Spin 1 Ising Model on the Cubic Lattices: Critical Temperature

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ABSTRACT

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The "i-δ relations" are used, in conjunction with three different decoupling methods for the evaluation of certain correlation functions which arise in the three-dimensional spin 1 Ising ferromagnet problem. The critical temperatures T_c for cubic lattices are calculated, and compared with results known from the analysis of series expansions. The results from indirect decoupling are consistent with the series results to within .3%, while those from direct and ratio decoupling are within .8% and .75%, respectively, of the series results. The values of the multispin correlation functions at T_c are also given.

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1 INTRODUCTION

Until recently, there has been no simple algebraic theory capable of giving, consistently, the transition temperature T_c of spin 1/2 Ising ferromagnets to within 1% of the more complex, accepted, methods. One has had to rely on series and/or Monte Carlo calculations for accurate values of T_c.

The i-δ theory of Frank, Cheung and Mouritsen (to be referred to as FCM) (1982) based on earlier work by Frank and Mitrán (1977, 1978), is now able, through the use of an approximation designed specifically for the critical region, to provide consistent estimates of T_c to within 0.5% of the results of series analysis for the three-dimensional cubic lattices. Moreover, higher-order correlation functions which are calculated within the theory, are within 3% of Monte Carlo results for the simple cubic lattice. This theory was designed for spin 1/2.

The question arises, whether this theory can be generalized to higher spin values. An attempt in this direction has been made by Zhang and Min (1980) (to be referred to as ZM). They have generalized a theory based on an early theory of Frank and Mitran (1978), the CCFA, to higher spin. Their results for T_c are generally not closer to series and Monte Carlo values than 2.7% for the SC, 3.3% for the BCC and 4.9% for the FCC lattices for spin 1/2 and for spin 1 their results differ by .88% for the SC, 1.8% for the BCC and 3.16% for the FCC lattices (ZM). These large discrepancies are not surprising since a consistent application of the CCFA approximation to spin 1/2 has been shown (FCM § 4) to lead to very inaccurate values of T_c.

Here, an attempt is made to first generalize a "criticality equation" to the case of Ising ferromagnets with arbitrary spin, in a zero external magnetic field, in the critical region, through the use of a linearization assumption. Starting in § 4, the i-δ theory of FCM is applied to the spin 1 case. In this case, and also for higher spin cases, when the i-δ equation is expanded some complications arise due to the fact that the average of S_δ^2, the square of the spin at site δ, has not a definite numerical value independent of the temperature, as it has in the spin 1/2 case. Hence, we investigate various techniques to decouple the different combinations of multispin correlation function containing an S_δ^2. Once decoupled, these functions are then substituted into the i-δ equation in order to obtain the higher order correlation functions T_4, T_6, ... required to predict T_c. One of the decoupling methods, "indirect decoupling", allows us to apply the i-δ equation without involving autocorrelation function decoupling. With this method the resulting critical temperatures for the cubic lattices are within .3% of the series values. The simplest decoupling method "direct decoupling", (e.g., $< O_i^2 S_\delta^2 > = < O_i^2 >< S_\delta^2 >$), and a third decoupling method, "ratio decoupling", are also applied to the spin 1 case. This is done to obtain an idea of the errors introduced by these decouplings; this will be useful in higher spin cases where the indirect decoupling method cannot be applied: for higher spin we have to balance out accuracy with ease of calculation.

The direct and ratio decoupling methods result in critical temperatures for the cubic lattices which are within .8% and .75% of the series values respectively. Other three-dimensional lattices can be treated as well, given a knowledge of the Watson sum F(1) for these lattices.

The theory is presented in §'s 2-5. In § 6, the calculation process is outlined, as well as the values of T_c and $< S_i^2 >$ for all cubic lattices, resulting from the different decoupling methods, for the spin 1 Ising model.

2. CRITICALITY EQUATION

Basic theory spin s, Ising model:

The physical system considered consists of magnetic ions localized at lattice sites. If there were no magnetic interactions, the magnetic moments would, in the absence of a field, be thermally disordered at any temperature, and the vector moments of the magnetic ions would average to zero. In some solids, however, individual magnetic ions have nonvanishing thermal average vector moments below a critical temperature T_C. Such solids are called magnetically ordered. The individual localized moments in a magnetically ordered solid may or may not add up to give a net non-zero magnetization for the solid as a whole. If they do, the microscopic bulk magnetization (even in the absence of an applied field) is known as the spontaneous magnetization, and the ordered state is described as ferromagnetic. The critical temperature T_C above which magnetic ordering vanishes is known as the Curie temperature in ferromagnets.

The critical region of temperatures is probably the most difficult to handle theoretically.

In this thesis the system Hamiltonian considered for the spin s Ising ferromagnet is

$$H = -1/2 \sum_i \sum_j J_{ij} S_i S_j - \sum_i h_i S_i , \qquad (2.1)$$

where S_i is the z - component of a spin operator, localized on the site $\vec{R}_i$ of a three-dimensional lattice, with eigenvalues $-s, -(s-1), \ldots, (s-1), s$. J_{ij} is the exchange coupling (exchange integral) which has a non-zero value, J ($J>0$), only if i and j are nearest neighbours, h_i represents an external magnetic field that acts locally on the spin at the i^{th} site.

In spite of the above simplified Hamiltonian, calculating the partition function is still a task of formidable difficulty; hence we will generalize, for spin s, an approach defined in FCM.

The first task is to define the "criticality equation" from which the critical temperature will be found. In this theory one defines the ordinary thermal average <...> as

$$<(\ldots)> = \frac{Tr\,[(\ldots)\,\exp\,(-\beta H)]}{Tr\,[\exp\,(-\beta H)]}, \qquad (2.2)$$

where H is the system Hamiltonian defined in (2.1),

$$Tr = \sum_{S_i} \sum_{S_j} \sum_{S_f = -s}^{+s} \ldots\ldots \text{ and } \beta = 1/k_B T,$$

where k_B is Boltzmann's constant and T is the absolute temperature.

With the Hamiltonian H from (2.1), and applying Callen's identity or Suzuki's method (1965) as in Appendix A, one obtains (equation (A.9)) the exact equation

$$< \{\bar{i}\}\, S_i^p > = < \{\bar{i}\} \frac{\sum_{S_i = -s}^{+s} S_i^p \exp\beta\,(\theta_i + h_i)\,S_i}{\sum_{S_i = -s}^{+s} \exp\beta\,(\theta_i + h_i)\,S_i} > \qquad (2.3)$$

where $\{\bar{i}\}$ is any combination of S_j's which does not include S_i, and

$$Q_i = \sum_j J_{ij} S_j = J * (\text{sum of spins of neighbours of } i) .$$

With the choice p = 1, (2.3) becomes (as shown in Appendix A, equation (A.15))

$$< \{\bar{i}\} S_i > = < \{\bar{i}\} B_s (\beta E_i) > \quad \text{where } E_i = Q_i + h_i \tag{2.4}$$

and $B_s(x) = (s + 1/2) \coth [(s + 1/2) x] - 1/2 \coth (x/2)$.

$B_s(x)$ is the "Brillouin function".

From equation (2.4) one easily obtains the two-spin correlation function relation for the spin s Ising model

$$< S_i S_j > = < S_j B_s (\beta E_i) > , \quad i \neq j. \tag{2.5}$$

Also, by choosing p = 2 and $\{\bar{i}\} = 1$ in (2.3), one obtains (Appendix B, equation (B.6)).

$$< S_i^2 > = < S_i B_s (\beta E_i) > + < B'_s (\beta E_i) > \tag{2.6}$$

where $B'_s(x) = dB_s(x)/dx$.

Combining (2.5) and (2.6), one obtains the general two-spin correlation function equation

$$< S_i S_j > = < S_j B_s (\beta E_i) > + \delta_{ij} < B'_s (\beta E_i) > . \tag{2.7}$$

Also useful will be the relation

$$< S_i B_s(\beta E_i) > = < B_s^2 (\beta E_i) > \tag{2.8}$$

which comes from (2.3) with $\{\ \bar{i}\ \} = B_s\ (\beta\ E_i)$ and $p = 1$.
The two-spin correlation function in (2.7) is of particular interest, since the $\vec{q} \to 0$ limit of its Fourier transform,

$$G_s\ (\vec{q}\ ) = \sum_j \langle S_i\ S_j \rangle \exp\{\ i\ \vec{q} \cdot (\vec{R}_j - \vec{R}_i)\ \} \tag{2.9}$$

determines T_c through the relation (Brout 1965)

$$\lim_{\vec{q} \to 0} G_s\ (\vec{q}\ ) \to \infty \text{ at } T = T_c\ . \tag{2.10}$$

In order to apply the condition (2.10), it would be useful to linearize (2.8) completely in terms of two-spin correlation functions. The way we choose to accomplish this is by introducing a linearization assumption, according to which (as in Frank and Mitran (1977))

$$\langle O_i^{2n+1} \rangle \text{ and } \langle O_i \rangle \qquad (n = 0,\ 1,\ 2,\ \ldots\ )$$

approach zero in the same way for $T = T_c$, whichever order is taken for $h_k \to 0$. Hence one may write

$$\langle O_i^{2n+1} \rangle = R_n \langle O_i \rangle\ ,$$

then one differentiates w.r.t. h_j, and then takes the limit as all $h_k \to 0$.

As a consequence,

$$\langle O_i^{2n+1}\ S_j \rangle = R_n \langle O_i\ S_j \rangle, \text{ where } R_n \text{ is independent of } j, \tag{2.11}$$

$$n = 0,\ 1,\ 2,\ \ldots,\ 2sz\ .$$

By applying (2.11) to the expansion of the odd function

$B_s\ (\beta\ O_i\ )$ inside $<S_j\ B_s\ (\ \beta\ O_i\ )>$, one obtains

$$< S_j\ B_s\ (\beta\ O_i\ ) > = \sum_{n=0}^{sz-1} C_n < S_j\ O_i^{2n+1} >$$

$$= \sum_{n=0}^{sz-1} C_n\ R_n\ < S_j\ O_i >.$$

Defining a site-independent quantity A_s by

$A_s = J(0) \sum_n C_n R_n$, one has

$$\frac{<S_j\ B_s\ (\beta\ O_i)>}{<S_j\ O_i>} = A_s/J(0) \text{ independent of } j, \qquad (2.12)$$

where C_n and R_n are site independent quantities.

Here, $J(0) = \sum_j J_{ij} = zJ$ where z is the number of nearest neighbours of any lattice site and where

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

In (2.12), one may choose, for convenience, j to be a nearest neighbour of i, or i itself, which gives a better result as pointed out by Girvin (1978). Choosing j=i and applying (2.4) with $\{\ \bar{i}\ \} = O_i$ (for calculating the denominator of (2.12)) and $\{\ \bar{i}\ \} = B_s\ (\ \beta\ O_i\ )$ (for the numerator of (2.12)),

$$A_s/J(0) = \frac{< B_s^2 (\beta O_i) >}{< O_i B_s (\beta O_i)>} \qquad (2.13)$$

Substituting (2.12) into (2.8), one obtains the two-spin correlation equation, as the $h_k \to 0$

$$< S_i S_j > = \frac{A_s}{J(0)} < S_j O_i > + \delta_{ij} < B'_s (\beta O_i) >. \qquad (2.14)$$

Using (2.14) and (2.9), one readily solves for $G_s(\vec{q})$ (Appendix C, equation (C.7)):

$$G_s(\vec{q}) = \frac{L_s}{1 - A_s (J(\vec{q})/J(0))} \qquad (2.15)$$

where

$$L_s = < B'_s (\beta O_i) >.$$

The condition (2.10) applied to (2.15) leads to the "criticality equation" from which the transition temperature T_c will be determined:

$$A_s = 1 \quad (T=T_c) \qquad (2.16)$$

and, from (2.15) and the identity (C.9), $G_s(\vec{q})$ may further be written (see (C.11)).

$$G_s(\vec{q}) = \frac{< S_i^2 >}{F(1) (1 - J(\vec{q})/J(0))} \quad (T=T_c) \qquad (2.17)$$

where F(1) is the well-known Watson (1939) sum:

$$F(1) = \frac{1}{N} \sum_{\vec{q}} [1/(1-J(\vec{q})/J(0))].$$

The numerator and denominator of (2.13) are functions of even powers of O_i/J; therefore, combining (2.16) and (2.13) one obtains as the criticality equation

$$\frac{A_2' < (O_i/J(0))^2 > + A_4' < (O_i/J(0))^4 > + \ldots + A_{2n}' < (O_i/J(0))^{2n} > + \ldots}{B_2' < (O_i/J(0))^2 > + B_4' < (O_i/J(0))^4 > + \ldots + B_{2n}' < (O_i/J(0))^{2n} > + \ldots} = 1 \qquad (2.18)$$

where A_{2n}' and B_{2n}' are explicit functions of β.

Fortunately, as shown in § 3, the numerator and denominator of (2.18) can be reduced to a form containing a finite number of terms. As in FCM, one defines

$$T_{2n} = < O_i^{2n}/J^{2n}(0)> . \qquad (2.19)$$

Equation (2.18) can then be rewritten as

$$\frac{A_2' T_2 + A_4' T_4 + \ldots + A_{2n}' T_{2n} + \ldots}{B_2' T_2 + B_4' T_4 + \ldots + B_{2n}' T_{2n} + \ldots} = 1 \qquad (2.20)$$

valid at $T = T_c$ in zero external field.

Using (2.17) and the fact that

$$T_2 = (1/N) \sum_{\vec{q}} G(\vec{q})\, J^2(\vec{q})/J^2(\vec{0}) \quad \text{(FCM and C.14)}$$

one obtains at T_c

$$T_2 = \langle S_i^2 \rangle (1-1/F(1)) \tag{2.21}$$

3. CALCULATION OF THE T_{2n}, USING THE EXISTENCE OF A SPIN-OPERATOR REDUCTION RELATION (from (FCM))

It appears at first sight that to solve (2.20) for T_c, one needs the values T_2, T_4, T_6, ... T_∞. Because of the existence of the spin-operator reduction relation (FCM) (Zhelifonov and Galiullin 1973)

$$(z (O_i/J(0)) \prod_{n=1}^{sz} \{ (z\, O_i /J(0))^2 - n^2 \} \equiv 0, \qquad (3.1)$$

all higher-order T_{2n} may be expressed in terms of the sz quantities T_2, T_4, T_6, ... T_{2sz}; consequently there exist coefficients A_2, ..., A_{2sz}, B_2, ... B_{2sz} such that

$$\frac{A_2 T_2 + A_4 T_4 + \dots A_{2sz} T_{2sz}}{B_2 T_2 + B_4 T_4 + \dots B_{2sz} T_{2sz}} = 1 \qquad (3.2)$$

The identity (3.1) expresses the fact that the eigenvalues of O_i/J are sz, (sz-1), ..., - (sz-1), - sz.

Since A from (2.13) and $< S_i^2 >$ from (2.6) are also expressible in terms of T_2, T_4 ... T_{2sz} (Appendix E), there are sz+1 variables (including T_c), but so far only two equations: (2.16) and (2.6).

As in FCM, the method for calculating the higher-order correlation functions T_{2n} (n>1) will be that using the "i-δ relations".

4. The "i-δ RELATIONS", SPIN 1 CASE.

One considers a spin operator S_δ where δ is a specific chosen nearest neighbour of i. One forms the sum of spin operators at sites neighbouring on i, but excluding that at δ; this sum may be written $O_i/J-S_\delta$.

Following the same assumption as in (2.11), one obtains at $T=T_c$ for $h_j=0$ (all j)

$$\frac{\langle (O_i/J - S_\delta)^{2n+1} \; S_j \rangle}{\langle (O_i/J - S_\delta) \; S_j \rangle} = R'_n \quad \text{for } n=1, 2, \ldots sz-1 \qquad (4.1)$$

where R'_n is a site-independent quantity.

Using (4.1) with j=i and j=δ successively leads to the i-δ relations

$$\frac{\langle (O_i/J - S_\delta)^{2n+1} \; S_i \rangle}{\langle (O_i/J - S_\delta) \; S_i \rangle} = \frac{\langle (O_i/J- S_\delta)^{2n+1} \; S_\delta \rangle}{\langle (O_i/J -S_\delta) \; S_\delta \rangle} \qquad (4.2)$$

In equation (4.2) when the left-hand side binomial expansions are performed, among the terms that appear are terms like

$$\langle (O_i/J\,(0))^{2m+1} \; S_i \rangle \quad \text{and} \quad \langle (O_i/J\,(0))^{2m} \; S_\delta S_i \rangle \qquad (4.3)$$

where $0 \leq m$ (integer) $\leq sz-1$. The right-hand side of (4.2) contains, among others, terms like

$$< (0_i/J (0))^{2m+1} S_\delta > = T_{2m+2} \qquad (4.4a)$$

and

$$< (0_i/J (0))^{2m} > = T_{2m} \qquad (4.4b)$$

We now show that the terms in (4.3) (as well as in (4.4)) can be written in terms of the T_{2n} alone.

Defining

$$U_{2n} = < (0_i/J (0))^{2n-1} S_i > \qquad (4.5)$$

we have from (2.16) and (2.14) (see (C.17)) that

$$U_2 = T_2 \qquad (T = T_c). \qquad (4.6)$$

Using (2.11) with j one of the nearest neighbours of i (i.e. $R_{n-1} = T_{2n}/T_2$), (2.11) with j = i (i.e. $R_{n-1} = U_{2n}/U_2$) and (4.6), one obtains

$$U_{2n} = T_{2n} \qquad (n = 1, 2, 3, \ldots). \quad (T = T_c) \qquad (4.7)$$

Consequently, the terms in (4.3) may be rewritten as

$$< (0_i /J (0))^{2m+1} S_i > = U_{2m+2} \qquad (4.8a)$$

$$= T_{2m+2}$$

and, using symmetry,

$$< (O_i/J(0))^{2m} S_\delta S_i> = U_{2m+2} \qquad (4.8b)$$

$$= T_{2m+2} .$$

Thus, if (4.2) contained only the terms in (4.3) and (4.4), then no new variables would be introduced, and equation (4.2) would provide the missing sz-1 equations necessary for the determination of T_c. However additional terms like

$< O_i^{2m+1} S_\delta^{2k} S_i >$ (k=1, 2, ...) also appear in (4.2) because $S_\delta^2 \neq 1/4$ when $s \neq 1/2$. Therefore, techniques must be developed to cope with this type of term.

The present theory for the spin s Ising ferromagnet, for the case $s > 1/2$, involves the thermal average of the square of the spin. Its value may be found by summing (2.9) over q, in which case (Appendix C)

$$< S_\delta^2> = \frac{1}{N} \sum_q G_s(\vec{q}) \qquad (T=T_c) \qquad (4.9)$$

or, from the exact equation (Appendix B, (B.8)), valid at all T

$$< S_\delta^2 > = < B_s^2 (\beta O_\delta) > + < B_s'(\beta O_\delta)> . \qquad (4.10)$$

Up to here the theory holds for general spin s. We will now examine the new terms in the binomial expansions of (4.2) for the spin 1 case.

5. DECOUPLING OF MULTISPIN-CORRELATION FUNCTIONS: SPIN 1

In the spin 1 case we have the identity, for all j, (since $S_j = 1, 0, -1$)

$$S_j^{2k} = S_j^2 \qquad k = 1, 2, \ldots \tag{5.1a}$$

$$S_j^{2k+1} = S_j \qquad k = 1, 2, \ldots \tag{5.1b}$$

Substitution of (5.1a,b) into the binomial expansion of the numerators of (4.2) leads to only two new terms:

$$< (O_i/J)^{2p+1} \quad S_\delta^2 \; S_i > \tag{5.2a}$$

$$p = 0, 1, 2, \ldots, \; z - 2$$

and $$< (O_i/J)^{2p+2} \quad S_\delta^2 > \tag{5.2b}$$

We now investigate various techniques to decouple the combinations (5.2a) and (5.2b) of the multispin functions.

5a. DIRECT DECOUPLING

A first naive attack on the problem leads one to the decoupling

$$< (O_i/J)^{2p+1} \quad S_\delta^2 \, S_i > = < (O_i/J)^{2p+1} S_i > < S_\delta^2 > \tag{5.3a}$$

where p=0, 1, 2,..., z-2. That is, "the average of the product is the product of the averages".

From (4.5), (5.3a) becomes

$$< O_i^{2p+1} S_\delta^2 S_i > = J^{2p+1}(0) \, U_{2p+2} < S_\delta^2 > . \qquad (5.3b)$$

Similarly (5.2b) may be replaced by

$$<(O_i/J)^{2p+2} S_\delta^2 > = <(O_i/J)^{2p+2} > < S_\delta^2 > . \qquad (5.4a)$$

or, from (2.19)

$$< O_i^{2p+2} S_\delta^2 > = J^{2p+2}(0) \, T_{2p+2} <S_\delta^2> . \qquad (5.4b)$$

The decoupling method used in (5.3) and (5.4) is called "direct decoupling".

From (4.2), the higher-order correlation functions may now be determined successively in terms of lower-order ones, and in conjunction with the approximation (4.7) ($U_{2n} \simeq T_{2n}$) one obtains

$$T_{2n+2} = < S_\delta^2 > z^{-(2n+1)} a_n + \sum_{k=1}^{n} [P_{2k}^{2n+1} b_n + P_{2k-1}^{2n+1} a_n] T_{2n+2-2k} \qquad (5.5)$$

where

$$a_n = [1-(1-(2n+1)/z) (1-< S_\delta^2 > /zT_2) (1-1/z)^{-1}]^{-1} \qquad (5.6)$$

$$b_n = (1-< S_\delta^2 > /zT_2)(1-1/z)^{-1} a_n$$

and P_{2k}^{2n+1} is given in terms of the binomial coefficients, ${}^{n}C_k$ as follows:

$$P_{2k}^{2n+1} = ({}^{2n+1}C_{2k} < S_\delta^2 > - {}^{2n+1}C_{2k+1} /z) z^{-2k}$$

5b. INDIRECT DECOUPLING

Here we allow the extra terms (5.2a) and (5.2b) to be determined by the equations

$$<(0_i/J-S_\delta)^{2p+1} S_\delta^2 S_i> = <(0_i/J-S_\delta)^{2p+1} S_i> < S_\delta^2 > \quad (5.7)$$

and

$$<(0_i/J-S_\delta)^{2p+2} S_\delta^2 > = <(0_i/J-S_\delta)^{2p+2} > < S_\delta^2 > . \quad (5.8)$$

where $p = 0, 1, 2, \ldots, (z - 2)$.

This is a better approach in decoupling the combination of multispin correlation functions, because $(0_i/J-S_\delta)^{2p+1}$ does not contain the spin at site δ.

Thus, self-correlations are treated with respect. (Implied decouplings like $< S_\delta^4 > = < S_\delta^2 >^2$ are hence avoided.) As shown in Appendix D, the binomial expansion of (5.7) and (5.8), using (5.1), leads to the replacement of (5.2a) by

$$<(0_i/J)^{2p+1} S_\delta^2 S_i> = <(0_i/J-S_\delta)^{2p+1} S_i> [< S_\delta^2 > -1] + <(0_i/J)^{2p+1} S_i> \quad (5.9)$$

where p = 0, 1, 2, ..., z - 2

and of (5.2b) by

$$<(0_i/J)^{2p+2} S_\delta^2> = <(0_i/J-S_\delta)^{2p+2} >[<S_\delta^2 > -1] + <(0_i/J)^{2p+2} > . \quad (5.10)$$

This is called "indirect decoupling". The last terms on the right-hand sides of (5.9) and (5.10) are expressible in terms of the U's or T's . The first right-hand side terms, when expanded, contain averages like

$<(0_i/J)^{2r+1} S_\delta^2 S_i>$ and $<(0_i/J)^{2r+2} S_\delta^2 >$, but with $r < p$. One may thus return to (5.9) and (5.10) and continue the calculation recursively.

In a manner similar to that used for direct decoupling, the T_{2n+2} may be written, from (4.2) and with the use of (5.9), (5.10), and (5.1a, b), as

$$T_{2n+2} = \langle S_\delta^2\rangle z^{-(2n+1)} a_n + \sum_{k=1}^{n}\{[\,{}^{2n+1}D_{2k}\, b_n$$

$$+ a_n\,{}^{2n+1}D_{2k-1}]\, T_{2n+2-2k}\}$$

$$+ [\langle S_\delta^2\rangle -1]\, z^{-(2n+1)} \sum_{k=1}^{n}\{[\, b_n\,{}^{2n+1}C_{2k}\langle(O_i/J-S_\delta)^{2n+1-2k}\, S_i\rangle]$$

$$+ [\, a_n\,{}^{2n+1}C_{2k-1}\langle(O_i/J-S_\delta)^{2n+2-2k}\rangle]\} \qquad (5.11)$$

where a_n and b_n are given by (5.6) and

$${}^{2n+1}D_r = ({}^{2n+1}C_r - {}^{2n+1}C_{r+1}/z)\, z^{-r}.$$

In order to be able to solve (5.11) we need to first evaluate

$$\langle(O_i/J-S_\delta)^{2n+1-2k}\, S_i\rangle \text{ and } \langle(O_i/J-S_\delta)^{2n+2-2k}\rangle$$

then to substitute the result back into (5.11).

For example, if T_6 needs to be calculated (n=2), with T_2 and $\langle S_\delta^2\rangle$ assumed, T_4 must first be evaluated, which implies that the term $\langle(O_i/J-S_\delta)^2\rangle$ appears on the right hand side of (5.11).

Expanding this term yields,

$$\langle(O_i/J-S_\delta)^2\rangle = \langle(O_i/J)^2\rangle - 2\langle S_\delta\, O_i/J\rangle + \langle S_\delta^2\rangle$$

$$= z^2\, T_2 - 2zT_2 + \langle S_\delta^2\rangle \quad . \qquad (5.12)$$

Since every term on the right-hand side of (5.12) is known, hence when n = 1 T_4 can be easily evaluated. Also when n = 2 a new term $\langle(O_i/J-S_\delta)^4\rangle$ must be expanded in order to evaluate it,

$$\langle(O_i/J-S_\delta)^4\rangle = \langle(O_i/J)^4\rangle - 4\langle(O_i/J)^3\, S_\delta\rangle + 6\langle(O_i/J)^2\, S_\delta^2\rangle$$

$$-4\langle(O_i/J)\, S_\delta^3\rangle + \langle S_\delta^4\rangle \qquad (5.13)$$

$$= z^4\, T_4 - 4\, z^3\, T_4 + 6\langle(O_i/J)^2\, S_\delta^2\rangle$$

$$- 4\langle(O_i/J)\, S_\delta^3\rangle + \langle S_\delta^4\rangle \, .$$

From (5.1a, b)

$$\langle(O_i/J)\, S_\delta^3\rangle = \langle(O_i/J)\, S_\delta\rangle \qquad (5.14a)$$

$$= z\, T_2$$

$$\langle S_\delta^4\rangle = \langle S_\delta^2\rangle \qquad (5.14b)$$

and from (5.10), one obtains

$$\langle(O_i/J)^2\, S_\delta^2\rangle = \langle(O_i/J-S_\delta)^2\rangle\, [\, \langle S_\delta^2\rangle - 1\,] + \langle(O_i/J)^2\rangle . \qquad (5.15)$$

Since $\langle(O_i/J-S_\delta)^2\rangle$ can be evaluated from (5.12) and since $\langle(O_i/J)^2\rangle = z^2\, T_2$, every term in (5.15) is known.

From (5.12), (5.15) and (5.14a, b) one can easily evaluate (5.13); hence, every term needed in (5.11), when n=2, may be calculated, and T_6 is easily evaluated.

5c. RATIO DECOUPLING METHOD

Following the spirit of the derivation of (2.11), a new set of relations for the higher-order correlation functions is obtained by establishing the following assumption, at $T = T_c$ and $h_k \to 0$ (all k), that :

$$\frac{\langle (O_i/J)^{2p+1} S_\delta^2 S_j \rangle}{\langle (O_i/J) S_\delta^2 S_j \rangle} = R_p \text{ independent of } j. \qquad (5.16)$$

Using (5.16) with j=i and j=δ successively and knowing that for spin one $S_\delta^3 = S_\delta$ (5.1b) a ratio decoupling equation is obtained, at $T=T_c$

$$\frac{\langle (O_i/J)^{2p+1} S_\delta^2 S_i \rangle}{\langle (O_i/J) S_\delta^2 S_i \rangle} = \frac{\langle (O_i/J)^{2p+1} S_\delta \rangle}{\langle (O_i/J) S_\delta \rangle} \equiv T_{2p+2}/T_2 \qquad (5.17)$$

for p=0, 1, 2, ..., z-2 ;

and similarly using (5.16) with S_j replaced by O_i/J and then with $S_j = S_\delta$ leads to (at $T=T_c$)

$$\frac{\langle (O_i/J)^{2p+2} S_\delta^2 \rangle}{\langle (O_i/J)^2 S_\delta^2 \rangle} = \frac{\langle (O_i/J)^{2p+1} S_\delta \rangle}{\langle (O_i/J) S_\delta \rangle} \equiv T_{2p+2}/T_2 \qquad (5.18)$$

for $p = 0, 1, 2, \ldots, z-2$

These two equations will allow us to decouple (5.2a,b) only if the two averages $\langle (O_i/J)\, S_\delta^2\, S_i \rangle$ and $\langle (O_i/J)^2\, S_\delta^2 \rangle$ can be evaluated. This is done using the indirect decoupling method of (5.6).

Using (5.17) and (5.18), we now can evaluate (5.2a) and (5.2b) which permits us to solve (4.2) for T_{2n+2}:

$$T_{2n+2} = \langle S_\delta^2 \rangle\, z^{-(2n+1)}\, a_n + \sum_{k=1}^{n} \{ {}^{2n+1}P_{2k}\, b_n + {}^{2n+1}D_{2k-1}\, a_n \}\, T_{2n+2-2k} \tag{5.19}$$

where a_n and b_n are given by (5.6),

$${}^{2n+1}P_{2k} = ({}^{2n+1}C_{2k}\, W - {}^{2n+1}C_{2k+1}/z)\, z^{-(2k)}$$

$${}^{2n+1}D_{2k-1} = ({}^{2n+1}C_{2k-1}\, F - {}^{2n+1}C_{2k}/z)\, z^{-(2k-1)}$$

$$F = \langle S_\delta^2 \rangle \{ 2/z \langle S_\delta^2 \rangle - 1/z^2\, T_2 + 1 - 2/z + \langle S_\delta^2 \rangle / z^2\, T_2 \}$$

and

$$W = \langle S_\delta^2 \rangle (1 - 1/z) + 1/z .$$

6. CALCULATION PROCESS.

Once a decoupling method is chosen, initial values of $< S_i^2 >$ and T_c are assumed. T_2 is evaluated from (2.21), and all higher-order correlation functions can be completely determined from the T_{2n+2} equations. Equations (2.16) (for A_s) and (4.10) (for $<S_i^2>$) are used in a two-variable Newton-Raphson procedure to calculate new values of $<S_i^2>$ and T_c. This process is continued until convergence is obtained. The values of T_c from the different decoupling methods are listed in Table 1 for the cubic lattices. Similarly, the values of T_{2n} are given in Tables 3 (SC lattice), 4 (BCC lattice) and 5 (FCC lattice). The T_c values vary from those obtained from series analysis by a small percentage ($\sim$.5%) that depends on the particular decoupling method used.

It is of interest to investigate, at this juncture, the consistency of our approach with the approximation $U_{2n} = T_{2n}$. From (2.4) with $\{ \bar{i} \} = O_i, O_i^3, \ldots, O_i^{2z-1}$ successively, and $h_i = 0$, one has, exactly,

$$U_{2n} = < (O_i/J)^{2n-1} \; B_s \; (\beta \, O_i) > , \qquad n=1, 2,\ldots, sz \quad (6.1)$$

With the method of Appendix E, and the values of the T_{2n} (from Tables 3, 4,5), one readily evaluates U_{2n} at T_c. The results are presented in Table 6 (for SC), Table 7 (for BCC) and Table 8 (for FCC). The ratios U_{2n}/T_{2n} which for consistency should be close to unity, vary, for example, from 0.994 (for 2n = 2, z = 12) to 0.935 (for 2n = 24, z = 12) for the direct case.

Table 1. Values of $3k_B T_c/2zJ$ for the cubic lattices at T_c (s=1).

Cubic Lattices	Mean Field	Zhang and Min (1980) $n^2 = \langle O_i^3 \rangle / \langle O_i \rangle$	Zhang and Min (1980) $n^2 = \langle O_i^4 \rangle / \langle O_i^2 \rangle$	Present Work Decoupling Method: Direct	Present Work Decoupling Method: Indirect	Present Work Decoupling Method: Ratio	Series
SC	1	0.806	0.767	0.8110	0.8015	0.7916	0.7989 (1)
BCC	1	0.850	0.818	0.8402	0.8327	0.8271	0.8346 (2)
FCC	1	0.884	0.856	0.8550	0.8498	0.8465	0.8523 (3)

(1) Camp & Van Dyke (1974)

(2) Zinn-Justin (1981)

(3) Camp, Saul, Van Dyke, Wortis (1976)

(4) n^2 is from the Zhang and Min assumption that $\langle O_i^{2n+1} \rangle / \langle O_i^{2n-1} \rangle = \langle O_i^{2n+2} \rangle / \langle O_i^{2n} \rangle \equiv n^2$ is independent of the order n near the transition temperature.

Table 2. Values of $<S_i^2>$ at T_c for the cubic lattices.
a*: direct; b*: indirect; c*: ratio methods

	SC	BCC	FCC
direct decoupling	0.7347	0.7213	0.7155
indirect decoupling	0.7345	0.7212	0.7155
ratio decoupling	0.7351	0.7215	0.7155

Table 3. Values of T_{2n} for the SC lattice at T_c (s = 1).
a*:direct; b*:indirect; c*: ratio methods

2n	a*	b*	c*
2	0.25019	0.25013	0.25034
4	0.1198	0.1326	0.1328
6	0.06652	0.09081	0.08307
8	0.03796	0.07078	0.05429
10	0.02145	0.05973	0.03557
12	0.01194	0.05309	0.02309

Table 4. Values of T_{2n} for the BCC lattice at T_c (s = 1)
a*: direct; b*: indirect; c*: ratio methods

2n	a*	b*	c*
2	0.20357	0.20356	0.20364
4	0.08480	0.09202	0.09209
6	0.04303	0.05520	0.05126
8	0.02335	0.03849	0.03083
10	0.01287	0.02954	0.01902
12	0.007063	0.02420	0.01176
14	0.003829	0.02080	0.007232
16	0.002053	0.01851	0.004408

Table 5. Values of T_{2n} for the FCC lattice at T_c (s=1).

a*: direct; b*: indirect; c*: ratio methods

2n	a *	b *	c *
2	0.18341	0.18341	0.18345
4	0.06998	0.07419	0.07422
6	0.03319	0.03975	0.03765
8	0.01742	0.02481	0.02108
10	0.009487	0.01710	0.01235
12	0.005240	0.01265	0.007379
14	0.002896	0.009870	0.004428
16	0.001590	0.008025	0.002649
18	0.0008649	0.006747	0.001574
20	0.0004658	0.005830	0.0009287
22	0.0002485	0.005154	0.0005434
24	0.0001315	0.004643	0.0003157

Table 6. Values of U_{2n} for the SC lattice at T_c (s=1).
a*: direct; b*: indirect; c*: ratio methods

2n	a*	b*	c*
2	0.24831	0.24699	0.24784
4	0.1147	0.1231	0.1259
6	0.06314	0.08132	0.07760
8	0.03611	0.06923	0.05064
10	0.02045	0.05143	0.03322
12	0.01144	0.04521	0.02165

Table 7. Values of U_{2n} for the BCC lattice at T_c (s=1).
a*: direct; b*: indirect; c*: ratio methods

2n	a*	b*	c*
2	0.20222	0.20159	0.20199
4	0.08103	0.08604	0.08738
6	0.04048	0.04979	0.04770
8	0.02187	0.03388	0.02849
10	0.01206	0.02554	0.01755
12	0.006634	0.02065	0.01085
14	0.003605	0.01757	0.006694
16	0.001936	0.01551	0.004087

Table 8. Values of U_{2n} for the FCC lattice at T_c (s=1).
a*: direct; b*: indirect; c*: ratio methods

2n	a *	b *	c *
2	0.18234	0.18201	0.18223
4	0.06692	0.06998	0.07069
6	0.03126	0.03629	0.03510
8	0.01619	0.02214	0.01944
10	0.008790	0.01500	0.01134
12	0.004853	0.01095	0.006764
14	0.002685	0.008452	0.004060
16	0.001476	0.006812	0.002432
18	0.0008048	0.005685	0.001448
20	0.0004342	0.004882	0.0008555
22	0.0002321	0.004293	0.0005013
24	0.0001230	0.003850	0.0002916

7. DISCUSSION

As in FCM, in this thesis, we assume the same basic assumptions i.e (i) "$A_s = 1$" the "criticality equation" (2.16); (ii) the i-δ relations, this time coupled with three different methods of decoupling higher order correlation functions in which S_δ^2 is involved, and (iii) the $U_{2n} = T_{2n}$ equations. From Table 1, the values of T_c obtained from the direct decoupling method differ from the series values by 1.5% for the SC lattice, 0.67% for the BCC lattice and 0.31% for the FCC lattice; also for the indirect case the critical temperatures differ from the series values by 0.32%, 0.22% and 0.29% for the SC, BCC and FCC lattices respectively; finally for the ratio case the T_c's differ from the series values by 0.91%, 0.89% and 0.68% for the SC, BCC and FCC lattices respectively.

The most accurate critical temperatures are obtained by applying the indirect decoupling method within the i-δ relations. This is expected since, as in the spin 1/2 case, we were careful about the splitting up of autocorrelations. The direct decoupling results are not as good; this is as one might expect due to the fact the O_i contains S_δ, hence S_δ^3 and S_δ^4 are effectively treated as $S_\delta < S_\delta^2 >$ and $< S_\delta^2 > < S_\delta^2 >$) respectively which, by (5.1 a & b) is manifestly incorrect. The ratio decoupling method though less accurate than the indirect method, has a pedagogical value for the spin 1 case but will be, as well as the direct method, very useful for the spin $s > 1$ case. For example the direct method applied to the spin 3/2 Ising case yields critical temperatures that differ from the series values by 0.79% for the SC lattice, 0.82% and 0.099% for the BCC and FCC lattices respectively; for the ratio case applied to spin 3/2, the T_c's differ from series values by 0.18%, 0.29% and 0.1853% for the SC, BCC and FCC lattices respectively. For spin $s > 1$ the ratio and direct decoupling methods give accurate values of T_c and are easily applied.

From Table II, one notices that the thermal average of the square of the spin (namely $< S_\delta^2 >$),evaluated at the critical temperature for the different decoupling methods, are nearly equal.

From the other tables, the U_{2n}/T_{2n} ratios which for consistency should be close to unity, vary from 0.994 (for 2n = 2, z = 12) to .935 (for 2n = 24, z = 12) for the direct case; from 0.992 (for 2n = 2, z = 12) to 0.829 (for 2n = 24, z = 12) for the indirect case and from 0.993 (for 2n = 2, z = 12) to 0.923 (for 2n = 24, z = 12) for the ratio case. The decoupling method that yields the best critical temperature values is the one for which the U_{2n}/T_{2n} ratio differs most from unity. It is important to note that the $U_{2n} = T_{2n}$ equality is used only in a part of the calculation where the final results are not extremely sensitive to the exact value of the U_{2n}/T_{2n} ratios.

This work shows that it is possible to extend the i-δ theory to higher-spin cases, with no sacrifice in accuracy. It also indicates that a trade-off between the ease of application of one of the tested decoupling techniques against the accuracy of another might well be worthwhile.

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Appendix A: Generalized exact formula for the Ising model correlation functions (Suzuki (1965)).

From the Suzuki paper the Hamiltonian considered is

$$H = - \sum_i \sum_j J_{ij} S_i S_j - \sum_i h_i S_i \tag{A.1}$$

Letting $\{ \bar{i} \}$ = any function of S_j's at sites other than the i^{th},

one considers the following general correlation function:

$$< \{ \bar{i} \} S_i^p > \equiv \frac{1}{Z} \, Tr [\{ \bar{i} \} S_i^p \exp (- \beta H)] \tag{A.2}$$

where the partition function Z is defined as

$$Z = Tr \exp (- \beta H) \quad , \qquad (\beta = 1/k_B T). \tag{A.3}$$

In general the symbol Tr is defined as

$$Tr = \sum_{S_1} \sum_{S_2} \ldots \sum_{S_n = -s}^{+s} ;$$

we also define

$$Tr_i = \sum_{S_i = -s}^{+s} \; ; \quad Tr' = \sum_{S_1} \ldots \sum_{S_2} \ldots \sum_{S_j = -s}^{+s} \ldots \sum_{S_n} \; j \neq i$$

$$= \sum_{\text{all } S_j = -s}^{+s} \; (j \neq i) \tag{A.4}$$

In general, we consider a Hamiltonian H which can be expressed as

$$H = H' - E_i\, S_i \qquad (A.5)$$

where H' is that part of H that does not contain S_i.

Expressing (A.1) in the form of (A.5), one obtains

$$H' = -\,1/2 \sum_{\substack{f \\ f \neq i}} \sum_{\substack{j \\ j \neq i}} J_{fj}\, S_f\, S_j - \sum_{\substack{f \\ f \neq i}} h_f\, S_f \qquad (A.6)$$

and

$$E_i = O_i + h_i \qquad (A.7)$$

where $O_i = \sum_j J_{ij}\, S_j$.

One substitutes (A.5) into (A.2):

$$< \{ \bar{i} \}\, S_i^p > = (1/Z)\ \mathrm{Tr}\ \{ \{ \bar{i} \}\, S_i^p \exp(-\beta H' + \beta E_i S_i) \},$$

and from A(4) one obtains

$$<\{ \bar{i} \}\, S_i^p > = \frac{1}{Z}\, \mathrm{Tr}'\ \mathrm{Tr}_i\ [\{ \bar{i} \}\, S_i^p \exp(\beta E_i S_i) \exp(-\beta H')] .$$

Since $\{ \bar{i} \} \exp(-\beta H')$ does not contain S_i,

$$<\{ \bar{i} \}\, S_i^p > = \frac{1}{Z}\, \mathrm{Tr}'[\{ \bar{i} \} \exp(-\beta H')\ \mathrm{Tr}_i\, S_i^p \exp(\beta E_i S_i)] .$$

Multiplying and dividing by the same factor within Tr' ,

$$<\{\bar{i}\} S_i^p> = \frac{1}{Z} Tr'[\{\bar{i}\} \exp(-\beta H') Tr_i \exp(\beta E_i S_i) \frac{Tr_i S_i \exp(\beta E_i S_i)}{Tr_i \exp(\beta E_i S_i)}]$$

$$= \frac{1}{Z} Tr' Tr_i [\exp[-\beta(H'-E_i S_i)] \{\bar{i}\} \frac{Tr_i S_i^p \exp(\beta E_i S_i)}{Tr_i \exp(\beta E_i S_i)}]$$

hence from (A.4) and (A.5)

$$<\{\bar{i}\} S_i^p> = \frac{1}{Z} Tr\{[\{\bar{i}\} \frac{Tr_i S_i^p \exp(\beta E_i S_i)}{Tr_i \exp(\beta E_i S_i)}] \exp(-\beta H)]\} \quad (A.8)$$

Using (A.2), (A.8) becomes

$$<\{\bar{i}\} S_i^p> = <\{\bar{i}\} \frac{Tr_i[S_i^p \exp(\beta E_i S_i)]}{Tr_i[\exp(\beta E_i S_i)]}> . \quad (A.9)$$

Equation (A.9) is the required generalized formula for the correlation functions of an Ising model of spin S.

Letting $k = S_i + S$, (A.9) may be now expressed as

$$<\{\bar{i}\} S_i^p> \equiv <\{\bar{i}\} \frac{\sum_{k=0}^{2s} (k-s)^p \exp[\beta(k-s) E_i]}{\sum_{k=0}^{+2s} \exp(\beta(k-s) E_i)}>$$

with s representing the values of the spin, or,

$$<\{\bar{i}\} S_i^p> \equiv <\{\bar{i}\} T_s^{(p)}(\beta E_i)> \quad (A.10)$$

where

$$T_s^{(p)}(x) = \frac{\sum_{k=0}^{2s} (k-s)^p \exp kx}{\sum_{k=0}^{2s} \exp kx} . \quad (A.11)$$

Using equation (A.10) for s=1/2 and letting $\{ \bar{i} \} = 1$ and p=1

$$< S_i > = < T_{\frac{1}{2}}^{(1)}(\beta E_i) > .$$

Since from (A.11)

$$T_{\frac{1}{2}}^{(1)}(x) = \frac{\sum_{k=0}^{1} (k-\frac{1}{2}) \exp kx}{\sum_{k=0}^{1} \exp kx}$$

$$= 1/2 \left[\frac{e^x - 1}{e^x + 1}\right]$$

$$= 1/2 \tanh (x/2)$$

one obtains, for spin $\frac{1}{2}$,

$$< S_i > = 1/2 < \tanh (\beta E_i/2) > . \qquad (A.12)$$

Similarly for spin s, using (A.10) and letting p=1 one obtains

$$<\{ \bar{i} \} S_i> = <\{ \bar{i} \} T_s^{(1)} (\beta E_i) > .$$

$T_s^{(1)}(x)$ may be easily found from (A.11)

$$T_s^{(1)}(x) = \frac{\sum_{k=0}^{2s} k \exp kx}{\sum_{k=0}^{2s} \exp kx} - s$$

$$= \frac{d}{dx}\left(\ell n \sum_{k=0}^{2s} \exp(kx)\right) - s \quad . \qquad (A.13)$$

Since from the formula for a geometric progression,

$$\sum_{k=0}^{2s} \exp(xk) = \frac{e^{x(2s+1)} - 1}{e^{x} - 1}$$

$$= \frac{e^{x(s+\frac{1}{2})}\left[e^{x(s+\frac{1}{2})} - e^{-x(s+\frac{1}{2})}\right]}{e^{x/2}\left[e^{x/2} - e^{-x/2}\right]}$$

$$= e^{xs}\,\frac{\sinh(x(s+\frac{1}{2}))}{\sinh(x/2)}, \qquad (A.14)$$

(A.13) leads to

$$T_s^{(1)}(x) \equiv \frac{d}{dx}\left[\ell n \sinh x(s+\tfrac{1}{2})\right] - \frac{d}{dx}\sinh(x/2)$$

$$= (s+\tfrac{1}{2})\coth x(s+\tfrac{1}{2}) - \tfrac{1}{2}\coth(x/2)$$

$$\equiv B_s(x) \quad \text{, the "Brillouin function".}$$

Therefore, for spin s, $<\{\bar{i}\}\, S_i> = <\{\bar{i}\}\, B_s(\beta E_i)>$ (A.15).

Appendix B: Two-spin correlation function

From Appendix A we have

$$<\{\bar{i}\} S_i^p> = < \frac{\{\bar{i}\} \sum_{S_i=-s}^{+s} S_i^p \exp \beta E_i S_i}{\sum_{S_i=-s}^{+s} \exp \beta E_i S_i} > \quad \text{(B.1)}$$

Letting $\{\bar{i}\} = 1$ and p=1 in (B.1) one obtains (A.15) with

$$\{\bar{i}\} = 1: < S_i > = < B_s(\beta E_i)> \quad \text{(B.2)}$$

$$\equiv < \frac{\partial}{\partial \beta E_i} \ell n \sum_{S_i=-s}^{+s} \exp (\beta E_i S_i)>$$

If one lets p=1 and $\{\bar{i}\} = S_j$ ($j \neq i$) in (B.1), one obtains the two-spin correlation function

$$< S_i S_j > = < S_j B_s(\beta E_i) > , \quad j \neq i . \quad \text{(B.3)}$$

Also from (B.1) one may obtain $< S_i^2 >$ by letting

p = 2 and $\{\bar{i}\} = 1$

$$< S_i^2 > = < \frac{\sum_{S_i=-s}^{+s} S_i^2 \exp (\beta E_i S_i)}{\sum_{S_i=-s}^{+s} \exp (\beta E_i S_i)} > . \quad \text{(B.4)}$$

Since

$$\frac{\partial}{\partial(\beta E_i)} \ell n \sum_{S_i} S_i \; e^{\beta E_i S_i} = \frac{\sum_{S_i} S_i^2 \, e^{\beta E_i S_i}}{\sum_{S_i} S_i \, e^{\beta E_i S_i}} \qquad \text{(B.5a)}$$

and since, from Appendix A,

$$\ell n \sum_{S_i} S_i \; e^{\beta E_i S_i} = \ell n \, B_s(\beta E_i) + \ell n \sum_{S_i} e^{\beta E_i S_i} , \qquad \text{(B.5b)}$$

(B.4) becomes

$$<S_i^2> = < B_s(\beta E_i)[\frac{\partial}{\partial(\beta E_i)} \ell n \, B_s(\beta E_i) + \frac{\partial}{\partial(\beta E_i)} \ell n \sum_{S_i} e^{\beta E_i S_i}] >.$$

From the definition of $B_s(x)$ (A.13), one obtains

$$\frac{\partial}{\partial(\beta E_i)} \ell n \sum_{S_i} e^{\beta E_i S_i} = B_s(\beta E_i) \quad ;$$

therefore,

$$< S_i^2 > = < B_s' (\beta E_i) > + < B_s^2 (\beta E_i) > . \qquad \text{(B.6)}$$

From (B.1) $< B_s^2 (\beta E_i) >$ may also be expressed as

$$< B_s^2 (\beta E_i) > = < S_i \, B_s(\beta E_i) > . \qquad \text{(B.7)}$$

This is obtained by letting, in (A.15), $p = 1$ and $\{\bar{i}\} = B_s(\beta E_i)$.

Thus one may write (B.6) as

$$< S_i^2 > = < B_s' (\beta E_i) > + < S_i B_s(\beta E_i) > \qquad (B.8)$$

and combining (B.3) and (B.8), one obtains

$$< S_i S_j > = < S_j B_s (\beta E_i) > + \delta_{ij} < B_s' (\beta E_i) > . \qquad (B.9)$$

Appendix C: Correlation Functions: Fourier Transforms

We define $G_s(\vec{q})$ and $J(\vec{q})$ as the space Fourier transforms of $< S_i S_j >$ and J_{ij} respectively.

$$G_s(\vec{q}) = \sum_{\substack{j \\ (j \neq i)}} < S_i \, S_j > \exp [\, i \, \vec{q} . (\vec{R}_i - \vec{R}_j)] \qquad (C.1)$$

from which

$$< S_i \, S_j > = \frac{1}{N} \sum_{q} G_s \, (\vec{q}) \exp [\, i \, \vec{q} . (\vec{R}_j - \vec{R}_i)] \qquad (C.2)$$

And

$$J(\vec{q}) = \sum_j J_{ij} \exp [\, i \, \vec{q} . (\vec{R}_i - \vec{R}_j)] \qquad (C.3)$$

$\vec{q}$ is a wave number in the first Brillouin zone of the reciprocal lattice. N is the number of lattice sites. By the definition of J_{ij}, from (C.3), $J(0) = \sum_j J_{ij} = zJ$

where z is the number of nearest neighbours of any lattice site and J is the exchange integral.

Now since

$$< S_i \, S_j > = \frac{A_s}{J(0)} < S_j \, O_i > + \delta_{ij} < B'_s \, (\beta O_i) > \qquad (C.4)$$

from (2.14), one substitutes (C.4) into (C.1) to get

$$G_s(\vec{q}) = \frac{A_s}{J(0)} \sum_j < S_j\, 0_i > \exp [i\, \vec{q}.\, (\vec{R}_i - \vec{R}_j\,)]$$

$$+ \sum_j \delta_{ij} < B_s'(\beta 0_i) > \exp (\, i\, \vec{q}.\, (\vec{R}_i - \vec{R}_j)$$

$$= \frac{A_s}{J(0)} \sum_j \sum_\ell J_{i\ell} < S_\ell\, S_j > \exp [\, i\, \vec{q}.(\vec{R}_i - \vec{R}_j)]$$

$$+ < B_s' \,(\beta 0_i) > \qquad (C.5)$$

From (C.1), (C.2) and (C.3), (C.5) becomes

$$G_s\,(\vec{q}) = A_s\, G_s(\vec{q})\, J(q)/J(\vec{0}) + < B_s' \,(\beta 0_i) > \quad .$$

Solving for $G_s\,(\vec{q})$

$$G_s\,(\vec{q}) = \frac{< B_s' \,(\beta 0_i) >}{1 - A_s \quad J(\vec{q})/J(\vec{0})} \quad . \qquad (C.6)$$

Since $\lim_{\vec{q}\to 0} G_s\,(\vec{q}) \to \infty$ at $T = T_c$ (C.6) leads to the criticality equation $A_s = 1$ at $T = T_c$

Thus

$$G_s(\vec{q}) = < B_s' \,(\beta 0_i) > / \,(1 - J(\vec{q}) \,/\, J(\vec{0}))\ \text{at}\ T = T_c; \qquad (C.7)$$

also, from (C.1)

$$\sum_{\vec{q}} G_s(\vec{q}) = \sum_j \,[\, \sum_{\vec{q}} \exp\ i\ \vec{q}.\,(\,\vec{R}_i - \vec{R}_j\,)] < S_i\, S_j > \qquad (C.8)$$

Since $\sum_{\vec{q}} \exp\, i\,\vec{q}\,.\,(\vec{R}_i - \vec{R}_j) = N\,\delta_{ij}$

(C.8) becomes

$$\sum_{\vec{q}} G_s(\vec{q}) = N < S_i^2 > \quad . \qquad (C.9)$$

From (C.7) we get at $T = T_c$

$$(1/N) \sum_{\vec{q}} G_s(\vec{q}) = < B_s' \,(\beta 0_i) > \frac{1}{N} \sum_{\vec{q}} \frac{1}{1 - J(\vec{q})/J(\vec{0})} \qquad (C.10)$$

The summation on the right-hand side, given the name F(1): $F(1) = (1/N) \sum_{\vec{q}} \dfrac{1}{1 - J(\vec{q})/J(\vec{0})}$

is the Watson (1939) sum. F (1) = 1.51638, 1.3932, 1.34466, for the SC, BCC and FCC lattices respectively.

Comparing (C.7) and (C.10)

$$< S_i^2 > = F(1) < B_s'(\beta 0_i) > , \qquad \text{at } T = T_c$$

(also, from Appendix B, at all T $< S_i^2 > = < B_s^2\,(\beta 0_i) > + < B_s'(\beta 0_i) >$)

(C.7) may then be written

$$G_s(\vec{q}) = \frac{<S_i^2>}{F(1)\,(\,1 - J(\vec{q})/J(\vec{0})} \quad , \; T = T_c \quad . \qquad (C.11)$$

Example :

$T_2 = < \frac{O_i^2}{J^2(0)} >$ may be evaluated from (C.1), (C.2) and (C.3)

$$< \frac{O_i^2}{J^2(0)} > = \frac{1}{J^2(0)} \sum_j \sum_\ell J_{ij} J_{i\ell} < S_j S_\ell > .$$

From (C.2)

$$< \frac{O_i^2}{J^2(0)} > = \frac{1}{N J^2(0)} \sum_{\vec{q}} G_s(\vec{q}) [\sum_j e^{i \vec{q}. (\vec{R}_i - \vec{R}_j)} J_{ij}] \sum_\ell J_{i\ell} e^{i(\vec{R}_\ell - \vec{R}_i).\vec{q}} ,$$

then from (C.3)

$$< \frac{O_i^2}{J^2(0)} > = \frac{1}{N} \sum_{\vec{q}} G_s(\vec{q}) J^2(\vec{q})/J^2(\vec{0}) \quad (C.12)$$

$$< \frac{O_i^2}{J^2(0)} > = \frac{1}{N} \sum_{\vec{q}} G_s(\vec{q}) [J^2(\vec{q})/J^2(\vec{0}) - 1] + \frac{1}{N} \sum_{\vec{q}} G_s(\vec{q}) \quad (C.13)$$

Substituting (C.9) and (C.11) into (C.13), we get

$$< \frac{O_i^2}{J^2(0)} > = \frac{1}{N} \frac{<S_i^2>}{F(1)} \sum_{\vec{q}} [(J^2(\vec{q})/J^2(\vec{0}) - 1)/(1 - J(\vec{q})/J(\vec{0})] + <S_i^2>$$

$$= <S_i^2> [1 - \frac{1}{NF(1)} \sum_{\vec{q}} (1 + J(\vec{q})/J(\vec{0}))]$$

i.e.

$$T_2 = \langle S_i^2 \rangle (1 - 1/F(1)) \qquad (C.14)$$

since $\sum_{\vec{q}} 1 = N$ and $\sum_{\vec{q}} J(\vec{q}) = J_{ii} = 0$.

Example:

From (C.14) ,(C.4) and (2.16) one may prove that

$U_2 = T_2$, that is, $\langle \frac{0_i}{J(0)} S_i \rangle = \langle \frac{0_i^2}{J^2(0)} \rangle$.

Knowing that $\langle S_i S_j \rangle = \frac{A_s}{J(0)} \langle S_j 0_i \rangle + \delta_{ij} \langle B_s' (\beta 0_i) \rangle$

(from (C.14)) and that, at $T = T_c$,

$$\langle S_i^2 \rangle = \langle S_i \frac{0_i}{J(0)} \rangle + \langle B_s' (\beta 0_i) \rangle \qquad (C.15)$$

Since $\langle S_i^2 \rangle = F(1) \langle B_s'(\beta 0_i) \rangle$

(C.15) becomes

$$\langle S_i^2 \rangle = \langle S_i \frac{0_i}{J(0)} \rangle + \langle S_i^2 \rangle /F(1) .$$

Solving for $\langle S_i \frac{0_i}{J(0)} \rangle$

$$\langle S_i \frac{0_i}{J(0)} \rangle = \langle S_i^2 \rangle (1 - 1/F(1)) . \qquad (C.16)$$

Comparing (C.14) and (C.16), one obtains

$$< \frac{0_i^2}{J^2(0)} > \; = \; < S_i \frac{0_i}{J(0)} > \qquad \text{at } T = T_c \qquad (C.17)$$

The same result may be obtained directly from (C.4).

Appendix D: Indirect Decoupling. Derivation of (5.9) and (5.10).

For the spin 1 case, knowing that ((5.1a,b))

$$S_j^{2k} = S_j^2 \qquad k = 1, 2, \ldots \qquad (D.1)$$

$$S_j^{2k+1} = S_j \qquad k = 1, 2, \ldots \qquad (D.2)$$

one obtains the following binomial expansions

$$<(0_i/J - S_\delta)^{2p+1} S_i> = <(0_i/J)^{2p+1} S_i> - {}^{2p+1}C_1 <(0_i/J)^{2p} S_\delta S_i>$$

$$+ \sum_{k=1}^{p} {}^{2p+1}C_{2k} <(0_i/J)^{2p+1-2k} S_\delta S_i> \qquad (D.3)$$

$$- \sum_{k=1}^{p} {}^{2p+1}C_{2k+1} <(0_i/J)^{2p-2k} S_\delta^2 S_i>$$

and

$$<(0_i/J - S_\delta)^{2p+1} S_\delta^2 S_i> = <(0_i/J)^{2p+1} S_\delta S_i> - {}^{2p+1}C_1 <(0_i/J)^{2p} S_\delta S_i>$$

$$+ \sum_{k=1}^{p} {}^{2p+1}C_{2k} <(0_i/J)^{2p+1-2k} S_\delta S_i> - \sum_{k=1}^{p} {}^{2p+1}C_{2k+1} <(0_i/J)^{2p-2k} S_\delta S_i>.$$

(D.4)

One subtracts (D.4) from (D.3), which leads to

$$<(O_i/J)^{2p+1} S_\delta^2 S_i> = <(O_i/J - S_\delta)^{2p+1} S_\delta^2 S_i>$$

$$- <(O_i/J - S_\delta)^{2p+1} S_i> + <(O_i/J)^{2p+1} S_i> \quad (D.5)$$

for p = 0, 1, 2, ..., z - 2.

(D.5) is exact. In indirect decoupling one uses (5.7), namely

$$<(O_i/J - S_\delta)^{2p+1} S_\delta^2 S_i> = <(O_i/J - S_\delta)^{2p+1} S_i> <S_\delta^2> \quad (D.6)$$

Substituting (D.6) into (D.5) leads to the first decoupling equation

$$<(O_i/J)^{2p+1} S_\delta^2 S_i> = <(O_i/J-S_\delta)^{2p+1} S_i> \{<S_\delta^2> - 1\} + <(O_i/J)^{2p+1} S_i> \quad (D.7)$$

Similarly, using (5.1), one obtains the following binomial expansions

$$<(O_i/J-S_\delta)^{2p+2}> = <(O_i/J)^{2p+2}> + \sum_{k=1}^{p+1} {}^{2p+2}C_{2k-1} <(O_i/J)^{2p+2-2k} S_\delta^2>$$

$$- \sum_{k=1}^{p+1} {}^{2p+2}C_{2k-1} <(O_i/J)^{2p+3-2k} S_\delta> \quad (D.8)$$

and

$$\langle (O_i/J-S_\delta)^{2p+2} S_\delta^2 \rangle = \langle (O_i/J)^{2p+2} S_\delta^2\rangle + \sum_{k=1}^{p+1} {}^{2p+2}C_{2k-1} \langle (O_i/J)^{2p+2-2k} S_\delta^2\rangle$$

$$- \sum_{k=1}^{p+1} {}^{2p+2}C_{2k-1} \langle (O_i/J)^{2p+3-2k} S_\delta\rangle \qquad \text{(D.9)}$$

for $p = 0, 1, 2, \ldots, z-2$.

One now assumes (5.8), namely

$$\langle (O_i/J-S_\delta)^{2p+2} S_\delta^2 \rangle = \langle (O_i/J-S_\delta)^{2p+2}\rangle \langle S_\delta^2\rangle \quad . \qquad \text{(D.10)}$$

Using (D.10) and subtracting (D.9) from (D.8), one solves for

$\langle (O_i/J)^{2p+2} S_\delta^2\rangle$ and gets

$$\langle (O_i/J)^{2p+2} S_\delta^2\rangle = \langle (O_i/J-S_\delta)^{2p+2}\rangle \{ \langle S_\delta^2\rangle - 1 \}$$

$$+ \langle (O_i/J)^{2p+2}\rangle \qquad \text{(D.11)}$$

Hence, equations (5.9) and (5.10).

Appendix E

Any function of the operator 0_i which has a Taylor expansion in 0_i^2 may be written as a finite series ending in 0_i^{2sz} (0_i^{2z} for the spin 1 case) due to the existence of the spin-operator reduction relations (3.1). That is, one may write (if F (0) = 0)

$$< F (0_i^2) > = A_2 < \frac{0_i^2}{J^2 (0)} > + A_4 < \frac{0_i^4}{J^4 (0)} > + \ldots + A_{2sz} < \frac{0_i^{2sz}}{J^{2sz} (0)} > \qquad \text{(E.1a)}$$

$$\equiv A_2 T_2 + A_4 T_4 + \ldots A_{2sz} T_{2sz} \quad . \qquad \text{(E.1b)}$$

The A_n are functions of β which are determined by putting $(0i/J)^2$ successively equal to its eigenvalues $0, 1^2, 2^2, \ldots, (sz)^2$ from (E.1a) before the thermal average is taken, as explained in FCM, which leads to

$$F (0_i^2) = A_2 \frac{0_i^2}{J^2 (0)} + A_4 \frac{0_i^4}{J^4 (0)} + \ldots + A_{2sz} \frac{0_i^{2sz}}{J^{2sz} (0)} \qquad \text{(E.2)}$$

$$F (1) = A_2 + A_4 + \ldots + A_{2sz}$$

$$F (2^2) = A_2 (2^2/Z^2) + A_4 (2^4/Z^4) + \ldots + A_{2sz} (2^{2sz}/Z^{2sz})$$

$$F((SZ)^2) = A_2 S^2 + A_4 S^4 + \ldots + A_{2sz} S^{2sz}$$

where $J(0) = z J$.

One has then sz simultaneous linear equations in the sz unknowns, A_2, A_4, ... A_{2sz} which may then be substituted into (E.1b). (The procedure is completely analogous to that used by Fisher (1959), the difference being that one is here dealing with the spin sums O_i rather than with individual spins.)

APPENDIX F

THE FORTRAN PROGRAM TO CALCULATE T_c FOR THE SPIN 1 ISING FERROMAGNET

```
     PROGRAM SPIN 1 (INPUT,OUTPUT)

TO CALCULATE THE CRITICAL TEMPERATURE FOR THREE
DIMENSIONAL LATTICES,SPIN 1 ISING FERROMAGNET

     DIMENSION TT(100),AS(50),BS(50),DS(50),OISI(50),OISD(50)
     DIMENSION US(50),UU(100)
     COMMON N,Z,ICASE,F1
     READ*,Z,BJO,SDS,F1,ICASE
Z NUMBER OF NEAREST NEIGHBOURS
BJO IS B*J())=J(0)/KB/TC
SDS IS AN INITIAL VALUE OF <S**2>
F1 IS THE WATSON SUM

     N=Z
     DO 1 I=1,50

TWO-VARIABLE NEWTON-RAPHSON METHOD

     X1=SDS
     Y1=BJO
     CALL AWRTS(X1,Y1,APS)
     CALL AWRTB(X1,Y1,APB)
     CALL SWRTS(X1,Y1,SPS)
     CALL SWRTB(X1,Y1,SPB)
     DJ=APS*SPB-APB*SPS
     SDS=SDS-((A(X1,Y1))*SPB-(S(X1,Y1))*APB)/DJ
     BJO=BJO+((A(X1,Y1))*SPS-(S(X1,Y1))*APS)/DJ
     ERR1=ABS(X1-SDS)
     ERR2=ABS(Y1-BJO)
     IF(ERR1.LE.1.E-10.AND.ERR2.LE.1.E-10)GO TO 11
   1 CONTINUE
```

```
   11 PRINT*,"SDS=",SDS
      PRINT*,"BJO=",BJO
      PRINT*,"F1=",F1
      TCTM=3/(2*BJO)
C TCTM IS THE RATIO OF CRITICAL TEMPERATURE TO MEAN FIELD
C CRITICAL TEMPERATURE
      PRINT*,"TCTM=",TCTM
      NN=2*N
      IF(ICASE.EQ.1)PRINT*,"SPIN 1 INDIRECT DECOUPLING"
      IF(ICASE.EQ.2)PRINT*,"SPIN 1 RATIO DECOUPLING"
      IF(ICASE.EQ.3)PRINT*,"SPIN 1 DIRECT DECOUPLING"
      IF(ICASE.EQ.1)CALL GETT1(SDS,TT)
      IF(ICASE.EQ.2)CALL GETT2(SDS,TT)
      IF(ICASE.EQ.3)CALL GETT3(SDS,TT)
      PRINT*,"TT=",(TT(I),I=2,NN,2)
      CALL UGET(SDS,BJO,UU)
      PRINT*,"UU=",(UU(I),I=2,NN,2)
      STOP
      END
C------------------------------------------------------------
C THE FOLLOWING FOUR SUBROUTINES DIFFERENTIATE THE FUNCTIONS
C A(SDS,BJO) AND S(SDS,BJO) W.R.T. SDS AND BJO
      SUBROUTINE AWRTS(SDS,BJO,APS)
      COMMON N,Z,ICASE
      H=.001
      DO 2 II=1,50
```

```
      S1=SDS-2.*H
      S2=SDS-H
      S3=SDS+H
      S4=SDS+2.*H
      A5=APS
      APS=(A(S1,BJO)-8.*A(S2,BJO)+8.*A(S3,BJO)-A(S4,BJO))
     1/(12.*H)
      ERR3=ABS(A5-APS)
      IF(ERR3.LE.1.E-10)GO TO 21
      H=H/2.
    2 CONTINUE
   21 RETURN
      END

      SUBROUTINE AWRTB(SDS,BJO,APB)
      COMMON N,Z,ICASE
      H=.001
      DO 3 K=1,50
      B1=BJO-2.*H
      B2=BJO-H
      B3=BJO+H
      B4=BJO+2.*H
      B5=APB
      APB=(A(SDS,B1)-8.*A(SDS,B2)+8.*A(SDS,B3)-A(SDS,B4))
     1/(12.*H)
      ERR4=ABS(B5-APB)
      IF(ERR4.LE.1.E-10)GO TO 21
```

```
      H=H/2.
    3 CONTINUE
   21 RETURN
      END

      SUBROUTINE SWRTS(SDS,BJO,SPS)
      COMMON N,Z,ICASE
      H=.001
      DO 4 KK=1,50
      S1=SDS-2.*H
      S2=SDS-H
      S3=SDS+H
      S4=SDS+2.*H
      S5=SPS
      SPS=(S(S1,BJO)-8.*S(S2,BJO)+8.*S(S3,BJO)-S(S4,BJO))
     1/(12.*H)
      ERR5=ABS(S5-SPS)
      IF(ERR5.LE.1.E-10)GO TO 41
      H=H/2.
    4 CONTINUE
   41 RETURN
      END

      SUBROUTINE SWRTB(SDS,BJO,SPB)
      COMMON N,Z,ICASE
      H=.001
      DO 5 L=1,50
```

```
      B1=BJO-2.*H
      B2=BJO-H
      B3=BJO+H
      B4=BJO+(2.*H)
      B5=SPB
      SPB=(S(SDS,B1)-8.*S(SDS,B2)+8.*S(SDS,B3)-S(SDS,B4))
     1/(12.*H)
      ERR6=ABS(B5-SPB)
      IF(ERR6.LE.1.E-10)GO TO 51
      H=H/2.
    5 CONTINUE
   51 RETURN
      END
C------------------------------------------------------
EVALUATION OF S=<S**2>-...
      FUNCTION S(SDS,BJO)
      COMMON N,Z,ICASE
      DIMENSION AS(50),TT(100)
      CALL SCOEF(BJO,AS)
      IF(ICASE.EQ.1)CALL GETT1(SDS,TT)
      IF(ICASE.EQ.2)CALL GETT2(SDS,TT)
      IF(ICASE.EQ.3)CALL GETT3(SDS,TT)
      NN=N*2
      SUM=0
      DO 5 I=2,NN,2
      J=I/2
```

```
      SUM=SUM+(AS(J)*TT(I))
    5 CONTINUE
      S=SDS-2./3.-SUM
      RETURN
      END

      SUBROUTINE SCOEF(BJO,AS)
C SOLVE FOR MATRICES WITH HELP OF LEQT2F
      DIMENSION D(50,50),AS(50),WK(200)
      COMMON N,Z,ICASE
      DO 40 I=1,N
      DO 30 J=1,N
      AI=FLOAT(I)
      D(I,J)=(AI/Z)**(2*J)
   30 CONTINUE
   40 CONTINUE
      X=BJO/(2.*Z)
      DO 50 I=1,N
      BI=FLOAT(I)*X
      AS(I)=4./3.+.5*(COTH(BI))**2-1.5*(COTH(3.*BI))*(COTH(BI))
   50 CONTINUE
      CALL LEQT2F(D,1,N,50,AS,0,WK,IER)
      RETURN
      END

C-----------------------------------------------------------
C CALCULATION OF A=1

      FUNCTION A(SDS,BJQ)
```

```
      DIMENSION DS(50),BS(50),TT(100)
      COMMON N,Z,ICASE
      CALL ANCOEF(BJO,DS)
      IF(ICASE.EQ.1)CALL GETT1(SDS,TT)
      IF(ICASE.EQ.2)CALL GETT2(SDS,TT)
      IF(ICASE.EQ.3)CALL GETT3(SDS,TT)
      CALL ADCOEF(BJO,BS)
      NN=2*N
      SUM=0
      DO 5 I=2,NN,2
      J=I/2
      SUM=SUM+(TT(I)*DS(J))
    5 CONTINUE
      AN=SUM
      ASUM=0
      DO 6 I=2,NN,2
      J=I/2
      ASUM=ASUM+(TT(I)*BS(J))
    6 CONTINUE
      AD=ASUM
      A=AN/AD-1.
      RETURN
      END

      SUBROUTINE ANCOEF(BJO,DS)
      DIMENSION D(50,50),DS(50),WK(200)
      COMMON N,Z,ICASE
```

```
      DO 40 I=1,N
      DO 30 J=1,N
      AI=FLOAT(I)
      D(I,J)=(AI/Z)**(2*J)
   30 CONTINUE
   40 CONTINUE
      DO 50 I=1,N
      Y=BJO/(2*Z)
      BI=FLOAT(I)*Y
      DS(I)=(1.5*COTH(3.*BI)-.5*(COTH(BI)))**2
   50 CONTINUE
      CALL LEQT2F(D,1,N,50,DS,0,WK,IER)
      RETURN
      END

      SUBROUTINE ADCOEF(BJO,BS)
      DIMENSION D(50,50),BS(50),WK(200)
      COMMON N,Z,ICASE
      DO 40 I=1,N
      DO 50 J=1,N
      AI=FLOAT(I)
      D(I,J)=(AI/Z)**(2*J)
   50 CONTINUE
   40 CONTINUE
      DO 30 I=1,N
      A=BJO/(2*Z)
      BI=FLOAT(I)
```

```
      BS(I)=(BI/Z)*(1.5*COTH(3.*A*BI)-.5*COTH(A*BI))
   30 CONTINUE
      CALL LEQT2F(D,1,N,50,BS,0,WK,IER)
      RETURN
      END
C---------------------------------------------
      FUNCTION COEFA(L,SDS,T2)
      COMMON N,Z,ICASE
      Z1=(1.-1./Z)**(-1)
      Z2=1.-(SDS/(Z*T2))
      AL=FLOAT(L)
      COEFA=(1.-(1.-(2.*AL+1.)/Z)*(Z1*Z2))**(-1)
      RETURN
      END
C---------------------------------------------
      FUNCTION COEFB(L,SDS,T2)
      COMMON N,Z,ICASE
      Z1=(1.-1./Z)**(-1)
      Z2=1.-(SDS/(Z*T2))
      COEFB=Z1*Z2*COEFA(L,SDS,T2)
      RETURN
      END
C---------------------------------------------
      FUNCTION BIN(K,L)
      COMMON N,Z,ICASE
      BIN=1.
      DO 8 I=1,L
```

```
      AL=FLOAT(L)
      AI=FLOAT(I)
      AK=FLOAT(K)
      PROD=(AK-AL+AI)/AI
      BIN=BIN*PROD
    8 CONTINUE
      RETURN
      END
C-----------------------------------------------------------------
EVALUATES T'S BASED ON THE "INDIRECT DECOUPLING" METHOD

      SUBROUTINE GETT1(SDS,TT)
      DIMENSION TT(100),OISI(50),OISD(50)
      COMMON N,Z,ICASE,F1
      T2=SDS*(1.-1./F1)
      TT(2)=T2
      NN=2*N-2
      DO 1 I=2,NN,2
      M=I/2
      SUM=SDS*COEFA(M,SDS,T2)*(Z**(-(2*M+1)))
      ASUM4=0
      DO 2 J=1,M
      OISI(1)=TT(2)*(Z-1.)
      OISD(2)=(Z**2)*(TT(2)*(1.-2./Z))+SDS
      L=2*M+1-2*J
      IF(L-1.EQ.0)GO TO 8
      LL=(L-1)/2
```

```
      ASUM1=0
      COEF1=(Z**L)*(1.-FLOAT(L)/Z)*TT(L+1)
      DO 5 II=1,LL
      ASUM1=ASUM1+DDJ(L,2*II)*(Z**L)*TT(L+1-2*II)
     1+(SDS-1.)*BIN(L,2*II)*OISI(-2*II+L)
    5 CONTINUE
      OISI(L)=COEF1+ASUM1
    8 JJ=2*M+2-2*J
      IF(JJ-2.EQ.0)GO TO 9
      COEF2=(Z**JJ)*TT(JJ)
      ASUM2=0
      K=JJ/2
      DO 4 KK=1,K
      ASUM2=ASUM2-(Z**(JJ+1-2*KK))*(BIN(JJ,2*KK-1)*TT(-2*KK+JJ+2))
     2+(BIN(JJ,2*KK)*TT(-2*KK+JJ))*Z**(JJ-2*KK)
     2+(SDS-1.)*BIN(JJ,2*KK)*OISD(-2*KK+JJ)
    4 CONTINUE
      OISD(JJ)=ASUM2+COEF2
    9 ASUM4=ASUM4+COEFB(M,SDS,T2)*DDJ(2*M+1,2*J)*TT(2*M+2-2*J)
     1+COEFA(M,SDS,T2)*DDJ(2*M+1,2*J-1)*TT(2*M+2-2*J)
     1+(SDS-1.)*Z**(-(2*M+1))*(COEFB(M,SDS,T2)*BIN(2*M+1,2*J)
     1*OISI(2*M+1-2*J)+COEFA(M,SDS,T2)*BIN(2*M+1,2*J-1)*
     1OISD(2*M+2-2*J))
    2 CONTINUE
      K=I+2
      TT(K)=SUM+ASUM4
    1 CONTINUE
```

```
      RETURN
      END

      FUNCTION DDJ(M,J)
      COMMON N,Z,ICASE
      DDJ=(BIN(M,J)-BIN(M,J+1)/Z)*Z**(-J)
      RETURN
      END

C-----------------------------------------------------

      FUNCTION COTH(X)
      COTH=(EXP(X)+EXP(-X))/(EXP(X)-EXP(-X))
      RETURN
      END

C-----------------------------------------------

C EVALUATES T'S BASED ON THE DIRECT DECOUPLING METHOD

      SUBROUTINE GETT3(SDS,TT)
      DIMENSION TT(100)
      COMMON N,Z,ICASE,F1
      T2=SDS*(1.-1./F1)
      TT(2)=T2
      NN=2*N-2
      DO 1 I=2,NN,2
      M=I/2
      SUM=SDS*COEFA(M,SDS,T2)*(Z**(-(2*M+1)))
```

```
      ASUM4=0
      DO 2 J=1,M
      ASUM4=ASUM4+COEFB(M,SDS,T2)*DJ(2*M+1,2*J,SDS)*TT(2*M+2-2*J)
     1+COEFA(M,SDS,T2)*DJ(2*M+1,2*J-1,SDS)*TT(2*M+2-2*J)
    2 CONTINUE
      K=I+2
      TT(K)=SUM+ASUM4
    1 CONTINUE
      RETURN
      END

      FUNCTION DJ(M,J,SDS)
      COMMON N,Z,ICASE
      DJ=((BIN(M,J))*SDS-BIN(M,J+1)/Z)*Z**(-J)
      RETURN
      END

C-----------------------------------------------------

EVALUATES T'S BASED ON THE RATIO DECOUPLING METHOD

      SUBROUTINE GETT2(SDS,TT)
      DIMENSION TT(100)
      COMMON N,Z,ICASE,F1
      T2=SDS*(1.-1./F1)
      TT(2)=T2
      NN=2*N-2
      DO 1 I=2,NN,2
```

```
      M=I/2
      SUM=SDS*COEFA(M,SDS,T2)*(Z**(-(2*M+1)))
      ASUM4=0
      DO 2 J=1,M
      ASUM4=ASUM4+COEFB(M,SDS,T2)*SS(2*M+1,2*J,SDS)*TT(2*M+2-2*J)
     1+COEFA(M,SDS,T2)*EE(2*M+1,2*J-1,SDS,T2)*TT(2*M+2-2*J)
    2 CONTINUE
      K=I+2
      TT(K)=SUM+ASUM4
    1 CONTINUE
      RETURN
      END

      FUNCTION SS(M,J,SDS)
      COMMON N,Z,ICASE,F1
      XICASE=SDS+(1.-SDS)/Z
      SS=((BIN(M,J))*XW-BIN(M,J+1)/Z)*Z**(-J)
      RETURN
      END

      FUNCTION EE(M,J,SDS,T2)
      COMMON N,Z,W,F1
      XF=SDS*((2./(Z*SDS))-1./(T2*(Z**2))+1.-(2./Z))
     1+SDS*(SDS/(T2*(Z**2)))
      BB=BIN(M,J)*XF
      CC=BIN(M,J+1)/Z
      DD=BB-CC
```

```
      EE=DD/(Z**(J))
      RETURN
      END
C-----------------------------------------
C     EVALUATION OF U'S FROM THE KNOWN T VALUES
      SUBROUTINE UGET(SDS,BJO,UU)
      COMMON N,Z,ICASE
      DIMENSION TT(100),US(50),UU(100)
      IF(ICASE.EQ.1)CALL GETT1(SDS,TT)
      IF(ICASE.EQ.2)CALL GETT2(SDS,TT)
      IF(ICASE.EQ.3)CALL GETT3(SDS,TT)
      NN=2*N
      DO 6 II=2,NN,2
      CALL USCOEF(BJO,II,US)
      SUM=0
      DO 5 I=2,NN,2
      J=I/2
      SUM=SUM+(US(J)*TT(I))
    5 CONTINUE
      UU(II)=SUM
    6 CONTINUE
      RETURN
      END

      SUBROUTINE USCOEF(BJO,II,US)
      COMMON N,Z
```

```
      DIMENSION D(50,50),US(50),WK(200)
      DO 4 I=1,N
      DO 5 J=1,N
      AI=FLOAT(I)
      D(I,J)=(AI/Z)**(2*J)
    5 CONTINUE
    4 CONTINUE
      A=BJO/(2.*Z)
      DO 3 I=1,N
      BI=FLOAT(I)
      US(I)=((BI/Z)**(II-1))*(1.5*COTH(3.*A*BI)-.5*COTH(A*BI))
    3 CONTINUE
      CALL LEQT2F(D,1,N,50,US,0,WK,IER)
      RETURN
      END
```