td>
<td>0.08384</td>
<td>0.06978</td>
</tr>
<tr>
<td></td>
<td>FCM</td>
<td>0.08368</td>
<td>0.06958</td>
</tr>
<tr>
<td></td>
<td>series analysis</td>
<td>0.0827</td>
<td>0.0683</td>
</tr>
</tbody>
</table>

^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)

TO FIND CRITICAL TEMPERATURE AND CRITICAL ENERGY FOR
THREE DIMENSIONAL LATTICES AND D-DIMENSIONAL
HYPERCUBIC LATTICES WITH NUMBER OF NEAREST
NEIGHBOURS = 2*D (FIXED POINT OR INTEGRAL VALUE)

DIMENSION U(100), COL(100)
DIMENSION UC(100)

UC(2) IS THE CRITICAL ENERGY
COMMON N,Z,T2,IOPTA,T(100)
COMMON/UUU/IOPOTION
CALL UERSET(0,LEVOLD)

TO GET RID OF ERROR MESSAGE
101 PRINT*, "ENTER NUMBER OF NEAREST NEIGBOURS AND GUESSED CRITEMP"
READ*, N, XX
Z=FLOAT(N)
X=2./(2**XX)
ND=N/2

C
IF (N-4) 2, 14, 16
14 T2=.25

C
GO TO 9

16 IF (N-6) 2, 3, 4
3 T2=0.851343323821

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)/(1.1/2)
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 NRIVAR(X)
XX=2./(X*Z)
PRINT *, "CRITEMP=", XX
Y=X
PRINT *, "T2N="
PRINT 100, (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="
PRINT 100, (COL(K), K=1, ND)
PRINT *, "CRITENERGY = ", UC(2)
100 FORMAT (1P5E22.10)
2 GO TO 101
STOP
END

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

----------------------------------------
SUBROUTINE LEQSOL(D,COI,ND,NI)
FROM FORTRAN IV - PROGRAMMING AND COMPUTING BY J.T. GOLDEN
THIS SOLVES SIMULTANEOUS LINEARLY INDEPENDENT EQUATIONS.
DIMENSION D(I00,101) COI(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,NI
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,NI)/D(L,I)
GO TO 103
99 PRINT*,"NO UNIQUE SOLUTION FROM LEQSOL"
103 RETURN
END

----------------------------------------
SUBROUTINE T2N(T2,N,T)
THIS GIVES T'S BASED ON I-DELTA EQUATIONS
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.
  DO 14 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

FUNCTION DDJ(Z,M,J)
  DDJ=(BIN(M,J)-BIN(M,J+1)/Z)*(2.*Z)**(-J).
RETURN
END

FUNCTION BIN(K,L)
  BIN=1.
  IF(L.EQ.0)GO TO 19
  DO 18 I=1,L
     AI=FLOAT(I)
     AL=FLOAT(L)
     AK=A(I)+AI
     TERM=(AK-AL)/AI
     BIN=BIN*TERM
  18 CONTINUE
  19 CONTINUE
RETURN
END

FUNCTION COEFB(Z,T2,L)
  ZI=1./((1.-1./Z)
  ZT2=1./((4.*Z*T2)
  COEFB=2.*ZT2*ZI*COEFA(Z,T2,L)
RETURN
END

FUNCTION COEFA(Z,T2,L)
  ZI=1./((1.-1./Z)
  ZT2=1./((4.*Z*T2)
  AL=FLOAT(L)

COEFA = .5/(1.-(Z.*AL+1.)/Z)*ZI*ZT2
RETURN
END

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)**2*(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)=2**N*(TANH(BI*YY))**2
46 CONTINUE
GO TO 95
55 DO 56 I=1,ND
AI=FLOAT(I)
D(I,NP)=2**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)=2**N*(TANH(AI*YY))**4
66 CONTINUE
GO TO 95
75 DO 76 I=1,ND
AI=FLOAT(I)
D(I,NP)=2**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)=2**N*(AI/Z)**2
86 CONTINUE
GO TO 95
95 CALL LEQSOL(D, COL, ND, NP)
RETURN
END

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

FUNCTION SIG(K)
   SIG=0.
   DO 56 I=1,K
      SIG=SIG+1.
   56 CONTINUE
   RETURN
END

SUBROUTINE DIF(X,FPRIM)
   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

SUBROUTINE U2N(T2,U,N,Y)
   THIS FINDS U'S BASED ON SUZUKI IDENTITY (EXACT)
   DIMENSION DOL(100),U(N),T(100)
   COMMON/UUL/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 T2NF1(PBAR,N,T)
IF(IOPTION.EQ.3)CALL T2NIT(T2,N,T,U,XY)
DO 86 L1=2,N,2
L1=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

SUBROUTINE T2NF1(P,N,TPP)
C
C CALCULATES T'S BASED ON FM1
C
C P=.25*(TANH(BETA*.54)**2=.25*(TANH(.5X)**2 FOR S.G.
C
DIMENSION TPP(100)
Z=FLOAT(N)
TPF(2)=.25*(Z-1.)*P/Z
TPF(4)=FAC(N)/Z**4*(P**2/FAC(N-4)+P*(1.5/FAC(N-3)+
1.0/FAC(N-2))/4.+P*(.5/FAC(N-3)+1./FAC(N-1))/.16.)
TPF(6)=FAC(N)/Z**5*(P**2/FAC(N-5)+P**2*(15./FAC(N-4)+
10./FAC(N-3)+3./FAC(N-2)+1./FAC(N-1))/64.)
TPF(8)=FAC(N)/Z**7*(P**3/FAC(N-7)+P**3*(14./FAC(N-6)+
10./FAC(N-5)+3./FAC(N-4)+1./FAC(N-3))/128.)
TPF(10)=FAC(N)/Z**10*(P**5/FAC(N-10)+P**5*120./FAC(N-9)
1+45./FAC(N-8))/4.+P**3*(176./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(N-
6))/256.+(1./FAC(N-1)+3./FAC(N-2)+210./FAC(N-
3)+105./FAC(N-4))/256.)
TPF(12)=FAC(N)/Z**12*(P**6/FAC(N-12)+P**6/16.*
1+.1365./FAC(N-11)+220./FAC(N-10)+P**4/16.*
1.+1485./FAC(N-10)+8415./
2.*FAC(N-9)+10032./FAC(N-8)+P**3/64.*
3.*13860./FAC(N-9)+
3*97020./FAC(N-8)+183876./FAC(N-7)+90112./FAC(N-6)+P**2*
4.*51975./FAC(N-8)+381150./FAC(N-7)+807345./FAC(N-
6)+3*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)/454506./FAC(N-3)+1024./FAC(N-2)+1./FAC(N-1))
RETURN
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(2i-1))
DIMENSION T1(100), TIT(100), UN(100), DOL(100)
ND=N/2
Z=FLOAT(N)
CALL T2N(T2, N, T7)
DO 201 I=2, N, 2
T1(I)=T1(I)
201 CONTINUE
DO 203 IJ2=1, 100
TIT(I)=T1(I)
203 CONTINUE
C MERGE THE PROGRAM FOR U2N
DO 86 L1=2, N, 2
L1H=L1/2
CALL GOLSOL(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
FACT=Z**(I+1)
M=I/2
SUM1=.5**(I+2)
FACT2=(T2*Z-.25)/((UN(2)**(I-1.
ASUM1=0.
DO 30 J=1, M
III2=I+2-2*J
XY=(2.*Z)**(2*J-1)
ASUM1=ASUM1+(FACT)*TIT(IIJ2)*(Z**IIJ2)*XY*DDJ(Z, I+1, 2*J-1)
30 CONTINUE
II2=II+2
SUM2=UN(III2)*(Z**(I+1)-I+1)*I
ASUM2=0.
DO 40 J=1, M
IIIJ1=I+1-2*J
IIIJ2=IIIJ1+1
XZ=(2.*Z)**(2*J)
ASUM2=ASUM2+(Z**IIIJ1)*UN(IIIJ2)*(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 SUBROUTINE U2NFM1(P,U,N,Y)
C CALCULATES U'S BASED ON FM1 AT A TEMPERATURE (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 SUBROUTINE INTBES(ND,T2)
C FOR INTEGRATION OF BESSSEL FUNCTION
COMMON/IBESS/ND1
INTEGER IER
REAL DCADRE,FBESS,A,B,AERR,ERRR,ERROR,C
EXTERNAL FBESS
ND1=ND
A=0.
B=1000000000.
AERR=0.0000000001
ERRR=0.0000000001
C=DCADRE(FBESS,A,B,AERR,ERRR,ERROR,IER)
CC=C/4.
F1=FLOAT(ND)*C
FF1=1./F1
C T2=.25*(1.+.1./F1)
PRINT*," INDECA="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
REAL FUNCTION FBESS(X)
MODIFIED BESSSEL FUNCTION OF THE FIRST KIND OF ORDER ZERO
COMMON/IBESS/ND1
INTEGER IOPT, IER
REAL MMBSSIO, ARG, Y, X
ND=ND1
IOPT=2
ARG=X
Y=MMBSSIO(IOPT, ARG, IER)
ZZ=Y**ND
FBESS=ZZ
RETURN
END

FUNCTION FOF1(ND)
ANOTHER METHOD TO CALCULATE F(1)
NOT GOOD FOR SMALL D'S
N=2*ND
Z=FLOAT(N)
FOF1=1.261/Z+3/Z**2+12/Z**3+60/Z**4+355/Z**5+2380/Z**6
1+174.30/Z**7+36.190/Z**8+1027.56/Z**9+6922/146/Z**10+
2.21248073/Z**11-601.7044143/Z**12-20802115620/Z**13
RETURN
END

SUBROUTINE NR1VAR(X)
NEWTON-RAPHSON METHOD TO FIND SOLUTION OF ONE VARIABLE
DO 10 J=1,50
X=X
CALL DIF(X,FPRIM)
X=X-FUN(X)/FPRIM
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

K. Nath and B. Frank

Department of Physics, Concordia University, Montreal, Quebec, Canada H3G 1M8

The critical temperatures $K_c$ and the nearest-neighbour correlation functions $U_i$ 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 $U_i$ are found to approach the spherical model values. Polynomial expansions 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. $U_i/(1 - K_c)$, 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 [1], 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 $K_c = -T_c / T_N$ (Mean Field) of the critical temperature $K_c = -T_c / T_N^*$ (1/d expansion) at $H = 0$.

Possible extensions of the MCRG work to $d = 4$ suggest 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 expansion of the susceptibility. They have, as well, produced (possibly asymptotic) expansions of $K_c$ in powers of the inverse dimensionality, up to $d^{-8}$. It is not clear how one obtains numerical estimates of $K_c$ from this expansion, especially as a similar expansion for the nearest-neighbour correlation function $U_i$ at the critical temperature (so called because of its relation to the critical energy per spin: $E_i = (\text{energy}) / (2N)$) proves identical to that for the spherical model up to the term in $d^{-2}$, whereas the known respective values of $K_c$ differ by $\Delta K_c$. The 1/d expansion for $K_c$ has been calculated for the spherical model by Gärber and Fisher [4]. That for $U_i$ is easily derived from it through the spherical model formula $U_i = (1 - K_c)^{1/d}$. The exact Ising 1/d expansion of $U_i$ 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 $K_c$, $U_i$, and other correlation functions consistent with within 1% with the Monte Carlo data [5] for the three-dimensional cubic lattice, it was considered of interest to apply it to the d-dimensional hypercubic case for $d = 4$, 5, ... , 30. In the expectation that, if the theory holds for all values of $d_i$, to yield better than $1\%$ accuracy, such a calculation could serve both to provide such values of $K_c$ and $U_i$ and to check whether the terms up to $d^{-2}$ in the expansion of $K_c$ derived from high-
temperature series do indeed give accurate results for $d = 4$.

In order to organise the theoretically-derived data, and for purposes of comparison, 1/d expansions are derived, as well, for $K_c$ and $U_i$ from the numerical results of the 1/d theory. It is too difficult to derive these expansions analytically, as to obtain expansion coefficients are found essentially by fitting the expansion to the data for $d = 20$ to $30$, 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 $U_i/(1 - K_c)$ being exactly 1/d 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 $d = 5$ and different lattice structures, the values of this expression are clustered around 0.33, while for $d = 2$ they are clustered around 0.60.

In this paper values are presented, in tabular form, for $K_c$ and $U_i$ for $d = 4$ to 30 for the 1/d theory and the spherical model, and for $d = 5$, 6, 7, and 8 from susceptibility series analysis [3]. The method used for fitting the results of the 1/d theory to a 1/d formula extending to $d = 20$ 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 is considered as

$$H = -\frac{1}{2} \sum_{i, j} S_i \cdot S_j$$

where $S_i$ are the Ising spins ($S_i = \pm 1$) placed in d-dimensional hypercubic lattices; $J_{ij} = J$ if $i$ and $j$ are nearest neighbours and zero otherwise; and $\phi$ is the generally non-uniform external field at site $i$.

The basic approximation of the 1/d theory is that odd correlation functions involving spins localized around site $i$, all go to zero in the same way as the
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 $A_i$ of (3) exactly up to and including $n^j=1$, and approximately for $n^j$, one attempts to fit the natural logarithm of $1-k_c(1-6)^{-n^j}M_1^j/d^n$, regarded as our data points, to the one term $\ln(A_{i+1}/d^j)$ asymptotically in the limit of large $d$. In doing so, $A_{i+1}$ 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 $A_i$ is adjusted until $j$ extrapolates (for $1/(d-6)$ to $d+1$, this adjustment following the principle of analogy with the spherical model coefficients. One then accepts the corresponding value of $A_{i+1}$ as approximate. It eventually reaches a value of $j$ such that the extrapolation of $j$ (large) is unreliable. Then $j$th defines $M_i$ in (3). As we have found $M^4$, we report only up to $M^4$ 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 $A_i$; 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 [1], and the Bethe approximation [5].

![Fig. 2. Sensitivity of the extrapolated value of $j$ to various adjusted values of $A_i$. Here, $j=4$. $A_i$ vary: 52/96, 51.5/96, and 51/96 for the upper, middle and lower curves respectively.](image)

Table II. Values of $j$ in the expansion $K = A_j/d^j$ of $K_c$ and $U_c$.

<table>
<thead>
<tr>
<th>$n$</th>
<th>$j$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1</td>
<td>1/2</td>
</tr>
<tr>
<td>2</td>
<td>1/6</td>
</tr>
<tr>
<td>3</td>
<td>1/14</td>
</tr>
<tr>
<td>4</td>
<td>1/22</td>
</tr>
<tr>
<td>5</td>
<td>1/30</td>
</tr>
</tbody>
</table>

![Table I. Values of $K_c$ and $U_c$ for the hypercubic Ising lattices for selected values of $d$.](image)
Finally, in Tables III and IV are presented values of \( U_c/(1-K_c) \), constructed from Ref. 11, for some three- and two-dimensional lattices. These values appear to be clustered about 0.33 and about 0.40 for the \( d=1 \) 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 (HT) \( d=3 \) lattices. Values for \( U_c \) and \( K_c \) are taken from Domb [8].

<table>
<thead>
<tr>
<th>SC</th>
<th>BCC</th>
<th>FCC</th>
<th>DIA</th>
<th>HP</th>
<th>HT</th>
</tr>
</thead>
<tbody>
<tr>
<td>.332</td>
<td>.3318</td>
<td>.3368</td>
<td>.3371</td>
<td>.3127</td>
<td>.3210</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>HC</th>
<th>SQ</th>
<th>PT</th>
<th>K</th>
<th>D</th>
</tr>
</thead>
<tbody>
<tr>
<td>.3897</td>
<td>.4085</td>
<td>.4239</td>
<td>.4007</td>
<td>.4191</td>
</tr>
</tbody>
</table>

**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 \( U_c \) (spherical) for \( d=4 \) is closer to \( U_c \) (series) than in \( U_c \) (spherical) for \( d=3 \) (Ref. 5); (ii) the coefficients in the \( d \) and spherical 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 \( d \)-theory values of \( K_c \) and \( U_c \) are consistent with the series values to within \( 10^{-4} \) for \( d=4 \); (iv) \( K_c \) (spherical) and \( K_c \) (dimer) approach each other much faster than either one approaches the mean field value, as \( d \rightarrow \infty \); (v) for all entries, \( U_c \) as \( d \rightarrow \infty \); this is so for different reasons than for mean field theory, since the system energy per spin \( - \infty \) in mean field theory, while here it acquires an extra factor \( d \) (see Table II); (vi) the series formula gives values, for \( d \geq 4 \), consistent with 1-d theory to within 0.1%.

The motivation behind the present work is its relevance to MCRC calculations. Apart from that, however, this work shows to what extent the 1-d 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 \( 0.05\% \) between the formula and the calculated values.

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**References**

9. C. Syosi, ibid., Vol. 1, Ch. 7.