A COMPARATIVE STUDY OF TWO DECOUPLING PROCEDURES IN THE GREEN'S FUNCTION TREATMENT OF THE ISING FERROMAGNET

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ABSTRACT

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TABLE OF CONTENTS

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1. INTRODUCTION

Recently, Frank[1] made a moment comparison between two procedures for decoupling the infinite hierarchy of Green's function equations: a simpler procedure due to Tomita and Tanaka[2] (called hereafter the TTA procedure), and a more accurate but less tractable one due to Tahir-Kheli[3] (called hereafter the RPA procedure). The model, chosen for simplicity, was that of the Ising paramagnet. It was found that, as far as the first few moments are concerned, for large effective number of nearest neighbours z the results differ only to order $(1/z^2)$. This indicated that the TTA would constitute a reasonable and reasonably simple approach that might be carried a stage further than the more complicated RPA.

Some properties of the Ising ferromagnet, then, are here calculated in the first few stages of the TTA and compared with those calculated in the RPA[3]. It is found that for first- and second-stage decoupling the TTA results are indeed reasonable. For third-stage decoupling, however, they are no longer reasonable at low temperatures; an inconsistency arises due to the appearance of complex poles of the lowest-order Green's function in complex energy space. Such poles are ruled out by the general theory (see e.g., Reference 23, p. 325) and moreover such poles do not appear in the more exact third-stage RPA. The indications are, then, that the more general third-stage results of TTA must be regarded with suspicion close to the Ising limit. It is also interesting to note that a third-stage decoupling within a specified decoupling scheme may be a much more sensitive test of that scheme than a second-stage decoupling.

In the following section, a brief history of the development of the theory of ferromagnetism, with special emphasis on the Ising and Heisenberg models, is presented; and the importance of the Ising model and the use of the Green's function method as applied to ferromagnetism are also mentioned. In Section 2, the Green's function approach is described in detail. The RPA and TTA decoupling procedures are introduced and applied to the Ising model of ferromagnetism in Section 4. The results of the first- and second-stage RPA due to Tahir-Kheli[3] are presented in Section 5. In Section 6, several results of the first- and second-stage TTA are obtained and the third-stage TTA is shown to be inconsistent. In Section 7, some implications of these findings are discussed.

2. FERROMAGNETISM

Ferromagnetism is caused by the interaction of the spins of certain electrons at the various atomic sites in a crystal.[4] An assembly consisting of microscopic systems which interact, under certain conditions, exhibits co-operative phenomena. Statistical mechanics has shown that co-operative phenomena have characteristic singularities in their physical properties. In the case of a ferromagnetic, the physical properties show discontinuities at a critical temperature, T_C, known as the Curie temperature or Curie point.

At $T < T_C$, spontaneous magnetization is present and the magnetization, M, tends to a non-zero value as the external magnetic field is reduced to zero. The magnetization is a function of the temperature and reduces to zero at T_C. At $T > T_C$, there is no spontaneous magnetization, but the ferromagnetic possesses a paramagnetic susceptibility which becomes infinite at T_C. The specific heat of a ferromagnetic also shows a discontinuity at T_C.

The first theoretical attempt to account for the properties of a ferromagnetic was made by Weiss[5] (1907), who postulated the existence of a large "internal field". By means of this hypothesis, Weiss was able to reproduce such important physical properties of the ferromagnetic as: the Curie temperature, spontaneous magnetization, and a magnetic susceptibility proportional to $1/(T-T_C)$ above the Curie temperature. However, the origin of this "internal field" was not clear and a statistical formulation in terms of atomic interactions was not possible.

Attempts at such a formulation were made by Ising[6] (1925) and Heisenberg[7] (1928). Their models will be considered in more detail in parts 2.1 and 2.2 of this paper, respectively. Using simplifying approximations (mathematical) both models arrived at the same general results as the Weiss theory. But these mathematical approximations proved to be inadequate when it came to a detailed comparison with experiment.

Bragg and Williams[8] (1934) introduced the concept of long range order which is essential to a clear understanding of higher order transitions of which the Curie point of a ferromagnetic is an example. Bethe[9] (1935) showed how to introduce a parameter in order to take into account short range order, and hence laid the foundation for an improved approximation to the Ising model.

Onsager[10] (1944) solved exactly the Ising model for the two-dimensional quadratic lattice. The form of the specific heat curve obtained by Onsager differed markedly from both the experimental curve and curves obtained by various approximations. The differences between the Onsager results and the experimental results were thought to be due either to the inadequacy of the Ising model as a representation of the interactions, or to the two-dimensional nature of the Onsager solution.

Unfortunately the methods of Onsager and others for an exact solution of the Ising model fail completely in three dimensions, and there has still been virtually no progress with an exact solution to this problem. Theoretical research has been largely confined to improving closed-form approximations, and to deriving exact series expansions at high and low temperatures. Most of the progress has taken place in the second area, that is, with series expansions. Techniques[11,12,13] have been developed to extend these series, and predictions of critical properties of the model can be made with considerable confidence.

Theoretical developments regarding the Heisenberg model have proceeded more slowly. Series expansions are more difficult to derive and they therefore contain fewer terms. The spin wave picture introduced by Bloch[14] (1930) proved to be very helpful at low temperatures as did the spin wave interaction calculations of Dyson[15] (1956), but the formulae become invalid before the critical temperature is reached.

2.1 Ising Model of Ferromagnetism

The Ising model assumes a semi-classical type of interaction between the spins of certain electrons in the atoms making up the crystal. The interaction between two spins at sites labeled by i and j is taken as proportional to $S_i^z S_j^z$, the product of the z-components of the spins. The sites in the crystal are taken to be rigidly fixed, assuming that the vibrations of the crystal can either be neglected, or that they act independently of the spin configuration and that they can therefore be considered separately.[4] Therefore, in an external magnetic field H, the Hamiltonian may be written, for a crystal of N atoms (or ions) each of total spin S, as

$$\mathcal{H} = -\frac{J}{S^2}\sum_{i,j}^{N} S_i^z S_j^z - \frac{mH}{S}\sum_{i}^{N} S_i^z , \qquad (2.1)$$

where the summation is taken over all nearest-neighbour pairs i, j in the lattice, J is the interaction energy of parallel spins and m is the total magnetic moment of the site. The second term on the right-hand side of (2.1) arises because of the Zeeman effect in an external field. The Ising model therefore corresponds to extreme anisotropy since there is no interaction between the x and y components of spin.

It is therefore postulated that only nearest-neighbour lattice sites interact; that the energy is -J if the nearest neighbours have parallel spins and +J if they have antiparallel spins. The zero of energy is conveniently chosen to be the average of these two cases. J, which is a measure of the coupling, must be determined from the physical properties of the system. It is positive for a ferromagnetic system and negative for an antiferromagnetic system.

The original model considered by Ising was for $S = \frac{1}{2}$ and most theoretical work corresponds to this case. But it has also been possible, using series expansions, to study the effects of larger S's.[16]

Ising solved this model only in one dimension, and this case showed no ferromagnetism. Peierls[17] was the first to show that two- or three-dimensional models would exhibit ferromagnetism. But no one has as yet solved exactly (a) the three-dimensional Ising model; (b) the two-dimensional model in a magnetic field; (c) the two-dimensional model with interactions between next-nearest neighbours as well as nearest neighbours.

2.2 Heisenberg Model of Ferromagnetism

Dirac[18] had shown that the electronic spin and the Pauli exclusion principle combine in such a way as to produce between spins of two neighbouring electrons a possible coupling of the form

$$V = - J \underline{S}_1 \cdot \underline{S}_2 , \tag{2.2}$$

where $\underline{S}_1$ and $\underline{S}_2$ are the two neighbouring spins and J is a function of the distance between the spins called the exchange energy, or exchange coupling. Heisenberg[7] was the first to realize that if J was of positive sign it would provide an explanation of ferromagnetism. The Hamiltonian suggested by Heisenberg could then be written for a crystal of N atoms each of total spin S as

$$\mathcal{H} = -\frac{J}{S^2}\sum_{i,j}^{N} \underline{S}_i \cdot \underline{S}_j - \frac{mH}{S}\sum_{i}^{N} S_i^z \, , \qquad (2.3)$$

with the same notation as used in (2.1).

In contrast to the Ising model, the Heisenberg model corresponds to magnetic isotropy. In effect the Ising model ignores the off-diagonal elements of the spin operators and considers only the components along some fixed direction - usually the direction of the external magnetic field.

Calculations for the Heisenberg model being more difficult than for the Ising model, exact results have been obtained only for certain properties of the one-dimensional chain. No discontinuities were found to arise in one- or two-dimensional models.

High temperature series expansions are more reliable as $S \rightarrow \infty$, and for $S = \frac{1}{2}$ are less reliable than those for the Ising model. Only qualitative information has been obtained for the behaviour near the Curie point and the low temperature behaviour is much more complicated than that of the Ising model.

2.3 Importance of the Ising Model

Considering the facts that the spin interaction used in the Ising model is a scalar one and that lattice distances are fixed and do not depend upon spin orientation, one would tend to question the importance and usefulness of this model. However, the interest in the Ising model lies in the fact that it is one of the simplest descriptions of a system of interacting particles while still having some semblance of physical reality in it. The model forms an excellent test for any new approximative method for dealing with co-operative phenomena. If the new method cannot handle the Ising model, it certainly will not be able to deal with more complicated cases.

Even though the Ising model is not considered a realistic model of ferromagnetism, it is a very good model for a binary substitutional alloy and an interesting model of a gas, or liquid. Actually the Ising model can serve in any system where the configuration approximates a lattice on each site of which there is a binary choice with a certain favoured relative configuration of a pair.[19]

Lastly, the spin $\frac{1}{2}$ Ising model has served as a useful representation of the ferromagnetic behaviour of certain cobalt and rare earth salts at low temperatures.[20]

2.4 Green's Functions and Ferromagnetism

The various methods, that have been mentioned so far, for evaluating various properties of a ferromagnetic are valid only in each of their particular temperature range. Tyablikov and Bogolyubov[24,25] were the first to show that it is possible by using the Green's function method to develop one approximate method to evaluate the properties of a ferromagnetic which is valid in the whole temperature range. They had investigated the spin ½ Heisenberg model.

Much work has been done since in this area. Izyumov and Yakovlev[26] and Kawasahi and Mori[27] attempted to extend the Bogolyubov-Tyablikov theory to higher spin-values. Tahir-Kheli and ter Haar[28] tackled the same problem by a better method and also discussed the influence of higher-order decoupling. Tahir-Kheli developed a higher order random phase approximation (RPA) and applied it in the first two orders to the Heisenberg[29] and Ising[3] models of ferromagnetism.

In the following section, the Green's function approach is described in detail; applications to ferromagnetism follow in later sections.

3. GREEN'S FUNCTIONS

The type of Green's functions employed in statistical mechanics are the double-time temperature-dependent Green's functions[21,22]. There are three different basic kinds: the causal, $G_c(t,t')$; the retarded, $G_r(t,t')$; and the advanced, $G_a(t,t')$; respectively

$$G_c(t,t') = \langle\langle A(t)|B(t')\rangle\rangle_c = -i\langle TA(t)B(t')\rangle, \qquad (3.1a)$$

$$G_r(t,t') = \langle\langle A(t)|B(t')\rangle\rangle_r = -i\theta(t-t')\langle[A(t),B(t')]\rangle, \qquad (3.1b)$$

$$G_a(t,t') = \langle\langle A(t)|B(t')\rangle\rangle_a = i\theta(t'-t)\langle[A(t),B(t')]\rangle, \qquad (3.1c)$$

where the averages $\langle\ldots\rangle$ are grand canonical ensemble averages defined by the relation

$$\langle\ldots\rangle = \frac{\mathrm{Tr}(e^{-\beta\mathcal{H}_T}\ldots)}{\mathrm{Tr}(e^{-\beta\mathcal{H}_T})}, \qquad (3.2)$$

where

$$\beta = 1/k_BT \qquad (3.3)$$

with k_B, Boltzmann's constant; T, absolute temperature; and

$$\mathcal{H}_T = \mathcal{H} - \xi N, \qquad (3.4)$$

where $\mathcal{H}$ is the time-independent Hamiltonian operator of the system; N, the total number operator; and ξ is the chemical potential. In our particular case, N will be a constant and therefore will not enter in our calculations.

The A(t) and B(t') are time-dependent (Heisenberg) operators which are connected with the time-independent (Schrodinger) operators through the relation

$$A(t) = e^{i\mathcal{H}_Tt}Ae^{-i\mathcal{H}_Tt}, \qquad (3.5)$$

where, throughout, a system of units is used such that $\hbar = 1$.

The symbol T indicates a time-ordered product of operators defined as follows:

$$TA(t)B(t') = \theta(t-t')A(t)B(t') + \eta\,\theta(t'-t)B(t')A(t), \tag{3.6}$$

where $\theta(t)$ is a step function defined by the equations:

$$\theta(t) = 1, \quad t > 0 \; ; \quad \theta(t) = 0, \quad t < 0 \; ; \tag{3.7}$$

and

$$\eta = \pm 1 \; . \tag{3.8}$$

$[A,B]$ indicates the commutator or anti-commutator of the operators A and B:

$$[A,B] = AB - \eta BA \; , \; \eta = \pm 1 \; . \tag{3.9}$$

The sign of η in equations (3.6) and (3.9) is chosen according to convenience, depending on the nature of the particular problem.

Equations (3.1) can be rewritten, using equations (3.6) and (3.9), in the form

$$G_c(t,t') = -i\theta(t-t')\langle A(t)B(t')\rangle - i\eta\theta(t'-t)\langle B(t')A(t)\rangle, \tag{3.10a}$$

$$G_r(t,t') = -i\theta(t-t')\{\langle A(t)B(t')\rangle - \eta\langle B(t')A(t)\rangle\}, \tag{3.10b}$$

$$G_a(t,t') = i\theta(t'-t)\{\langle A(t)B(t')\rangle - \eta\langle B(t')A(t)\rangle\} \; , \tag{3.10c}$$

$$\eta = \pm 1 \; . \tag{3.10d}$$

It should be noted that the Green's functions (3.10a, b, c) are not defined for t = t' and also that

$G_r(t,t') = 0$ for $t < t'$ and $G_a(t,t') = 0$ for $t > t'$. It can be shown that the Green's functions $G_c(t,t')$, $G_r(t,t')$ and $G_a(t,t')$ depend on t and t' only through (t-t')[20].

3.1 Equations for the Green's Functions

Differentiating equations (3.10a, b, c) with respect to t, the following is obtained for all three Green's functions:

$$i\,\frac{dG}{dt} = \frac{d\theta(t-t')}{dt}\left\langle [A(t),B(t')] \right\rangle + \left\langle\!\left\langle i\,\frac{dA(t)}{dt} \middle| B(t') \right\rangle\!\right\rangle , \qquad (3.11)$$

where the subscripts on G and $\langle\langle \ldots \rangle\rangle$ have been omitted. Using the equation of motion for the Heisenberg operators:

$$i\,\frac{dA}{dt} = [A,\mathcal{H}] = A\mathcal{H} - \mathcal{H}A \quad , \qquad (3.12)$$

and the relation

$$\frac{d\theta(t-t')}{dt} = -\frac{d\theta(t'-t)}{dt} = \delta(t-t') \qquad (3.13)$$

in equation (3.11), the equation of motion for the Green's function G is obtained:

$$i\,\frac{dG}{dt} = \delta(t-t')\left\langle [A(t),B(t')] \right\rangle + \left\langle\!\left\langle [A(t),\mathcal{H}(t)] \middle| B(t') \right\rangle\!\right\rangle . \qquad (3.14)$$

The double-time Green's functions on the right hand side of (3.14) are usually of higher order than the one on the left-hand side of equation (3.14). One can construct equations of the form (3.14) for these higher order Green's functions and thus obtain a coupled chain of equations for the Green's functions. These equations would be exact, and their solution involves some type of approximation method to uncouple them at some stage. In Section 4 of this paper two decoupling schemes which have been used mainly in studying the properties of magnetic systems will be introduced as applied to the Ising ferromagnet.

It is often convenient to work in the energy representation of the Green's functions. Going over to the Fourier components of the Green's functions, i.e., writing

$$G(t,t') = \int_{-\infty}^{\infty} \langle\langle A|B\rangle\rangle_E \exp[-iE(t-t')] \, d(t-t'), \qquad (3.15)$$

and using the representation

$$\delta(t-t') = \frac{1}{2\pi} \int_{-\infty}^{\infty} \exp[-iE(t-t')] \, dE \qquad (3.16)$$

for the δ-function, one obtains from (3.14)

$$E \langle\langle A|B\rangle\rangle_E = \frac{1}{2\pi} \langle [A,B] \rangle + \langle\langle [A,\mathcal{H}] | B\rangle\rangle_E . \qquad (3.17)$$

3.2 Correlation Functions

Many quantities of physical interest can be derived from the correlation functions $\mathcal{F}_{AB}$ and $\mathcal{F}_{BA}$ which are defined as follows:

$$\mathcal{F}_{AB}(t,t') = \langle A(t)B(t')\rangle \; , \; \mathcal{F}_{BA}(t,t') = \langle B(t')A(t)\rangle . \qquad (3.18)$$

These time correlation functions depend, as do the Green's functions, only on t-t'; but, in contradistinction to the Green's functions, they are defined for t = t' since they do not contain the discontinuous factor $\theta(t-t')$.

Equations of motion can be obtained for the correlation functions:

$$i\,\frac{d\mathcal{F}_{BA}}{dt} = \left\langle B(t')\left[A(t),\mathcal{H}(t')\right]\right\rangle \quad , \tag{3.19a}$$

$$i\,\frac{d\mathcal{F}_{AB}}{dt} = \left\langle \left[A(t),\mathcal{H}(t\right] B(t')\right\rangle \quad , \tag{3.19b}$$

by differentiating (3.18) with respect to t taking into consideration the equations of motion of the operators.

The correlation functions can be obtained either from a direct integration of equations (3.19) using the necessary boundary conditions, or indirectly from an evaluation of the Green's functions from equation (3.17). This latter method is usually employed since it is easier to satisfy boundary conditions with the use of the spectral theorems.

3.3 Spectral Representations

a) Spectral Representations for the Time Correlation Functions

Using (3.18) and (3.2), $\mathcal{F}_{BA}$ can be written in an obvious notation as

$$\mathcal{F}_{BA}\,(t,t') = (\mathrm{Tr}\; e^{-\beta\mathcal{H}_T})^{-1} \sum_{\nu,\mu} \langle\nu|e^{-\beta\mathcal{H}_T - i\mathcal{H}_T(t-t')}B|\mu\rangle \langle\mu|e^{i\mathcal{H}_T(t-t')}A|\nu\rangle \; . \tag{3.20}$$

If use is made of a representation for the matrix elements such that $\mathcal{H}_T$ is diagonal, that is,

$$\langle\nu|\mathcal{H}_T|\mu\rangle = \delta_{\mu\nu}E_\nu \quad , \tag{3.21}$$

then from (3.20) one obtains

$$\mathcal{F}_{BA}(t,t') = (\mathrm{Tr}\ e^{-\beta\mathcal{H}_T})^{-1} \sum_{\nu,\mu} \exp[-\beta E_\nu - i(E_\nu - E_\mu)(t-t')] \langle\nu|B|\mu\rangle\langle\mu|A|\nu\rangle \ . \tag{3.22}$$

If one lets $J(\omega)$ be the Fourier transform of $\mathcal{F}_{BA}$, that is,

$$\mathcal{F}_{BA}(t,t') = \int_{-\infty}^{\infty} J(\omega)\ \exp[-i\omega(t-t')]\ d\omega \ , \tag{3.23}$$

then

$$J(\omega) = (\mathrm{Tr}\ e^{-\beta\mathcal{H}_T})^{-1} \sum_{\nu,\mu} \langle\nu|B|\mu\rangle\langle\mu|A|\nu\rangle e^{-\beta E_\nu} \delta(\omega - E_\nu + E_\mu) . \tag{3.24}$$

Similarly one obtains for the Fourier integral of $\mathcal{F}_{AB}$:

$$\mathcal{F}_{AB}(t,t') = \int_{-\infty}^{\infty} J(\omega) e^{\beta\omega} \exp[-i\omega(t-t')]\ d\omega . \tag{3.25}$$

Equations (3.23) and (3.25) are the required spectral representations of the time correlation functions, and $J(\omega)$ is the spectral intensity of $\mathcal{F}_{BA}(t,t')$.

b) Spectral Representations for the Green's Functions

The Fourier transform of $G_r(t,t')$ is $G_r(E)$, where

$$G_r(E) = \frac{1}{2\pi}\int_{-\infty}^{\infty} G_r(t,t')\ \exp[-iE(t-t')]\ d(t-t') . \tag{3.26}$$

$\theta(t)$ can be written in the form

$$\theta(t) = \int_{-\infty}^{t} e^{\epsilon t'} \delta(t') dt' \qquad \epsilon \to 0 \quad (\epsilon > 0) ; \tag{3.27}$$

or, since

$$\delta(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \exp(-ixt) dx \ , \tag{3.28}$$

in integral form

$$\theta(t) = \frac{i}{2\pi}\int_{-\infty}^{\infty} \frac{\exp(-ixt)}{x + i\epsilon}\ dx \ . \tag{3.29}$$

From (3.26), (3.10b), (3.23) and (3.25), it is found that

$$G_r(E) = \frac{1}{2\pi i}\int_{-\infty}^{\infty} d(t-t') \exp[i(E+i\epsilon)(t-t')]$$
$$\int_{-\infty}^{\infty} J(\omega)\ (e^{\beta\omega}-\eta) \exp[-i\omega(t-t')]d\omega \quad ,$$
$$= \frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{(e^{\beta\omega}-\eta)J(\omega)}{E-\omega+i\epsilon}\, d\omega. \tag{3.30}$$

Similarly, one obtains for the advanced Green's function

$$G_a(E) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{(e^{\beta\omega}-\eta)J(\omega)}{E-\omega-i\epsilon}\, d\omega. \tag{3.31}$$

From the theory of dispersion relations it can be shown that the function G(E) defined by the equation

$$G(E) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{(e^{\beta\omega}-\eta)J(\omega)}{E-\omega-i\epsilon}\, d\omega, \tag{3.32}$$

is an analytic function in the complex E-plane which is equal to $G_r(E)$ everywhere in the upper half-plane ($\text{Im } E > 0$) and to $G_a(E)$ ($\text{Im } E < 0$) everywhere in the lower half-plane, and which has singularities on the real axis. Therefore, if a cut is made along the real axis, the function

$$G(E) = \begin{cases} G_r(E) & \text{Im } E > 0 \\ G_a(E) & \text{Im } E < 0 \end{cases} \quad , \tag{3.33}$$

can be considered to be one analytic function consisting of two branches, one defined in the upper, and the other in the lower half-plane of complex values of E.

Therefore, from (3.33), (3.30) and (3.31),

$$G(\omega+i\epsilon) - G(\omega-i\epsilon) = \frac{1}{2\pi}\int_{-\infty}^{\infty}(e^{\beta\omega}-\eta)J(E)$$
$$\left[\frac{1}{\omega-E+i\epsilon} - \frac{1}{\omega-E-i\epsilon}\right] dE \ , \tag{3.34}$$

and if use is made of the symbolic identity of complex integration

$$\lim_{\epsilon \to +0} \frac{1}{x \pm i\epsilon} = P\frac{1}{x} \mp i\pi\delta(x) \quad , \tag{3.35}$$

where $P\frac{1}{x}$ indicates that in integrating we take the principal part of the integral, then the following relation is obtained:

$$G(\omega + i\epsilon) - G(\omega - i\epsilon) = -i(e^{\beta\omega} - \eta)J(\omega). \tag{3.36}$$

From (3.36), it is possible to write the correlation functions in terms of the Green's functions, for example:

$$\mathcal{F}_{BA}(t,t') = \lim_{\epsilon \to +0} i\int_{-\infty}^{\infty} \frac{G(\omega + i\epsilon) - G(\omega - i\epsilon)}{e^{\beta\omega} - \eta} \exp[-i\omega(t-t')]\, d\omega . \tag{3.37}$$

For t' = t, equation (3.37) can be put into a more convenient form as

$$\begin{aligned}\mathcal{F}_{BA}(0) &\equiv \langle BA \rangle \\ &= \lim_{\epsilon \to +0} (-2\ \mathrm{Im}) \int_{-\infty}^{\infty} \langle\langle A(t) | B(t) \rangle\rangle_{E=\omega+i\epsilon} \left[e^{\beta\omega} - \eta\right]^{-1} d\omega.\end{aligned} \tag{338}$$

3.4 Application to the Ising Model of Ferromagnetism

For the Ising model of spin S = ½, and for arbitrary range of interaction, the Ising Hamiltonian (2.1) becomes

$$\mathcal{H} = -\tfrac{1}{2} \sum_{i,j}^{N} J_{ij} S_i^z S_j^z - \mu H \sum_{i}^{N} S_i^z \quad , \tag{3.39}$$

where μ = magnetic moment per unit spin and where the summation is now not restricted to only nearest-neighbour pairs i,j in the lattice but is taken over all lattice sites.

The interaction potential, J_{ij}, depends on the separation $i - j$, and is taken to be zero when $i = j$.

The eigenvalues of the operators S are either $+\frac{1}{2}$ or $-\frac{1}{2}$ (in Dirac units). This restriction implies the well-known relations:

$$(S_i^+)^2 = (S_i^-)^2 = 0 \; ; \quad (S_i^z)^2 = \tfrac{1}{4} \; , \tag{3.40a}$$

where

$$S_i^{\pm} = S_i^x \pm i S_i^y \; . \tag{3.40b}$$

Therefore, the usual spin commutation relations combine with (3.40a) to yield the identities:

$$S_i^+ S_i^- + S_i^- S_i^+ = +1 \; ; \quad S_i^z S_i^+ = \tfrac{1}{2} S_i^+ \; . \tag{3.41}$$

By using the equation of motion for the Green's functions (3.14) and Fourier transforming with respect to energy via (3.26) the equation of motion for the (n + 1)th-order Green's function is obtained:

$$\begin{aligned} &\langle\langle S_{f_1}^z S_{f_2}^z \cdots S_{f_n}^z S_i^+ | S_l^- \rangle\rangle_E \; (E - \mu H) \\ &= \frac{\delta_{il}}{\pi} \langle f_1 \cdots f_n i \rangle \\ &+ \sum_j J_{ij} \langle\langle S_{f_1}^z \cdots S_{f_n}^z S_j^z S_i^+ | S_l^- \rangle\rangle_E \; , \end{aligned} \tag{3.42}$$

where $\langle f_1 f_2 f_3 \cdots \rangle \equiv \langle S_{f_1}^z S_{f_2}^z S_{f_3}^z \cdots \rangle$.

Using (3.42), the first two exact Green's functions are

$$(E - \mu H) \langle\langle S_i^+ | S_l^- \rangle\rangle_E = (\sigma/\pi)\delta_{il} + \sum_j J_{ij} \langle\langle S_j^z S_i^+ | S_l^- \rangle\rangle \tag{3.43}$$

and

$$(E - \mu H) \langle\langle S_j^z S_i^+ | S_l^- \rangle\rangle_E = (\delta_{il}/(2\pi))(2\langle ji \rangle - \delta_{ji}(\tfrac{1}{2} - \sigma)) + \sum_p J_{ip} \langle\langle S_p^z S_j^z S_i^+ | S_l^- \rangle\rangle_E , \tag{3.44}$$

where $\sigma = \langle S_i^z \rangle$, independent of i by translational symmetry.

4. DECOUPLING PROCEDURES FOR ISING MODEL

As pointed out in the theory of Green's functions, it is always necessary at some stage to make an approximation in order to decouple the hierarchy of Green's function equations (3.17). In the case of the Ising model under consideration, (3.39), this involves making some approximation to the (n + 2)th-order Green's function on the right-hand side of the equation for the (n + 1)th-order Green's function (3.42).

Tahir-Kheli[3] (T-K) used the random phase approximation (RPA) and worked out the details of the first-and second-stage approximations as applied to the system with the Hamiltonian of equation (3.39). Tomita and Tanaka[2] (TT) also made use of an approximation (TTA) for the decoupling of the hierarchy of Green's functions. TT, however, were interested in studying the paramagnetic resonance line shape problem and used an anisotropic magnetic Hamiltonian involving dipole-dipole interactions.

We are interested in the implications of applying the TTA to the Ising model (3.39), and how they compare with the results of T-K. These two approximations will now be presented.

4.1 Random Phase Approximation

The nth-order RPA is defined by Tahir-Kheli[30] as

$$-i\theta(t-t')\Big\{\hat{O}(n)\Big\langle S^z_{f_1}S^z_{f_2}\ldots S^z_{f_n}S^-_g(t')S^+_g(t)\Big\rangle_c - \hat{O}(n)\Big\langle S^z_{f_1}S^z_{f_2}\ldots S^z_{f_n}S^+_g(t)S^-_g(t')\Big\rangle_c\Big\} = 0 \quad , \qquad (4.1)$$

where $\theta(t)$ is the step function defined in (3.7), $\langle\ldots\rangle_c$ denotes a cumulant average[31,32], and $\hat{O}(n)$ is a projection operator such that it has zero eigenvalues whenever any two, or more, of the (n + 1) spatial locations $f_1,\ldots,f_n$ and g coincide; otherwise its eigenvalues are unity.

The semi-invariant thermal averages $\langle\ldots\rangle_c$ may be defined in terms of the usual thermal averages of products of quantum mechanical operators $M_1\ldots M_n$ by the (inverse) relations

$$\langle M_1\rangle = \langle M_1\rangle_c \quad ,$$

$$\langle M_1M_2\rangle = \langle M_1\rangle_c\,\langle M_2\rangle_c + \langle M_1M_2\rangle_c \,,$$

$\langle M_1M_2\ldots M_n\rangle$ = the sum of all possible products of semi-invariants, each M_j being involved in only one of the factors, and all the M_j's being used in each term. (4.2)

Approximation (4.1) actually expresses the Green's function $\hat{O}(n)\langle\langle S^z_{f_1}S^z_{f_2}\ldots S^z_{f_n}S^+_g|S^-_g\rangle\rangle_E$ in terms of a certain linear combination of all the lower order Green's functions. For example, by making use of (4.1), it can be shown that the first and second RPA's respectively are

$$(1 - \delta_{gf})\langle\langle S^z_f S^+_g | S^-_g \rangle\rangle_E \xrightarrow[\text{1st RPA}]{} (1 - \delta_{gf})\sigma\langle\langle S^+_g | S^-_g \rangle\rangle_E \qquad (4.3)$$

and

$$\hat{O}(2)\langle\langle S^z_{f_1} S^z_{f_2} S^+_g | S^-_g \rangle\rangle_E \xrightarrow[\text{2nd RPA}]{} \hat{O}(2)\Big[\sigma\langle\langle S^z_{f_1} S^+_g | S^-_g \rangle\rangle_E$$

$$+ \sigma\langle\langle S^z_{f_2} S^+_g | S^-_g \rangle\rangle_E + L_{f_1 f_2}\langle\langle S^+_g | S^-_g \rangle\rangle_E$$

$$- \sigma^2\langle\langle S^+_g | S^-_g \rangle\rangle_E\Big] , \qquad (4.4)$$

where

$$L_{f_1 f_2} \equiv \langle S^z_{f_1} S^z_{f_2} \rangle - \sigma^2 \; . \qquad (4.5)$$

We shall henceforth refer to $L_{f_1 f_2}$ as the system correlation function. It expresses the fluctuation of the S^z operator from its average value.

4.2 Tomita and Tanaka Approximation

The TTA involves defining a new Green's function of the cumulant type (in an obvious notation):

$$[12\ldots n+| \;\equiv\; [12\ldots n+|-]_E \;\equiv\; [S^z_{f_1}\ldots S^z_{f_n} S^+_g | S^-_g]_E \; , \qquad (4.6)$$

in terms of the usual Green's functions

$$(12\ldots n+| \;\equiv\; \langle\langle S^z_{f_1}\ldots S^z_{f_n} S^+_g | S^-_g \rangle\rangle_E \; , \qquad (4.7)$$

as follows:

$$(+| = [+| \;,$$
$$(1+| = \langle 1 \rangle [+| + [1+| \;,$$
$$(12+| = \langle 12 \rangle [+| + \langle 1 \rangle [2+| + \langle 2 \rangle [1+| + [12+| \;,$$

$$\cdot$$
$$\cdot$$
$$\cdot$$

$$(12\ldots n+| = \sum_{r} \left\langle O^{(r)} \right\rangle \left[O^{(n-r)} + \right| \;, \qquad (4.8)$$

where 1 stands for $S^z_{f_1}$ etc.; it will be obvious just where this notation is being used (sometimes, the notation will be mixed). The $O^{(r)}$ is a product of r S^z's, and $O^{(n-r)}$ is a product of (n-r) S^z's such that $O^{(r)}O^{(n-r)} = O^{(n)} = 12\ldots n$, and the symbol $\sum_{r}$ means that r runs over all its physically possible values, and for each of these values one adds together terms corresponding to all possible ways of dividing the n S^z's into groups of r and n-r (and where permutations of S^z within each group are not counted as "different").

The nth-stage of approximation consists in letting $[12\ldots n+| = 0$.

Applying the TTA (4.8) to the spin Green's functions, we obtain for the first two TTA's respectively

$$\left\langle\!\left\langle S^z_{f_1} S^+_g \middle| S^-_g \right\rangle\!\right\rangle_E \xrightarrow[\text{1st TTA}]{} \sigma \left\langle\!\left\langle S^+_g \middle| S^-_g \right\rangle\!\right\rangle_E \quad , \qquad (4.9)$$

and

$$
\begin{aligned}
\langle\langle S^z_{f_1} S^z_{f_2} S^+_g | S^-_g \rangle\rangle_E \xrightarrow{\text{2nd TTA}} & \ \sigma \langle\langle S^z_{f_1} S^+_g | S^-_g \rangle\rangle_E \\
& + \sigma \langle\langle S^z_{f_2} S^+_g | S^-_g \rangle\rangle_E + L_{f_1 f_2} \langle\langle S^+_g | S^-_g \rangle\rangle_E \\
& - \sigma^2 \langle\langle S^+_g | S^-_g \rangle\rangle_E \ . \qquad (4.10)
\end{aligned}
$$

Comparing (4.9) and (4.10) with the expressions (4.4) and (4.5), it is seen that the decoupling procedure of T-K is exactly equivalent, for unequal indices, to that of TT.

5. THE RPA FOR THE ISING MODEL

The following will be a summary of the main results obtained by T-K[3]. The detailed calculations will be omitted, as those presented for the TTA in Section 6 of this paper will be sufficient to show how T-K obtained his results.

The notation used in the remaining parts of this paper follow very closely the notation used by T-K[3].

5.1 The First RPA

As was seen in expression (4.3), the first RPA consists in completely ignoring correlations between spatially separated spins.

Making use of equation (3.38) with (4.3), first-stage decoupling gives

$$L_{fg} = (\tfrac{1}{4} - \sigma^2)\delta_{gf} \; . \tag{5.1}$$

For the single spin Green's function, (4.3) yields

$$\langle\langle S_g^+ | S_g^- \rangle\rangle_E = \frac{1}{e}\,\frac{\sigma}{\pi} \, , \tag{5.2}$$

where

$$e = E - \mu H - \sigma J(0) \; , \tag{5.3}$$

and $J(0) = \Sigma_f\, J_{gf}$. Here, use was made of the Fourier transform notation $J(\underline{K})$ (for $\underline{K} = 0$) given by

$$J(\underline{K}) = \Sigma_j \, J_{ij} \exp\left[i \, \underline{K} \cdot \underline{(i-j)} \right] . \tag{5.4}$$

Applying the spectral theorem, that is, equation (3.38), to (5.2) yields the system magnetization:

$$2\,\sigma = \tanh\left[\frac{\beta \tilde{E}(0)}{2}\right], \tag{5.5}$$

where

$$\tilde{E}\,(0) = \mu H + \sigma J(0). \tag{5.6}$$

In the limit $\mu H \rightarrow +0$, the system is found to be spontaneously magnetized as long as $T<T_C$. The Curie temperature is found to be

$$T_C = \frac{J(0)}{4k_B} \quad , \tag{5.7}$$

where k_B is Boltzmann's constant.

For $T>T_C$, the system is paramagnetic with susceptibility χ :

$$\chi = \frac{\beta/4}{1 - T_C/T} \quad . \tag{5.8}$$

At temperatures much lower than T_C, the system is nearly fully aligned and the magnetization in the limit of zero magnetic field is

$$\sigma = \tfrac{1}{2} - \exp\left[-\beta J(0)/2 \right] \quad (1 + \epsilon), \tag{5.9}$$

where $\epsilon \ll 1$ and tends to zero exponentially as $T \rightarrow 0$.

5.2 The Second RPA

The approximation (4.4) yields for the single spin Green's function

$$\langle\langle S_g^+ | S_g^- \rangle\rangle_E = \frac{1}{\pi}\,\frac{A + \sigma(E - E(0))}{[E - E(+)]\,[E - E(-)]}\ , \qquad (5.10)$$

where

$$E(\pm) = E(0) \pm \Phi\ , \qquad (5.11a)$$

$$E(0) = \mu H + \sigma J(0)\left(\frac{z-1}{z}\right), \qquad (5.11b)$$

$$\Phi^2 - x^2 = \Sigma_{f_1}\Sigma_{f_2} J_{f_1 g} J_{f_2 g} L_{f_1 f_2} \equiv \Psi\ , \qquad (5.11c)$$

$$x = \sigma J(0)/z\ , \qquad (5.11d)$$

$$A = \Sigma_f J_{fg} L_{fg}\ , \qquad (5.11e)$$

and where z = the number of nearest neighbours of any individual spin. In deriving (5.9) use was made of the following reduction resulting from the nearest-neighbour approximation (see Appendix I):

$$\Sigma_f (J_{gf})^n = z\left[\frac{J(0)}{z}\right]^n . \qquad (5.12)$$

The second RPA result for the system magnetization is

$$1 = [\mathcal{T}(+) + \mathcal{T}(-)] + \left[\frac{A + \sigma x}{\Phi}\right][\mathcal{T}(+) - \mathcal{T}(-)]\ , \qquad (5.13a)$$

where

$$\mathcal{T}(\pm) = \coth\left[\frac{\beta E(\pm)}{2}\right]. \qquad (5.13b)$$

For $T > T_C$ and in the limit $\mu H \rightarrow +0$, Tahir-Kheli reports:

$$\chi = \beta/4\left[1 + (\beta/4)J(0) + (\beta/4)^2 J^2(0)\frac{(z-1)}{z}\right] + (\beta/4)^4 J^3(0)\left[1 - \frac{7}{3z} - \frac{a}{36}\right] + 0(\beta^5) \ , \qquad (5.14)$$

where a = 0, for sc and bcc lattices and is equal to +1 for fcc lattice. The results for the specific heat, C_V, were also computed:

$$C_V = \left[\frac{\beta J(0)}{4}\right]^2 (Nk_B)\left[\frac{1}{2z} + \frac{a}{36}\frac{\beta J(0)}{4}\right] + 0(\beta^4) \ . \qquad (5.15)$$

For $T \ll T_C$ and for $\mu H \rightarrow +0$,

$$\sigma = \tfrac{1}{2} - \exp\left[-\frac{\beta J(0)}{2}\right] - z\exp\left[-\beta J(0)\frac{(z-1)}{z}\right](1 + \epsilon), \qquad (5.16)$$

where ϵ is exponentially vanishing as $\beta \rightarrow \infty$.

The Curie temperature was found to obey the relation:

$$k_B T_C = \left[\frac{J(0)}{4}\right] y \ , \qquad (5.17a)$$

where

$$y = \begin{cases} 0.875 \text{ for sc (simple cubic)} \\ 0.898 \text{ for bcc (body-centered cubic)} \\ 0.908 \text{ for fcc (face-centered cubic)} \end{cases} \ . \qquad (5.17b)$$

Third order RPA was not investigated by T-K. An analysis of the results of the first two orders of the RPA will be made below when a comparison of RPA results are made with those obtained by means of the TTA.

6. THE TTA FOR ISING MODEL

The general equation of motion for the higher order cumulant Green's functions under the system with Hamiltonian (3.39) is obtained by using (3.17) and the equation arrived at is

$$
\begin{aligned}
e\left[S^z_{f_1}S^z_{f_2}\cdots S^z_{f_n}S^+_i \middle| S^-_l\right] = {} & T_{f_1f_2\ldots f_ni,l} + \sum_j J_{ij}\Big\{ \\
& \qquad \underbrace{\langle f_1f_2\ldots f_nj\rangle_c}_{(n+1)\text{ terms}}\left[S^+_i \middle| S^-_l\right] \\
& + \underbrace{\langle f_1f_3\ldots f_nj\rangle_c}_{n\text{ terms}}\left[\underbrace{S^z_{f_2}S^+_i}_{2\text{ terms}} \middle| S^-_l\right] + \text{all combinations} \\
& + \underbrace{\langle f_1f_4\ldots f_nj\rangle_c}_{(n-1)\text{ terms}}\left[\underbrace{S^z_{f_2}S^z_{f_3}S^+_i}_{3\text{ terms}} \middle| S^-_l\right] + \text{all combinations} \\
& + \ldots + \underbrace{\langle f_1j\rangle_c}_{2\text{ terms}}\left[\underbrace{S^z_{f_2}S^z_{f_3}\cdots S^z_{f_n}S^+_i}_{n\text{ terms}} \middle| S^-_l\right] + \text{all combinations} \\
& + \left[S^z_{f_1}S^z_{f_2}\cdots S^z_{f_n}S^z_jS^+_i \middle| S^-_l\right]\Big\}\,, \qquad (6.1a)
\end{aligned}
$$

where

$$
\begin{aligned}
T_{f_1f_2\ldots f_ni,l} = {} & (\delta_{il}/2\pi)\Big\{2\langle f_1f_2\ldots f_ni\rangle_c + \Big[\delta_{f_1i}\langle f_2f_3\ldots f_ni\rangle_c \\
& + \delta_{f_2i}\langle f_1f_3\ldots f_ni\rangle_c + \ldots + \delta_{f_ni}\langle f_1f_2\ldots f_{n-1}i\rangle_c\Big] \\
& + \Big[\delta_{f_1i}\delta_{f_2i}\langle f_3f_4\ldots f_ni\rangle_c + \text{all combinations}\Big] \\
& + \Big[\delta_{f_1i}\delta_{f_2i}\delta_{f_3i}\langle f_4f_5\ldots f_ni\rangle_c + \text{all combinations}\Big] \\
& + \ldots + \Big[\delta_{f_1i}\delta_{f_3i}\cdots\delta_{f_ni}\langle f_2i\rangle_c + \text{all combinations}\Big] \\
& - \delta_{f_1i}\delta_{f_2i}\cdots\delta_{f_ni}\left(\tfrac{1}{2} - \sigma\right)\Big\}\,, \qquad (6.1b)
\end{aligned}
$$

and where e is defined by equation (5.3).

Using equations (6.1a,b) the first three exact Green's function equations are

$$e\left[S_g^+\middle|S_g^-\right] = (\sigma/\pi) + \Sigma_f J_{fg}\left|S_f^z S_g^+\middle|S_g^-\right| \; , \tag{6.2}$$

$$\begin{aligned} e\left[S_{f_1}S_g^+\middle|S_g^-\right] &= 1/(2\pi)\left[2L_{f_1g} - (\tfrac{1}{2} - \sigma)\delta_{f_1g}\right] \\ &\quad + \Sigma_{f_2}J_{f_2g}L_{f_1f_2}\left[S_g^+\middle|S_g^-\right] \\ &\quad + \Sigma_{f_2}J_{f_2g}\left[S_{f_1}^zS_{f_2}^zS_g^+\middle|S_g^-\right] \; , \end{aligned} \tag{6.3}$$

$$\begin{aligned} e\left[S_{f_1}^zS_{f_2}^zS_g^+\middle|S_g^-\right] &= 1/(2\pi)\left[\, 2\langle f_1f_2g\rangle_c + \delta_{f_1g}L_{f_2g} \right. \\ &\quad \left. + \delta_{f_2g}L_{f_1g} - \delta_{f_1g}\delta_{f_2g}(\tfrac{1}{2} - \sigma)\right] \\ &\quad + \Sigma_{f_3}J_{f_3g}\left\{\langle f_1f_2f_3\rangle_c\left[S_g^+\middle|S_g^-\right]\right. \\ &\quad + L_{f_1f_3}\left[S_{f_2}S_g^+\middle|S_g^-\right] \\ &\quad \left. + L_{f_2f_3}\left[S_{f_1}^zS_g^+\middle|S_g^-\right] + \left[S_{f_1}^zS_{f_2}^zS_{f_3}^zS_g^+\middle|S_g^-\right]\right\} . \end{aligned} \tag{6.4}$$

It is worth noting here that the nth-stage of the TTA which consists in neglecting the cumulant Green's function $\left[S_{f_1}^zS_{f_2}^z\ldots S_{f_n}^zS_g^+\middle|S_g^-\right]$ implies letting $\langle f_1f_2\ldots f_ng\rangle_c$ equal zero (see Appendix II).

6.1 The First TTA

The first-stage TTA consists in neglecting the term $\Sigma_f J_{fg}\left[S_f^zS_g^+\middle|S_g^-\right]$ on the right-hand side of equation (6.2), giving

$$e[S_g^+ | S_g^-] = \sigma/\pi \ , \qquad (6.5)$$

which is exactly equivalent to the first RPA (5.2).

Applying spectral relation (3.38) to (6.5), the system magnetization obtained is (see Appendix III)

$$2\sigma = \tanh\left[\frac{\beta\tilde{E}(0)}{2}\right] \ . \qquad (6.6)$$

From (6.6) it is seen that for $\mu H = 0$ and $J(0) < 0$, the only solution is $\sigma = 0$. For $\mu H = 0$ and $J(0) > 0$, there exists in addition to the $\sigma = 0$ solution, a non-vanishing solution for $\beta J(0) > 4$. (This upper limit occurs because of the inequality $\tanh x \leq x$.) This nontrivial solution is clearly the correct one, since $J(0) > 0$ is the ferromagnetic coupling and at $T = 0$, the correct solution must be $\sigma = \pm\frac{1}{2}$.

Applying (3.38) again, this time to the relation (4.7) (1st-TTA), the correlation function is obtained:

$$L_{fg} \equiv \langle S_f^z S_g^z \rangle - \sigma^2 = \delta_{fg}(\tfrac{1}{2} - \sigma) \ . \qquad (6.7)$$

The correlation function obtained using the 1st-TTA differs from that obtained by using the 1st-RPA (5.1); besides (6.7) does not give the expected result, for if $f = g$, then L_{fg} must equal $(\frac{1}{4} - \sigma^2)$ since $(S_1^z)^2 = \frac{1}{4}$(3.40a). This will be taken care of by insisting that the spectral theorem (3.38) be used only for unequal indices and that the identity:

$$L_{gg} = \tfrac{1}{4} - \sigma^2, \tag{6.8a}$$

be used for equal indices. Then, the following is obtained:

$$L_{fg} = \delta_{fg}(\tfrac{1}{4} - \sigma^2). \tag{6.8b}$$

In effect, all that has been done is that L_{fg} has been normalized such that (6.8a) is satisfied (see (3.40a)).

Equations (5.1), (5.5), (6.6) and (6.8) are identical to the molecular field theory results and agree to order $(1/z)^0$ with the correct results as shown by the diagrammatic high density expansion results of Brout[19,33] and Horwitz and Callen[34].

At $T = T_C$, it takes but an infinitesimal H to establish a finite magnetization[35], σ; hence

$$\left(\frac{d\sigma}{d\mu H}\right)_{\substack{\mu H=0\\ T=T_C}} = \infty\ . \tag{6.9}$$

Using relation (6.9) as a definition for T_C, and substituting for σ from (6.6), the following Curie temperature is obtained:

$$T_C = J(0)/4k_B. \tag{6.10}$$

In the limit as $\mu H \rightarrow +0$, the system is spontaneously magnetized as long as $T < T_C$. As the temperature approaches T_C, the magnetization disappears, as is easily seen from the solution of equation (6.6).

Above T_C, the system is paramagnetic with zero-field susceptibility,

$$\chi = \frac{d\sigma}{d\mu H} = \frac{\beta/4}{1 - T_C/T}, \tag{6.11}$$

obtained by differentiating (6.6) implicitly with respect to H and then putting $\sigma = \mu H = 0$.

For temperatures much less than T_C and in the limit of zero magnetic field, the system magnetization can be solved for by writing $\tanh[\beta\tilde{E}(0)/2]$ in (6.6) in terms of exponentials and approximating σ in the exponentials by $\frac{1}{2}$. Therefore, one obtains

$$\begin{aligned} 2\sigma &= \tanh\frac{\beta\tilde{E}(0)}{2}, \\ &= \frac{1 - e^{-\beta J(0)/2}}{1 + e^{-\beta J(0)/2}}, \\ &= 1 - 2e^{-\beta J(0)/2} + O(e^{-\beta J(0)}), \\ \sigma &= \tfrac{1}{2} - e^{-\beta J(0)/2} + O(e^{-\beta J(0)}). \end{aligned} \tag{6.12}$$

The paramagnetic susceptibility (6.11) and the low temperature magnetization (6.12) are the same as those of the first RPA (5.8) and (5.9). These expansions (6.11) or (5.8) and (6.12) or (5.9) agree with the exact results to the first two terms. Disagreement with the exact results, however, appears immediately in the next order terms as indicated.

As Tahir-Kheli[30] points out, the above solution is internally inconsistent. Even though in the limit of vanishing fields the system magnetization disappears as $T \rightarrow T_C$ from below, and the paramagnetic susceptibility diverges as $T \rightarrow T_C$ from above, the correlation function L_{fg} doesn't show the existence of the phase transition. The range of L_{fg} is expected to grow inordinately as the Curie point is approached because the spin fluctuations will become exceedingly large. But (6.8), or (5.1), shows no fluctuations at any temperature. As T-K points out though, for the case $z = \infty$, the result is exact since in "... this case the correlation does not manifest any dominant change in its range with the changing of the system temperature for the reason that the infinite range of the interaction stabilizes the fluctuations".[30] In other words, the variation of the particular spin in question doesn't have much effect on the spin contributing to the field on it, since this second spin is locked in place by (z-1) other spins, where z is interpreted as the number of spins in the range of interaction.

The case of $z = \infty$ is the case of the molecular field theory approximation (MFA)[33,36]. Therefore, both the first RPA and the first TTA give the same results and in the limit as $z \rightarrow \infty$ are identical with those of the MFA.

6.2 The Second TTA

The second stage TTA consists in neglecting the term $\sum_{f_2} J_{f_2 g}[S^z_{f_1} S^z_{f_2} S^+_g | S^-_g]$ on the right-hand side of equation (6.3), giving:

$$e[S^z_{f_1} S^+_g | S^-_g] = 1/(2\pi)[2L_{f_1 g} - (\tfrac{1}{2} - \sigma)\delta_{f_1 g}] + \sum_{f_2}' J_{f_2 g} L_{f_1 f_2} [S^+_g | S^-_g] \; . \qquad (6.13)$$

Solving for $[S^z_{f_1} S^+_g | S^-_g]$ from (6.13) and substituting it in the left-hand side of (6.2), the following equation for the single spin Green's function is obtained:

$$\langle\langle S^+_g | S^-_g \rangle\rangle_E = \frac{1}{\pi} \frac{A + \sigma(E - \tilde{E}(0))}{[E - \tilde{E}(+)][E - \tilde{E}(-)]} \; , \qquad (6.14)$$

where

$$\tilde{E}(\pm) = \tilde{E}(0) \pm \phi \qquad (6.15)$$

$$\phi^2 = \sum_{p,j} J_{gp} J_{gj} L_{jp} \qquad (6.16)$$

$$A = \sum_f J_{fg} L_{fg} \quad . \qquad (6.17)$$

Equation (6.14) differs from the similar result of second RPA (5.10) in that ϕ, $\tilde{E}(\pm)$, and $\tilde{E}(0)$ have replaced the more complicated Φ, $E(\pm)$, and $E(0)$ respectively.

The use of relation (3.38) on equation (6.14) leads to the following expression for the system magnetization (see Appendix IV for derivation):

$$\sigma = \left[\tfrac{1}{2} - (A/\emptyset)(n(+) - n(-))\right]\left[n(+) + n(-) + 1\right]^{-1} , \qquad (6.18)$$

where

$$n(\alpha) = \left[e^{\beta\tilde{E}(\alpha)} - 1\right]^{-1} ; \alpha = +,-,0. \qquad (6.19)$$

Equation (6.18) constitutes the second TTA result for the system magnetization. Like the result obtained by the second RPA (5.13) it is a transcendental relation, but it is a little simpler than the result of second RPA since $\emptyset$ replaces the more complicated Φ . Its solution requires the computation of A and $\emptyset$ which in turn require the knowledge of the correlation function $L_{f_1f_2}$.

According to the second-stage TTA (4.6),

$$\left[S^z_{f_1}S^+_g | S^-_g\right] = \langle\langle S^z_{f_1}S^+_g | S^-_g\rangle\rangle_E - \sigma\langle\langle S^+_g | S^-_g\rangle\rangle_E . \qquad (6.20)$$

Substituting for $\left[S^z_{f_1}S^+_g | S^-_g\right]$ from (6.20) into (6.13), one obtains

$$\langle\langle S^z_{f_1}S^+_g | S^-_g\rangle\rangle - \langle\langle S^+_g | S^-_g\rangle\rangle = (1/e)(1/(2\pi))$$

$$\left[2L_{f_1g} - (\tfrac{1}{2} - \sigma)\delta_{f_1g}\right] + (1/e)\sum_{f_2} J_{f_2g}L_{f_1f_2}\langle\langle S^+_g | S^-_g\rangle\rangle_E . \qquad (6.21)$$

By applying relation (3.38) to both sides of (6.21), a relation for the correlation function is obtained:

$$L_{f_1g} \coth(\beta\tilde{E}(0)/2) = (\tfrac{1}{2} - \sigma)(n(0) + 1)\delta_{f_1g}$$

$$+ \frac{A_{f_1g}A}{\emptyset^2}\left[2n(0) - n(+) - n(-)\right]$$

$$+ \frac{A_{f_1g}\sigma}{\emptyset}\left[n(-) - n(+)\right] , \qquad (6.22)$$

where

$$A_{f_1 g} = \sum_{f_2} J_{f_2 g} L_{f_1 f_2} \cdot \tag{6.23}$$

Using the Fourier transform of J_{ij} (5.4), and the following inverse lattice Fourier transform of L_{ij}:

$$L_{ij} = 1/N \sum_{\underline{K}} L(\underline{K}) \exp\left[i\underline{K} \cdot (\underline{j-i}) \right] , \tag{6.24}$$

where $\underline{K}$ is a wave number in the first Brillouin zone of the reciprocal lattice of N sites, equation (6.22) can be written as

$$\begin{aligned} L(\underline{K}) \coth (\beta \tilde{E}(0)/2) = {} & (\tfrac{1}{2} - \sigma)(n(0) + 1) \\ & + \frac{J(\underline{K}) L(\underline{K}) A}{\beta^2} \left[2n(0) - n(+) - n(-) \right] \\ & + \frac{J(\underline{K}) L(\underline{K}) \sigma}{\beta} \left[n(-) - n(+) \right] . \end{aligned} \tag{6.25}$$

Use was made of the easily-established property (a consequence of translational symmetry):

$$\sum_{\underline{K}} \exp\left[i\underline{K} \cdot (\underline{j-i}) \right] = N\delta_{ji} . \tag{6.26}$$

Equations (6.18) and (6.22) or (6.25) are a coupled transcendental set of equations. Their self-consistent solution determines both the magnetization, σ, and the correlation, L_{ij}, or $L(\underline{K})$.

It should also be noted here that the second TTA expression for the correlation is a good deal simpler than that obtained for second RPA.

The set of equations (6.18) and (6.25) cannot be solved analytically at general temperatures; their solution must be computed numerically (this is also true of the much simpler results obtained by first-stage RPA or TTA). But, as T-K pointed out in his solution[3], in certain ranges of temperature rapidly convergent iteration procedures can be used which give the results in terms of suitable series expansions.

a) <u>High Temperature Solution</u>

The high temperature region will be investigated first. In this range the magnetization is much smaller than unity as long as $\mu H \ll kT$. In the limit of high temperatures and vanishing field, one obtains from (6.19):

$$n(\alpha) = \left[e^{\alpha\beta\phi} - 1\right]^{-1}; \quad \alpha = +,- . \tag{6.27}$$

Therefore, equation (6.18) yields

$$\frac{2A}{\phi} = \frac{1}{n(+) - n(-)} ,$$

$$\left.\frac{2A}{\phi}\right|_{\mu H=0;\ T\geq T_C} = \tanh\left(\beta\phi/2\right) . \tag{6.28}$$

Similarly equation (6.25) gives

$$\left.L(\underline{K})\right|_{\mu H=0;\ T\geq T_C} = \tfrac{1}{4} + \frac{J(\underline{K})L(\underline{K})A}{\phi^2} . \tag{6.29}$$

Therefore, in the limit of vanishing field and $T \geq T_C$,

$$L(\underline{K}) = \tfrac{1}{4}\left[1 - J(\underline{K})V(T)\right]^{-1} , \tag{6.30a}$$

where

$$V(T) = A/\phi^2 . \tag{6.30b}$$

Equations (6.30) are in essentially the same form as the result obtained by T-K^{37}. The differences between the two expressions are that equation (6.30a) contains ϕ instead of T-K's (5.11b) and that equation (6.30a) is not normalized. The normalized $L(\underline{K})$ from equation (6.30a) would be

$$L(\underline{K}) = \left[\frac{1}{1 - J(\underline{K})V(T)}\right]\left[\frac{4}{N}\sum_{\underline{Q}}\frac{1}{1 - J(\underline{Q})V(T)}\right]^{-1} . \qquad (6.31)$$

Equation (6.31) would then give $\sum_{\underline{K}} L(\underline{K}) = N/4$, which is the expected answer (see Appendix V).

The high-temperature susceptibility can be solved for by making use of the thermodynamic relation (see Appendix VI)

$$\left[L(\underline{K})\right]_{\lim\ \underline{K}=0} = \chi/\beta , \qquad (6.32)$$

and by making use of series expansions since for high temperature β is small.

Using (6.28) in (6.30b), it can be easily shown that

$$V = \beta/4 - \beta^3\phi^2/48 + O(\beta^5) . \qquad (6.33)$$

From equations (6.17), (5.4) and (6.24), it is seen that

$$A = 1/N\sum_{\underline{K}} J(\underline{K})L(\underline{K}) . \qquad (6.34)$$

Expanding $L(\underline{K})$ from (6.31) in terms of V, which is small, and substituting into (6.34) gives

$$A = \frac{1}{4}\sum_{\underline{K}} \frac{J(\underline{K})\left[1 + VJ(\underline{K}) + V^2J(\underline{K}) + V^3J^3(\underline{K}) + O(\beta^4)\right]}{\sum_{\underline{Q}}\left[1 + VJ(\underline{Q}) + V^2J^2(\underline{Q}) + V^3J^3(\underline{Q}) + O(\beta^4)\right]} . \qquad (6.35)$$

Equation (6.35) can be simplified using the following relations (see Appendix VII):

$$\sum_{\underline{K}} J(\underline{K}) = 0 \ , \qquad (6.36a)$$

$$\sum_{\underline{K}} J^2(\underline{K}) = NJ^2(0)/z \ , \qquad (6.36b)$$

$$\sum_{\underline{K}} J^3(\underline{K}) = \begin{cases} 0 \text{ for sc and bcc} \\ NJ^3(0)/36 \text{ for fcc} \end{cases} , \qquad (6.36c)$$

$$\sum_{\underline{K}} J^4(\underline{K}) = NJ^4(0)b/z^3 \ , \qquad (6.36d)$$

where b = 15 (sc); = 27 (bcc); = 45 (fcc). Therefore, equation (6.35) becomes

$$A = \tfrac{1}{4}VJ^2(0)/z + \tfrac{1}{4}\,\frac{V^2J^3(0)}{36}\,a + \tfrac{1}{4}\,\frac{V^3J^4(0)b}{z^3} + 0(\beta^4) \ , \qquad (6.37)$$

where a = 0 for sc and bcc lattices and is equal to +1 for fcc lattice and thus,

$$\phi^2 = \frac{A}{V} = \tfrac{1}{4}\,\frac{J^2(0)}{z} + \tfrac{1}{4}\,\frac{VJ^3(0)}{36}\,a + \tfrac{1}{4}\,\frac{V^2J^4(0)b}{z^3} + 0(\beta^3) \ . \qquad (6.38)$$

Substituting for ϕ^2 from (6.38) into (6.33) gives

$$V = \frac{\beta}{4} - \frac{\beta^3}{48}\left(\frac{J^2(0)}{4z}\right) + 0(\beta^4) \ . \qquad (6.39)$$

Now, from (6.32) and from employing the expansion for V(6.39) in the series expansion for $L(\underline{K})$, the susceptibility is obtained:

$$\chi = \beta\left[L(\underline{K})\right]_{\lim \underline{K}=0} \ ,$$

$$= \frac{\beta N}{4}\left\{\frac{1 + VJ(\underline{K}) + V^2J^2(\underline{K}) + V^3J^3(\underline{K}) + 0(\beta^4)}{\sum_{\underline{Q}}\left[1 + VJ(\underline{Q}) + V^2J^2(\underline{Q}) + V^3J^3(\underline{Q})\right] + 0(\beta^4)}\right\}_{\lim \underline{K}=0} ,$$

$$= \frac{\beta}{4}\ \frac{1 + J(0)\left[\frac{\beta}{4} - \frac{\beta^3}{48}\left(\frac{J^2(0)}{4z}\right)\right] + \left(\frac{\beta}{4}\right)^2 J^2(0) \quad \left(\frac{\beta}{4}\right)^3 J^3(0) + 0(\beta^4)}{1 + \left(\frac{\beta}{4}\right)^2\frac{J^2(0)}{z} + \left(\frac{\beta}{4}\right)^3\frac{J^3(0)a}{36} + 0(\beta^4)} \ ,$$

$$\chi = \frac{\beta}{4}\left\{1 + \frac{\beta}{4} J(0) + \left(\frac{\beta}{4}\right)^2 J^2(0)\,\frac{z-1}{z}\right] + \left(\frac{\beta}{4}\right)^4 J^3(0)\left[1 - 4/(3z) - a/36\right] + 0(\beta^5)\ . \tag{6.40}$$

The above result agrees with the exact one to order β^3 but the β^4-term is only approximately correct.

Comparing with (5.14), the second TTA gives the same result for high-temperature, zero-field susceptibility as the second RPA of T-K*.

The specific heat at constant volume, C_V, can be easily computed from

$$C_V = \frac{d\langle\mathcal{H}\rangle}{dT}\ . \tag{6.41}$$

For high temperature and vanishing field (6.41) yields (see Appendix VIII)

$$C_V = (Nk_B)\left(\frac{\beta J(0)}{4}\right)^2\left[\frac{1}{2z} + \left(\frac{a}{36}\right)\left(\frac{\beta J(0)}{4}\right) + \left(\frac{\beta J(0)}{4}\right)^2\left(\frac{6}{z^2}\right)\left(\frac{b}{z} - \frac{4}{3}\right)\right] + 0(\beta^5)\ . \tag{6.42}$$

* T-K using second RPA seems to have arrived at exactly the same result (see (5.14)) except that his β^4-term contains the factor $[1 - 7/(3z) - a/36]$ instead of $[1 - 4/(3z) - a/36]$. The 7/(3z)-term is due to what is an obvious error in his expansion for V(T); the β^3-term should be $-[\beta^3/(48z)][J^2(0)/(4z)]$ whereas T-K has $-[\beta^3/(48z)][J^2(0)/z]$.

Once again the above expression agrees with the exact result[13] to order β^3 and the β^4-term is again only approximately correct. T-K obtained exactly the same result for C_v to order β^3 (see (5.15)).

Therefore, for the high-temperature range, the results of the second TTA, as well as those of the second RPA, are equivalent to the diagrammatic, high density expansion[37] results computed to order (1/z).

b) Low Temperature Solution ($T \ll T_C$)

For the low temperature region rapidly convergent series expansions are again made use of. In the absence of a magnetic field ($\mu H=0$) and for $T \ll T_C$, expansions are made in powers of $\exp(-\beta J(0)/2)$ (the powers are not always integral, the factor (1/z) appearing in some instances).

Once again the solution must be obtained self-consistently through the coupled relations (6.18) and (6.25).

As $\beta \rightarrow \infty$, then $n(0) \rightarrow 0$, $n(+) \rightarrow 0$ and $n(-) \rightarrow 0$ if ϕ is small compared to $\sigma J(0)$ (which is the case); therefore, as a first approximation for very low temperatures relation (6.18) yields $\sigma = \frac{1}{2}$ and relation (6.25) yields $L(\underline{K}) = 0$, which are the expected results.

As a next approximation, σ is assumed to be $\frac{1}{2}$ and again $\emptyset$ is neglected with respect to J(0)/2. This yields

$$\begin{aligned} n(0) &= c + 0(c^2) \, , \\ n(+) &= c + 0(c^2) \, , \\ n(-) &= c + 0(c^2) \, , \end{aligned} \tag{6.43}$$

where

$$c \equiv \exp\left[-\beta J(0)/2\right] \, . \tag{6.44}$$

Substituting (6.43) into relation (6.18), the following is obtained for the system magnetization:

$$\sigma = \tfrac{1}{2}(1 - 2c) + 0(c^2) \, , \tag{6.45}$$

and (6.25) again gives $L(\underline{K}) = 0(c^2)$.

Proceeding in this manner, successive terms in the series expansions for σ and $L(\underline{K})$ are obtained. The result (6.45) agrees with the exact result of the low temperature series expansions to the order given[11,12,13,39,40]. The next step is to approximate σ by $\frac{1}{2}(1 - 2c)$ and proceed to find σ to higher order terms in c using (6.18) and (6.25). The following results are obtained (see Appendix IX):

$$V = \beta c + 0(c^2) \, , \tag{6.46a}$$

$$A = \frac{J^2(0)}{z}\beta c^2 + 0(c^3) \, , \tag{6.46b}$$

$$\emptyset^2 = \frac{J^2(0)}{z} c + 0(c^2) \, , \tag{6.46c}$$

$$\sigma = \tfrac{1}{2} - c + c^2\left[1 - \beta J(0) - \frac{\beta^2 J^2(0)}{2z}\right] + 0(c^3) \, . \tag{6.46d}$$

The results (6.46) are essentially the same as those obtained by T-K except of course for ϕ which is different from T-K's Φ. Another important difference occurs in equation (6.46d).

For the second RPA, T-K obtained, for low temperature and vanishing magnetic field, relation (5.16) for the system magnetization. If one solves for σ using second RPA, paying close attention to the orders, then one finds

$$\sigma = \tfrac{1}{2} - \exp\left[-\frac{\beta J(0)}{2}\right] - z\exp\left[-\beta J(0)\frac{(z-1)}{z}\right] + (z+1)\exp\left[-\beta J(0)\right] + O\left(\exp\left[-\frac{3\beta J(0)}{2}\right]\right). \qquad (6.47)$$

T-K did not carry out his calculation to the order treated above, though it was well within the limits of capability. Tanaka, Katsumori and Toshima[39], by means of low-temperature diagrammatic series expansions, obtained (6.47) plus other terms to higher orders. The interesting point here is that if one expands $\exp\left[-\beta J(0)(z-1)/z\right]$ according to:

$$\exp\left[-\beta J(0)\frac{(z-1)}{z}\right] = \exp\left[-\beta J(0)\right]\left[1 + \frac{\beta J(0)}{z} + \frac{1}{2!}\frac{\beta^2 J^2(0)}{z^2} + \ldots\right], \qquad (6.48)$$

and then substitutes (6.48) into (6.47) one obtains (6.46d) exactly to the order indicated.

When $z \to \infty$, one should obtain the MFA result which for the magnetization is

$$\sigma = \tfrac{1}{2} \tanh\left[\frac{\beta\sigma J(0)}{Z}\right]. \qquad (6.49)$$

By expanding (6.49) and whenever $\exp[-\beta\sigma J(0)]$ appears using

$$\begin{aligned}\exp[-\beta\sigma J(0)] &= \exp\left\{-\beta J(0)\left[\tfrac{1}{2} - e^{-\frac{\beta J(0)}{2}}\right]\right\}, \\ &= \exp[-\beta J(0)/2]\left\{1 + \beta J(0)\exp[-\beta J(0)/2]\right\} \\ &\quad + 0\left(\exp(-\beta J(0)3/2)\right),\end{aligned}$$

the following is obtained for the magnetization:

$$\begin{aligned}\sigma = \tfrac{1}{2} - \exp[-\beta J(0)/2] + [1 - \beta J(0)] \exp[-\beta J(0)] \\ + 0\left(\exp(-\beta J(0)3/2)\right). \qquad (6.50)\end{aligned}$$

Relation (6.50) is exactly the result obtained by second TTA (6.46d) as $z \to \infty$. The second RPA result (5.16) given by T-K is inconsistent as $z \to \infty$ but if the term $(z + 1)\exp[-\beta J(0)]$ is included then along with the second TTA it agrees with the exact results obtained[11,12,13,39,40] for β fixed (however large) and for z sufficiently large to order $(1/z)$.

The appearance of the third term on the right-hand side of (5.16) or (6.47) does not occur in the second TTA because the roots of the Green's function (6.14) (denominator) do not contain any $(z - 1)$ factor.

Of course, the second TTA is an improvement over the first TTA (6.12) just as the second RPA is an improvement over first RPA.

c) Solution Near Curie Point

Finally, the region in the immediate vicinity of the Curie temperature will now be considered. In this region, in the absence of the external field H, the system magnetization vanishes and simultaneously the spatial range of the correlation L_{gf} becomes macroscopically long. In other words, $L(\underline{K})$ becomes large as $\underline{K} \rightarrow \underline{0}$. From equation (6.31) it is seen that for this to be true:

$$V(T) \rightarrow V(T_C) = [J(0)]^{-1} \text{ .} \tag{6.51}$$

Now in the limit $\mu H = 0$, $T = T_C$ and $\sigma = 0$, equation (6.31) can be written as

$$L(\underline{K}) = \tfrac{1}{4}[F(-1)]^{-1} \frac{1}{1 - [J(0)]^{-1}J(\underline{K})}, \tag{6.52}$$

where

$$F(n) = \frac{1}{N} \sum_{\underline{K}} \left[\frac{J(0) - J(\underline{K})}{J(0)}\right]^{n} \text{ .} \tag{6.53}$$

Using (6.52) and (6.30b), the following can be shown:

$$\begin{aligned}
A(T_C) &= 1/N \sum_{\underline{K}} J(\underline{K})L(\underline{K}) \text{ ,} \\
&= \tfrac{1}{4}\,[F(-1)]^{-1}\; 1/N \sum_{\underline{K}} \frac{J(\underline{K})}{1 - [J(0)]^{-1}J(\underline{K})} \text{ ,} \\
&= \tfrac{1}{4}\,[F(-1)]^{-1}\; \frac{J(0)}{N} \sum_{\underline{K}} \frac{J(\underline{K}) + J(0) - J(0)}{J(0) - J(\underline{K})} \text{ ,} \\
&= \frac{J(0)}{4}[F(-1)]^{-1}\; \frac{1}{N}\sum_{\underline{K}}\left[\frac{J(0)}{J(0) - J(\underline{K})} - 1\right] \text{ ,} \\
&= \frac{J(0)}{4}[F(-1)]^{-1}[F(-1) - 1] \text{ ;}
\end{aligned} \tag{6.54}$$

$$\begin{aligned}
\phi(T_C) &= \left[\frac{A(T_C)}{V(T_C)}\right]^{\frac{1}{2}} \text{ ,} \\
&= [A(T_C)]^{\frac{1}{2}}[J(0)]^{\frac{1}{2}} \text{ ,} \\
&= [J(0)/2]\,[F(-1)]^{-\frac{1}{2}}\,[F(-1) - 1] \text{ .}
\end{aligned} \tag{6.55}$$

Therefore, substituting (6.54) and (6.55) into (6.28) a relation for the Curie temperature is obtained:

$$\tanh\left[\left(\frac{J(0)}{4k_BT_C}\right)\left(\frac{F(-1) - 1}{F(-1)}\right)^{\frac{1}{2}}\right] = \left[\frac{F(-1) - 1}{F(-1)}\right]^{\frac{1}{2}} . \qquad (6.56)$$

The solution of (6.56) is

$$k_BT_C = \left[\frac{J(0)}{4}\right]y , \qquad (6.57a)$$

where

$$y = \begin{cases} 0.875 & \text{for sc} \\ 0.898 & \text{for bcc} \\ 0.908 & \text{for fcc} \end{cases} . \qquad (6.57b)$$

Therefore, by using the normalized L(K) (6.31) of second TTA, exactly the same result is obtained as that of second RPA (5.17) near the Curie point.

T-K[3] has a table comparing the values of y obtained by the second RPA with those obtained using high-temperature diagrammatic series expansions[19,33,34] and by using the Padé approximant method[20] (high-temperature series extrapolation scheme). He found that the second RPA result for the Curie temperature was about 10% higher than the Padé estimate and the estimates of references 19, 33 and 34 were about 10% too low.

The Curie temperature obtained in (6.57) and (5.17) was computed on the assumption that the range of the correlation, in the absence of an applied field, becomes infinite as T approaches T_C from above. This is thermodynamically equivalent to the fact that the zero field susceptibility diverges at the Curie point. But as Englert[42] points out there is no "guarantee that the Curie point obtained by the divergence of the long-range order (or in the specific heat) coincides with the infinity of the susceptibility".

It should be noted that in the solution of the Ising model in the TTA the nearest-neighbour approximation was not made use of up to the point of solution.

So far, then, we have confidence that the TTA is not significantly worse than the RPA. However, as a general scheme, it is definitely not consistent. This will be shown in the next section.

6.3 Third-Stage Decoupling

The set of first three exact cumulant Green's function equations can be written as (see Eq. (6.1))

$$e\, G_0 = T_0 + G_1 \quad , \tag{6.58a}$$

$$e\, G_1 = T_1 + C_2 G_0 + G_2 \quad , \tag{6.58b}$$

$$e\, G_2 = T_2 + C_3 G_0 + 2C_2 G_1 + G_3 \quad , \tag{6.58c}$$

where

$$G_0 = \left[S_g^+ \middle| S_g^- \right] \quad , \tag{6.59a}$$

$$G_n = \sum_{f_1 \dots f_n} J_{gf_1} \dots J_{gf_n} \left[S^z_{f_1} \dots S^z_{f_n} S^+_g | S^-_g \right] , \qquad (6.59b)$$

$$n = 1, 2, 3, \dots ,$$

$$C_2 = \sum_{f_1, f_2} J_{gf_1} J_{gf_2} L_{f_1 f_2} , \qquad (6.59c)$$

$$C_3 = \sum_{f_1, f_2, f_3} J_{gf_1} J_{gf_2} J_{gf_3} \langle f_1 f_2 f_3 \rangle_c , \qquad (6.59d)$$

$$T_0 = T_{g,g} , \qquad (6.59e)$$

$$T_n = \sum_{f_1, \dots f_n} J_{f_1 g} \dots J_{f_n g} \, T_{f_1 f_2 \dots f_n g, g} . \qquad (6.59f)$$

In general, G_3 is decoupled as

$$G_3 = \alpha G_0 + \gamma G_1 + \delta G_2 , \qquad (6.60)$$

where for most decouplings $\alpha = 0$. Substituting for G_3 from (6.60) into (6.58), the solution for G_0 is obtained from the equation

$$(e-x_1)(e-x_2)(e-x_3)G_0 = A_1 e^2 + A_2 e + A_3 , \qquad (6.61)$$

where x_1, x_2, and x_3 are the roots of the equation

$$e^3 - \delta e^2 - e(3C_2 + \gamma) + (C_2 \delta - C_3) = 0 , \qquad (6.62)$$

and where

$$A_1 = T_0, \; A_2 = T_1 - \delta T_0, \text{ and } A_3 = T_2 - \delta T_1 - (2C_2 + \gamma) T_0 . \qquad (6.63)$$

The third-stage TTA involves simply putting $\left[S^z_{f_1} S^z_{f_2} S^z_{f_3} S^+_g \right| = 0$. Therefore, from (6.60), $\alpha = \gamma = \delta = 0$ and equation (6.62) becomes

$$e^3 - 3C_2 e - C_3 = 0 . \qquad (6.64)$$

An equation of the form: $y^3 + py + q = 0$, has three real roots[44] only if

$$4p^3 + 27q^2 < 0 . \tag{6.65}$$

This condition applied to (6.64) requires that $C_3^2 < 4C_2^3$. But at low temperature C_2 is small (see (A9.8)), and it can be shown (see Appendix X) that $C_3 \cong - JC_2$ (at low temperatures); therefore, $C_3^2 < 4C_2^3$ is not satisfied at low temperatures and equation (6.64) does not have three real roots. However, according to the theory of Green's functions, the roots must all be real since the Green's function is always analytic off the real axis (see Reference 22, p 325).

Thus, the third-stage TTA is inconsistent at low temperatures.

The third-stage RPA of T-K involves putting $[S^z_{f_1}S^z_{f_2}S^z_{f_3}S^+_g| = 0$ only when f_1, f_2, f_3, and g are unequal. When any two are equal, the equalities (for spin $\frac{1}{2}$) (see Eqs. (3.42) and (3.43)):

$$(S^z_f)^2 = \tfrac{1}{4} , \tag{6.66a}$$

$$S^z_f S^+_f = \tfrac{1}{2}S^+_f , \tag{6.66b}$$

are used to express $[123+|$ in terms of lower-order cumulant Green's functions (essentially).

For third-stage RPA, one obtains (see Appendix XI)

$$\delta = -6\sigma J , \tag{6.67a}$$

$$\gamma = J^2(1 - 12\sigma^2) - (6/z)C_2 \; . \qquad (6.67b)$$

At low temperatures, $\delta \cong -3J$ and $\gamma \cong -2J^2$, and $C_3 \cong - JC_2$ (see Appendix X). Therefore, equation (6.62) becomes

$$e^3 + 3Je^2 + 2J^2e + 2C_3 = 0 \; . \qquad (6.68)$$

Substituting $e = y - J$ in (6.68) one obtains the reduced equation

$$y^3 - 5J^2y + 4J^3 + 2C_3 = 0 \; . \qquad (6.69)$$

Equation (6.69) satisfies condition (6.65) and, therefore, has three real roots; thus, the three roots of (6.68) are real as required by the Green's function theory.

At high temperatures and vanishing field, $\sigma = 0$ and $C_3 \rightarrow 0$ and a third-stage TTA solution is feasible and, of course, a third-stage RPA solution definitely exists. The point, however, is that third-stage TTA is inconsistent (even if only at low temperatures) and that of the third-stage RPA is not. The question of which approximation is a "little worse" or a "little better" does not enter; the question of consistency does.

The reason why the work of Frank[1] did not indicate this tremendous failure of the third-stage TTA is that he was investigating paramagnetism, whereby $\sigma = 0$ at any temperature; i.e., J was never large enough to give a co-operative effect.

7. CONCLUSIONS

The first TTA, like the first RPA, has been shown to yield the same results as the MFA. The second TTA was a considerable improvement over the first TTA. Both at high temperatures as well as at low temperatures the results of the second TTA agreed more accurately (to order 1/z) than those of the first TTA with the exact low and high temperature series expansions.

In the immediate vicinity of the phase transition the second TTA is also an improvement over the molecular field results. Unlike the first TTA, the longitudinal correlation is shown to be non-zero even when the spins are spatially separated.

Therefore, the first- and second-stage TTA have been shown to give reasonable results for the Ising ferromagnet which were as exact as the results obtained by T-K for the first- and second-stage RPA but the calculations for the first- and second-stage TTA were shown to be simpler (less tedious mathematics) than those involved in the first two stages of the RPA.

For third-stage decoupling, however, the TTA results were no longer reasonable at low temperatures; an inconsistency arose due to the appearance of complex poles of the lowest-order Green's function in complex energy space. Such poles are ruled out by the general theory of Green's functions and moreover such poles did not appear in the more exact third-stage RPA.

Therefore, the more general third-stage results of TTA must be regarded with suspicion close to the Ising limit.

Finally, it has been shown that a third-stage decoupling within a specified decoupling scheme may be a much more sensitive test of that scheme than a second-stage decoupling.

Appendix I

Proof of Equation (5.12)

It is required to prove equation (5.12), that is,

$$\Sigma_f (J_{gf})^n = z\left[\frac{J(0)}{z}\right]^n . \qquad (A1.1)$$

The nearest-neighbour approximation consists in letting J_{gf} equal to zero when sites f and g are not nearest neighbours and equal to say J when f and g are nearest neighbours.

Therefore, if there exists z nearest neighbours, then

$$\Sigma_f J_{gf} = zJ . \qquad (A1.2)$$

Since $\Sigma_f J_{gf} \equiv J(0)$, then

$$J = \frac{J(0)}{z} . \qquad (A1.3)$$

Now using the nearest-neighbour approximation and (A1.3), relation (A1.1) follows immediately.

Appendix II

Proof of: $\left[S^z_{f_1}S^+_g \middle| S^-_g\right] = 0 \Longrightarrow \langle S^z_{f_1}S^z_g\rangle_c = 0$

It will be shown for the case of $n = 1$, that $\left[S^z_{f_1}S^z_{f_2}\ldots S^z_{f_n}S^+_g \middle| S^-_g\right]$ equals zero implies that $\langle f_1f_2\ldots f_ng\rangle_c = 0$.

Using the obvious simplifying notation,

$$\left[S^z_{f_1}S^z_{f_2}\ldots S^z_{f_n}S^+_g \middle| S^-_g\right] \equiv \left[12\ldots ng^+ \middle| g^-\right] , \qquad \text{(A2.1)}$$

the implication of $\left[1g^+ \middle| g^-\right] = 0$ is considered.

From (4.7), $\left[1g^+ \middle| g^-\right] = 0$ implies

$$\langle\langle 1g^+|g^-\rangle\rangle - \sigma\langle\langle g^+|g^-\rangle\rangle = 0. \qquad \text{(A2.2)}$$

Now, applying the spectral relation (3.38) to (A2.2) one obtains

$$\langle g^-1g^+\rangle - \sigma\langle g^-g^+\rangle = 0. \qquad \text{(A2.3)}$$

By using the commutations relations and $\langle g^-g^+\rangle = \frac{1}{2} - \sigma$, one obtains from (A2.3), if $g \neq f_1$,

$$\langle 1g\rangle - \sigma^2 = 0. \qquad \text{(A2.4)}$$

Therefore, from (4.2) it is seen (A2.4) implies

$$\langle 1g\rangle_c = 0. \qquad \text{(A2.5)}$$

Following the same procedure the relation can be proven for higher order Green's functions, that is, for $n = 2,3,\ldots$.

Appendix III

Derivation of System Magnetization (1st-TTA)

Spectral relation (3.38) can be used on (6.5) to obtain the system magnetization as follows:

Equation (6.5) can be rewritten in the form

$$\langle\langle S_g^+ | S_g^- \rangle\rangle_E = \frac{\sigma}{\pi} \frac{1}{E - \tilde{E}(0)} \; . \qquad \text{(A3.1)}$$

Apply $\lim_{\epsilon \to +0} (-2\mathrm{Im}) \int_{-\infty}^{\infty} \ldots (e^{\beta\omega} - 1)^{-1} d\omega$ to both sides of equation (A3.1). The left-hand side of (A3.1) will give, because of (3.38),

$$\begin{aligned} \langle S_g^- S_g^+ \rangle &= \langle S(S + 1) - S_g^z - (S_g^z)^2 \rangle , \\ &= (\tfrac{1}{2} - \sigma) \; . \end{aligned} \qquad \text{(A3.2)}$$

The right-hand side of (A3.1) will then give using identity (3.35)

$$(\sigma/\pi)(-2)(-\pi)(e^{\beta\tilde{E}(0)} - 1)^{-1} = 2\sigma(e^{\beta\tilde{E}(0)} - 1)^{-1}. \qquad \text{(A3.3)}$$

Equating the right-hand sides of (A3.2) and (A3.3),

$$\begin{aligned} \tfrac{1}{2} - \sigma &= 2\sigma(e^{\beta\tilde{E}(0)} - 1)^{-1}, \\ 2\sigma &= \tanh\left[\frac{\beta\tilde{E}(0)}{2}\right] , \end{aligned} \qquad \text{(A3.4)}$$

which is the result presented in equation (6.6).

Appendix IV

Derivation of Equation (6.18)

Spectral relation (3.38) must be applied to both sides of equation (6.14). Before (3.38) can be applied to the right-hand side of (6.14), this right-hand side must be re-arranged as follows:

$$\frac{1}{\pi}\,\frac{A + \sigma(E - \tilde{E}(0))}{[E - \tilde{E}(+)][E - \tilde{E}(-)]} = \frac{1}{2\phi\pi}\left\{\frac{A + \sigma\phi}{E - \tilde{E}(+)} - \frac{A - \sigma\phi}{E - \tilde{E}(-)}\right\}. \qquad (A4.1)$$

Applying (3.38) and identity (3.35) to the right-hand side of (A4.1) yields

$$\frac{(A + \sigma\phi)}{\phi}\, n(+) - \frac{(A - \sigma\phi)}{\phi}\, n(-) \ . \qquad (A4.2)$$

The application of (3.38) and identity (3.35) to the left-hand side of (6.14) yields

$$(\tfrac{1}{2} - \sigma) \ . \qquad (A4.3)$$

Equating (A4.3) to (A4.2) and solving for σ, equation (6.18) is obtained:

$$\sigma = \tfrac{1}{2} - \left[\frac{A}{\phi}(n(+) - n(-))\right]\left[1 + n(+) + n(-)\right]^{-1}. \qquad (A4.4)$$

Appendix V

Normalization of the Correlation Function

From (6.24),

$$L(\underline{K}) = \sum_{j} L_{ij} \exp[-i\underline{K}\cdot(\underline{j}-\underline{i})] \quad . \qquad (A5.1)$$

Therefore,

$$\sum_{\underline{K}} L(\underline{K}) = \sum_{j} L_{ij} \sum_{\underline{K}} \exp[-i\underline{K}\cdot(\underline{j}-\underline{i})] \quad ,$$

$$= \sum_{j} L_{ij}(N\delta_{ji}) \quad ,$$

$$= NL_{ii}$$

$$= N(\tfrac{1}{4} - \sigma^{2}) \quad . \qquad (A5.2)$$

Thus, the normalization requirement on the correlation function is that it satisfy (A5.2).

In the case of high temperatures ($\sigma \rightarrow 0$) and vanishing field, the correlation function obtained was (6.30a,b)

$$L(\underline{K}) = \tfrac{1}{4}[1 - J(\underline{K})V(T)]^{-1} \quad . \qquad (A5.3)$$

To normalize (A5.3) the following equation must be satisfied (from equation A5.2):

$$\sum_{\underline{K}} L(\underline{K}) = N/4 \quad . \qquad (A5.4)$$

If W is the normalization factor, then

$$\sum_{\underline{K}} \left\{\tfrac{1}{4}[1 - J(\underline{K})V(T)]^{-1}\right\} W = N/4 \quad ,$$

and therefore,

$$W = \left[\frac{1}{N} \sum_{\underline{K}} \frac{1}{1 - J(\underline{K})V(T)}\right]^{-1} . \qquad (A5.5)$$

Then, the correct normalized L($\underline{K}$) for high temperatures and vanishing field is

$$L(\underline{K}) = \left[\frac{1}{1 - J(\underline{K})V(T)}\right]\left[\frac{4}{N} \sum_{\underline{Q}} \frac{1}{1 - J(\underline{Q})V(T)}\right]^{-1} , \qquad (A5.6)$$

which is the result stated in (6.31).

It should be pointed out that the "correct" way of normalizing also leads to the same result as Equation (A5.6).

Appendix VI

Proof of Relation (6.32)

The partition function is

$$Z = \mathrm{tr}\left[\exp\left(-\beta\mathcal{H}\right)\right] , \qquad (A6.1)$$

where in our case the system Hamiltonian is

$$\mathcal{H} = -\tfrac{1}{2}\sum_{i,j}^{N} J_{ij}S_i^z S_j^z - \mu H \sum_i S_i^z . \qquad (A6.2)$$

Differentiating log Z with respect to $\beta\mu H$ gives

$$\begin{aligned}\frac{d \log Z}{d\,\beta\mu H} &= \frac{1}{Z}\,\mathrm{tr}\, e^{-\beta\mathcal{H}}\sum_i^N S_i^z ,\\ &= \left\langle \sum_i^N S_i^z \right\rangle ,\\ &= N\sigma , \qquad (A6.3)\end{aligned}$$

and

$$\begin{aligned}\frac{d^2 \log Z}{d(\beta\mu H)^2} &= N\frac{d\sigma}{d(\beta\mu H)} ,\\ &= \left\langle \left(\sum_i^N S_i^z\right)^2 \right\rangle - \left\langle \sum_i^N S_i^z \right\rangle^2 . \qquad (A6.4)\end{aligned}$$

The susceptibility is defined as

$$\chi \equiv \frac{dN\sigma}{d(\mu H)} = \beta\,\frac{dN\sigma}{d(\beta\mu H)} . \qquad (A6.5)$$

The right-hand side of (A6.4) can be rewritten as $\sum_{i,j}^{N} L_{ij}$ and, therefore, from (A6.5),

$$\chi = \beta\sum_{i,j}^{N} L_{ij} , \qquad (A6.6)$$

$$= \beta\left[L(\underline{K})\right]_{\lim \underline{K} = 0} . \qquad (A6.7)$$

This proof follows that given by Brout (see Reference 19, p. 20).

Appendix VII

Solution of $\sum_{\underline{K}} J^n(\underline{K})$ for n=1,2,3, and 4

According to the Fourier transform of J_{ij} (5.4),

$$J(\underline{K}) = \sum_{j} J_{ij} \exp[-i\underline{K}(\underline{j}-\underline{i})] \quad . \qquad (A7.1)$$

Therefore, using the origin for site i,

$$\begin{aligned}\sum_{\underline{K}} J(\underline{K}) &= \sum_{j} J_{oj} \sum_{\underline{K}} \exp[-i\underline{K}\cdot\underline{j}] \;, \\ &= \sum_{j} J_{oj} N\delta(\underline{j}) \;, \\ &= NJ_{oo} \;, \\ &= 0 \;, \qquad (A7.2)\end{aligned}$$

where $\delta(\underline{j})$ is zero if $j \neq \underline{o}$, and is equal to 1 if $\underline{j} = \underline{o}$; $\underline{o}$ indicates the vector to the origin o.

Similarly,

$$\begin{aligned}\sum_{\underline{K}} J^2(\underline{K}) &= \sum_{\underline{K}} \sum_{j} J_{oj} \exp[-i\underline{K}\cdot\underline{j}] \sum_{\underline{l}} J_{ol} \exp[+i\underline{K}\cdot\underline{l}] \;, \\ &= \sum_{j} \sum_{l} J_{oj} J_{ol} \sum_{\underline{K}} \exp[-i\underline{K}\cdot(\underline{j}+\underline{l})] \;, \\ &= \sum_{j} \sum_{l} J_{oj} J_{ol} N\delta(\underline{j}+\underline{l}) \;, \\ &= NzJ^2 \;, \\ &= \frac{NJ^2(0)}{z} \;, \qquad (A7.3)\end{aligned}$$

$$\begin{aligned}\sum_{\underline{K}} J^3(\underline{K}) &= N \sum_{j,l,m} J_{oj} J_{ol} J_{om} \delta(\underline{j} + \underline{l} + \underline{m}) \;, \\ &= NdzJ^3 \;, \\ &= \frac{NdJ^3(0)}{z^2} \;, \qquad (A7.4)\end{aligned}$$

where d = 0(sc and bcc); = 4(fcc).

The result (A7.4) is obtained by counting the number of ways one can get back to the origin using only three basis-vectors. For the sc and bcc lattices, there are no possible ways, but for the fcc lattice there are four ways for each nearest-neighbour.

Following the same procedure,

$$\begin{aligned}\sum_{\underline{K}} J^4(\underline{K}) &= N \sum_{j,l,m,n} J_{oj}J_{ol}J_{om}J_{on}\delta(\underline{j} + \underline{l} + \underline{m} + \underline{n}) \;, \\ &= Nbz\, J^4 \;, \\ &= \frac{NJ^4(0)b}{z^3} \;, \qquad\qquad (A7.5)\end{aligned}$$

where b = 15(sc); = 27(bcc); = 45(fcc). Use was made of relation (5.12) in deriving (A7.3) and (A7.5).

Another method for deriving results (A7.3), (A7.4) and (A7.5) involves using the definition of F(n) (see Eq. (6.53)) and the results obtained for F(n) for the various crystal structures (see Reference 43, Appendix A).

Appendix VIII

Calculation for the Specific Heat Using Second TTA

For the case of high temperature ($T \geq T_C$) and vanishing field ($\mu H=0$),

$$\begin{aligned} \langle \mathcal{H} \rangle &= -\tfrac{1}{2}\sum_{i,j} J_{ij} \langle S_i^z S_j^z \rangle , \\ &= -\tfrac{1}{2}\sum_{i,j} J_{ij} L_{ij} , \\ &= -\tfrac{1}{2} NA . \end{aligned} \tag{A8.1}$$

From (6.37) and (6.39), an expression for A is obtained:

$$\begin{aligned} A = \frac{1}{4}\Bigg\{ & \frac{\beta J^2(0)}{4z} + \left(\frac{\beta}{4}\right)^2 \frac{J^3(0)}{36}\, a \\ & + \left(\frac{\beta}{4}\right)^3 \left(\frac{J^4(0)}{z^2}\right)\left(\frac{b}{z} - \frac{4}{3}\right) + O(\beta^4) \quad . \end{aligned} \tag{A8.2}$$

Substituting for A from (A8.2) into (A8.1) and then differentiating with respect to T yields

$$\begin{aligned} C_V = \frac{d\langle \mathcal{H} \rangle}{dT} = (Nk_B)\left(\frac{\beta J(0)}{4}\right)^2 \Bigg\{ & \frac{1}{2z} + \frac{a}{36}\,\frac{\beta J(0)}{4} \\ & + \left(\frac{\beta J(0)}{4z}\right)^2 6\left(\frac{b}{z} - \frac{4}{3}\right)\Bigg\} + O(\beta^5) , \end{aligned} \tag{A8.3}$$

which is the required result (6.42).

Appendix IX

Low Temperature Second TTA Solution

Using equation (6.25), the definition of A (6.17) and ϕ^2 (6.16), and the relation (6.36a), the following expression for A is obtained:

$$A = \frac{\tanh(\beta\tilde{E}(0)/2)\ \phi\,\sigma\left[n(-) - n(+)\right]}{1 - D} , \qquad (A9.1)$$

where

$$D = \tanh(\beta\tilde{E}(0)/2)\left[2n(0) - n(+) - n(-)\right] . \qquad (A9.2)$$

For low temperature, vanishing magnetic field and approximating σ by $(\frac{1}{2} - c)$, it can be shown that

$$\tanh\left[\beta\tilde{E}(0)/2\right] = 1 - 2c + 2c^2\left[1 - \beta J(0)\right] + O(c^3) , \qquad (A9.3a)$$

$$n(0) + 1 = 1 + c + c^2\left[1 + \beta J(0)\right] + O(c^3) , \qquad (A9.3b)$$

$$n(-) - n(+) = 2ce^{\beta J(0)c}\sinh\beta\phi + 2c^2e^{2\beta J(0)c} \sinh 2\beta\phi + O(c^3) , \qquad (A9.3c)$$

$$n(-) + n(+) = 2ce^{\beta J(0)c}\cosh\beta\phi + 2c^2e^{2\beta J(0)c} \cosh 2\beta\phi + O(c^3) . \qquad (A9.3d)$$

In order to obtain an expression for ϕ^2, it is necessary to rewrite (6.25) as

$$L(\underline{K}) = \frac{(\frac{1}{2} - \sigma)\left[n(0) + 1\right]\tanh\left[\beta\tilde{E}(0)/2\right]}{1 - B} , \qquad (A9.4)$$

where

$$B = \tanh\left[\frac{\beta\tilde{E}(0)}{2}\right]\left\{\frac{J(\underline{K})A}{\phi^2}\left[2n(0) - n(+) - n(-)\right] + \frac{J(\underline{K})\sigma}{\phi}\left[n(-) - n(+)\right]\right\} . \qquad (A9.5)$$

From relations (A9.2) it is seen that B is at least of order c and therefore B is small compared to 1; thus, (A9.3) can be written as

$$L(\underline{K}) = (\tfrac{1}{2} - \sigma)[n(0) + 1] \tanh[\beta\tilde{E}(0)/2][1 + B + B^2 + O(c^3)] . \qquad (A9.6)$$

Using relations (A9.2),

$$\begin{aligned}(\tfrac{1}{2} - \sigma)[n(0) + 1] \tanh[\beta\tilde{E}(0)/2] &= c[1 + c + c^2(1 + \beta J) \\ &\qquad + O(c^3)] \\ &\quad \times [1 - 2c + 2c^2(1 - \beta J) + O(c^3)] , \\ &= c[1 - c + (1 - \beta J)c^2 + O(c^3)] , \\ &= c - c^2 + O(c^3) . \end{aligned} \qquad (A9.7)$$

Substituting (A9.6) into (A9.5) gives

$$\begin{aligned} L(\underline{K}) &= [c - c^2 + O(c^3)][1 + O(c)] , \\ &= c + O(c^2) . \end{aligned} \qquad (A9.8)$$

Now, using the definition of ϕ^2 (6.16), an expression for ϕ^2 is obtained:

$$\begin{aligned} \phi^2 &= \frac{1}{N} \sum_{\underline{K}} J^2(\underline{K}) L(\underline{K}) , \\ &= \frac{J^2(0)}{z} c + O(c^2) . \end{aligned} \qquad (A9.9)$$

Now, D in (A9.1) is of the order c^2 and is therefore small compared to 1, allowing (A9.1) to be rewritten as

$$\begin{aligned} A &= \tanh[\beta\tilde{E}(0)/2] \, \phi\sigma[n(-) - n(+)][1 + O(c^2)] , \\ &= [1 - 2c + 2c^2(1 - \beta J(0)) + O(c^3)] \, \phi(\tfrac{1}{2})(1 - 2c) \\ &\quad \times [2c(\beta\phi + \beta^2 J\phi c + \beta^3\phi^3/3!) + O(c^{5/2})][1 + O(c^2)] , \\ &= c\beta\phi^2 + O(c^3) , \\ &= \left[\frac{\beta J^2(0)}{z}\right] c^2 + O(c^3) . \end{aligned} \qquad (A9.10)$$

Using (A9.9) and (A9.10) in (6.18), the following is obtained for the magnetization:

$$\sigma = \tfrac{1}{2} - c + c^2(1 - \beta J) - \frac{\beta^2 J^2(0)}{2z} c^2 + O(c^3) \ . \qquad (A9.11)$$

The expansion for V is also obtained from (A9.9) and (A9.10) and is

$$V = \frac{A}{\phi^2} = \beta c + O(c^2) \ . \qquad (A9.12)$$

Appendix X

Proof of: $C_3 \cong - JC_2$,

in Low-Temperature Approximation (Third-Stage)

When the spectral relation (3.38) is applied to the third order Green's function equation (after third-stage decoupling) and when use is made of the low-temperature approximation: $n(\alpha)$ replaced by $\exp\left[-\beta J(0)/2\right]$; σ replaced by $\frac{1}{2}$, then to this approximation we are left with

$$-\left\langle S^z_{f_1} S^z_{f_2} S^z_g \right\rangle_c - \delta_{f_1g} L_{f_2g} - \delta_{f_2g} L_{f_1g} + (\tfrac{1}{2} - \sigma)\delta_{f_1g}\delta_{f_2g} =$$

$$\exp\left[-\beta J(0)/2\right]\Big(2\left\langle S^z_{f_1} S^z_{f_2} S^z_g \right\rangle_c + \delta_{f_2g} L_{f_1g} + \delta_{f_1g} L_{f_2g}$$

$$- (\tfrac{1}{2} - \sigma)\delta_{f_1g}\delta_{f_2g}\Big) \ . \qquad \text{(A10.1)}$$

Therefore, since $\left\langle S^z_{f_1} S^z_{f_2} S^z_g \right\rangle_c$ is equal to terms involving δ-functions only, then $\left\langle S^z_{f_1} S^z_{f_2} S^z_g \right\rangle_c = 0$ unless at least two indices are equal, to this order of approximation.

Using the result of (A10.1) then C_3 can be rewritten as

$$C_3 \cong \sum_{f_1,f_2,f_3} J_{f_1g} J_{f_2g} J_{f_3g} (\delta_{f_1f_2} + \delta_{f_1f_3} + \delta_{f_2f_3} - 2\delta_{f_1f_2}\delta_{f_1f_3})$$

$$\left\langle S^z_{f_1} S^z_{f_2} S^z_{f_3} \right\rangle_c \quad , \qquad \text{(A10.2)}$$

which, if σ is approximated by $\frac{1}{2}$, yields

$$C_3 \cong -3 \sum_{f_1,f_2} J^2_{f_1g} J_{f_2g} L_{f_1f_2} + 2JC_2 \ . \qquad \text{(A10.2)}$$

By going over to Fourier Transform Space and using the well-known relation[45] for spatially isotropic nearest-neighbour interactions (e.g. in lattices of cubic symmetry):

$$\frac{1}{N}\sum_{\underline{\lambda}} J(\underline{K}-\underline{\lambda})f(\underline{\lambda}) = \frac{J(\underline{K})}{J(0)}\frac{1}{N}\sum_{\underline{\lambda}} J(\underline{\lambda})f(\underline{\lambda}), \qquad (A10.3)$$

which follows whenever $f(\underline{\lambda}) = f(-\underline{\lambda})$ and using also relation (6.36b) one obtains from (A10.2)

$$C_3 \cong - JC_2 \quad , \qquad (A10.3)$$

which is the desired result.

Appendix XI

Third-Stage RPA

Third-stage RPA involves (following notation of (4.1) and (4.7)) simply putting $[123+| = 0$ when f_1, f_2, f_3 and g are unequal. Using this fact, G_3 (see (6.59b)) can be written as

$$G_3 = \sum_{f_1,f_2,f_3} J_{f_1g}J_{f_2g}J_{f_3g} \\ (\delta_{f_1f_2} + \delta_{f_1f_3} + \delta_{f_2f_3} - 2\delta_{f_1f_2}\delta_{f_1f_3}) \\ [123+| \quad . \qquad \text{(A11.1)}$$

By making use of (6.66a), one obtains from (A11.1)

$$G_3 = \sum_{f_1,f_2} J^2_{f_1g}J_{f_2g} - 6\sigma[12+| - 6L_{f_1f_2}[1+| \\ -2\sum_{f_1} J^3_{f_1g}(-\tfrac{1}{2} + 6\sigma^2)[1+| \quad . \qquad \text{(A11.2)}$$

Going over to Fourier Transform Space and using relation (A10.3), one obtains from (A11.2)

$$G_3 = -6\sigma JG_2 + \left[J^2(1 - 12\sigma^2) - 6/z\ C_2\right] G_1 \ , \qquad \text{(A11.3)}$$

from which equations (6.67a, b) follow.

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