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A SECOND ORDER GREEN FUNCTION THEORY OF THE HEISENBERG FERROMAGNET

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OF THE HEISENBERG FERROMAGNET

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CHAPTER I

INTRODUCTION

The Heisenberg Ferromagnet

The Heisenberg model of a ferromagnet is based on the concept of exchange forces which are present in a ferromagnetic solid.[1,2] The system of interest here is a solid consisting of a large number of atoms arranged on some crystal lattice. The atoms are close enough so that the orbital wave functions of the electrons of one atom overlap with the orbital wave functions of electrons in other atoms. As a result of the Pauli exclusion principle there is a correlation between the orbital symmetry and the spin alignment which produces a large spin-spin coupling. Dirac[3] showed that, apart from a constant term which has no importance here, the effective coupling between the two electrons on atoms i and j due to the exchange effect is equivalent to a potential of the form

$$V_{ij} = -2J_{ij}\vec{S}_i \cdot \vec{S}_j \qquad (1)$$

where $\vec{S}_i$ is the spin angular momentum operator of atom i measured in units of $\hbar$, and J_{ij} is the exchange integral given by

$$J_{ij} = \int \cdots \int \psi_i^*(1)\,\psi_j^*(2)\,\mathcal{H}_1\,\psi_j(2)\,\psi_i(1)\,d\tau_1\,d\tau_2 \qquad (2)$$

Here $\mathcal{H}_1$ denotes the Hamiltonian operator, and $\psi_i(1)$ is the wave function for electron (1) in a state i.

The so-called "Heisenberg Hamiltonian" for this system of atoms is then

$$\mathcal{H} = -\mu H \sum_j S_j^z - \sum_i \sum_j J_{ij} \vec{S}_i \cdot \vec{S}_j \qquad (3)$$

where the sums over i and j range over all of the atoms in the solid. The first term on the right hand side of this equation represents the interaction of an externally applied magnetic field, $\vec{H}$, with the magnetic moment, μ , associated with each unit of spin ($\hbar/2$). The direction of $\vec{H}$ defines the z-direction in space and S_j^z is the z-component of the total spin angular momentum operator for atom j. The last term of Eq. (3) represents the spin-spin coupling of each spin to other spins in the solid. It should be pointed out here that this term is correct only if all the electrons not in filled shells on a particular atom have the same exchange integrals. This assumption is in general not true for solids which have internal crystalline fields.[2]

If it is assumed that the wave function overlap is appreciable only for nearest neighbor atoms then Eq. (3) can be approximated by replacing J_{ij} by a non-zero constant if i and j are nearest neighbors and by zero otherwise. This is believed to be a good first approximation of Eq. (3) for physical systems. If, on the other hand, it is assumed that each spin interacts with every spin in the system with equal strength, that is, J_{ij} is a constant for $i \neq j$ and zero for $i=j$, then the Hamiltonian describes a system with an infinite range interaction. This problem has been solved exactly by Kittel and Shore.[4]

In either case Eq. (3) can be written in the form

$$\mathcal{H} = -\eta H \sum_j S_j^z - J \sum_j \sum_\rho \vec{S}_j \cdot \vec{S}_{j+\rho} \tag{4}$$

where J is the exchange integral, which is assumed to be independent of spatial co-ordinates, and ρ represents nearest neighbor distances in the case of the nearest neighbor approximation and all lattice vectors except j in the infinite range problem. If $J>0$ the above Hamiltonian describes a ferromagnet. The system has a well ordered ground state with all spins aligned in the z-direction, since this configuration gives the lowest possible energy for the system.

Excited states of this Hamiltonian can be obtained from the spin deviation operators $S_j^{\pm}(t)$. These operators are defined by

$$\begin{aligned} S_j^+ &= S_j^x + i S_j^y \\ S_j^- &= S_j^x - i S_j^y \end{aligned} \tag{5}$$

where S_j^x and S_j^y are the x and y components respectively of $\vec{S}_j$. The operators $S_j^{\pm}$ satisfy the equal time commutation rules

$$[S_j^+, S_\ell^-] = +2 S_j^z \delta_{\ell j} \tag{6}$$

$$[S_j^{\pm}, S_i^z] = \mp S_j^{\pm} \delta_{i,j} \tag{7}$$

The interpretation of these spin deviation operators is based on the effect that they have on the simultaneous eigenfunctions of $\mathcal{H}$ and S^z, where S^z is the total z-component of the spin angular momentum of the system.

$$S^z = \sum_j S_j^z \tag{8}$$

Let $\{|n\rangle\}$ represent the set of simultaneous eigenfunctions of S^z and $\mathcal{H}$, where n denotes the number of reversed spins with respect to the ground state. Then

$$\mathcal{H}\,|n\rangle = E_n\,|n\rangle \tag{9}$$

and

$$S^z|n\rangle = (N-2n)S\,|n\rangle \qquad (\hbar=1) \tag{10}$$

where S is the spin per atom, and N is the total number of atoms. Consider the state $S_j^{\pm}|n\rangle$. Using Eqs. (7) and (10)

$$S^z(S_j^{\pm}|n\rangle) = ([N-2n]S \pm 1)\,S_j^{\pm}|n\rangle \tag{11}$$

Thus the spin deviation operators have the effect of changing the total z-component of the spin of the system by one unit. For $S=\frac{1}{2}$ the S_j^- operator has the effect of flipping a spin down (in the negative z-direction) at the j-th lattice site, while S_j^+ has the effect of flipping a spin up (along the positive z-direction) at the j-th lattice site.

Therefore, it should be expected that the excited states of the system should be expressible in terms of these operators. Indeed, Bloch[5] has shown that the excited states with one reversed spin are given by

$$|P\rangle = \frac{1}{\sqrt{N}} \sum_n e^{i p\cdot n} S_n^- |0\rangle = \frac{1}{\sqrt{2S}} S_{\vec{p}}^- |0\rangle \tag{12}$$

The operator $S_{\vec{p}}^-$ defined by this equation is the spin-wave or magnon creation operator. The vector $\vec{p}$ is a reciprocal lattice vector which can take on the values $p=2\pi n_i/N^{1/3}$ where n_i is any integer. For any lattice with N lattice points this set can be reduced to a complete set of N non-equivalent vectors.[6] These sets of points are complete in the sense that

$$\delta_{m,n} = \frac{1}{N} \sum_p e^{i\vec{p}\cdot(\vec{n}-\vec{m})} \tag{13}$$

$$\delta_{P_1,P_2} = \frac{1}{N} \sum_m e^{i\vec{m}\cdot(\vec{P}_1-\vec{P}_2)}$$

where $\delta_{m,n}$ is the Kronecker delta function.

The energy of the spinwave (magnon) state with momentum $\vec{p}$ is given by

$$\mathcal{H}|P\rangle = 2JS(\gamma_0-\gamma_p)|P\rangle = E_p^0|P\rangle \tag{14}$$

$$\gamma_p = \sum_\rho e^{i\vec{p}\cdot\vec{\rho}} \tag{15}$$

Spinwave theory for the nearest neighbor approximation uses as a basis of states

$$|c\rangle = \prod_{\rho} (2S)^{-\frac{1}{2}c_\rho} (c_\rho !)^{-\frac{1}{2}} (S_\rho^-)^{c_\rho} |0\rangle \tag{16}$$

where c represents a set of non-negative integers $\{c_\rho\}$. For $\sum c_\rho > 1$, that is for states with two or more spinwaves, the states (16) are non-orthogonal and hence cannot be eigenfunctions of $\mathcal{H}$. In this case the number of states (16) exceeds the number of independent states for the system, which number $(2S+1)^N$.[1]

Dyson[7] has used these states to calculate the partition function for the system, from which all thermodynamic properties can be obtained. He obtains expressions for some of the properties which are correct for temperatures up to a value T for which the magnetization has decreased about one-fourth of its value at zero temperature.

The present work is concerned with the development of a consistent approach to this problem using the Green function theory. This formalism offers a method of solution at all temperatures. The problem with the Green function theory is that, in general, it generates an infinite set of coupled differential equations which must be solved. Approximate solutions are obtained by breaking up this hierarchy of equations. Previous work has been centered about a decoupling scheme in the first order equation.[8, 9, 10] The decoupling used here is in the second order equation.

CHAPTER II

DOUBLE TIME TEMPERATURE-DEPENDENT GREEN FUNCTIONS

Consider a system which is described by the Hamiltonian $\mathcal{H}$. Let A(t) and B(t) be any pair of operators in the Heisenberg representation which can be defined for this system. The advanced and retarded Green functions based on these operators are [11]

$$G_r(t,t') = -i\,\theta(t-t')\langle[A(t), B(t')]\rangle \tag{17}$$

$$G_a(t,t') = -i\,\theta(t'-t)\langle[A(t), B(t')]\rangle$$

$$\theta(t-t') = 0 \quad \text{if} \quad t'>t$$
$$\qquad\quad = 1 \quad \text{if} \quad t>t'$$

The square brackets represent the commutator or anti-commutator and the angular brackets indicate an average over a canonical ensemble. That is

$$\langle A(t)\rangle = Z^{-1}\,\mathrm{Tr}\,\left(e^{-\beta\mathcal{H}}A(t)\right) \tag{18}$$

$$Z = \mathrm{Tr}\,\left(e^{-\beta\mathcal{H}}\right)$$

The symbol β denotes the reciprocal of the product of Boltzmann's constant and the absolute temperature, Z is the partition function, and Tr indicates the trace of a matrix.

These double time Green functions depend on t and t' only through the time difference t-t'. This is easily demonstrated by recalling that the time dependence of the Heisenberg operators may be expressed as

$$A(t) = e^{i\mathcal{H}t} A(0)\, e^{-i\mathcal{H}t} \tag{19}$$

Let

$$[A, B] = AB - \eta BA \tag{20}$$

$\eta = 1$ for commutator

$\eta = -1$ for anti-commutator

Then

$$G_r(t,t') = -i\,\theta(t-t')\, Z^{-1}\, Tr\,\{ e^{\mathcal{H}[it-\beta]} A(0)\, e^{i\mathcal{H}[t'-t]} B(0)\, e^{-i\mathcal{H}t'} \tag{21}$$

$$- \eta\, e^{\mathcal{H}[it'-\beta]} B(0)\, e^{i\mathcal{H}[t-t']} A(0)\, e^{-i\mathcal{H}t} \}$$

Using the property of the invariance of the trace under cyclic permutations this equation becomes

$$G_r(t,t') = -i\,\Theta(t-t')\, Z^{-1}\, Tr\,\{ e^{\mathcal{H}[i(t-t')-\beta]} A(0)\, e^{i\mathcal{H}[t'-t]} B(0) \tag{22}$$

$$- \eta\, e^{\mathcal{H}[i(t'-t)-\beta]} B(0)\, e^{i\mathcal{H}(t-t')} A(0) \}$$

In a similar manner $G_a(t,t')$ can also be shown to have the same dependence on t and t', namely t-t'. Thus t' can be set equal to zero with no loss in generality.

In calculating physical properties of the system it is necessary that the average over the canonical ensemble of products of operators A and B be known. These averages are known collectively as time correlation functions. The two simplest correlation functions are

$$F_{AB}(t) = \langle A(t)\, B(o) \rangle \tag{23}$$

$$F_{BA}(t) = \langle B(o)\, A(t) \rangle$$

These time correlation functions can be obtained if the Green functions (17) are known. The direct connection can be established by means of a spectral representation of the functions involved.

Let $|c_n\rangle$ and E_n be eigenfunctions and eigenvalues of the Hamiltonian $\mathcal{H}$.

$$\mathcal{H}\,|c_n\rangle = E_n\,|c_n\rangle \tag{24}$$

The equation for $F_{AB}(t)$ is then

$$F_{AB}(t) = \langle A(t)\, B(o) \rangle = Z^{-1} \sum_n \langle c_n |\, A(t)\, B(o) \,| c_n \rangle\, e^{-\beta E_n} \tag{25}$$

$$Z = \sum_n e^{-\beta E_n}$$

Substituting Eq. (18) for A(t) and using the completeness of the set $\{|c_n\rangle\}$, $F_{AB}(t)$ becomes

$$\langle A(t)B(o)\rangle = Z^{-1}\sum_n\sum_m \langle C_n|A(o)|C_m\rangle\langle C_m|B(o)|C_n\rangle e^{i(E_n-E_m)t-\beta E_n} \tag{26}$$

Similarly

$$\langle B(o)A(t)\rangle = Z^{-1}\sum_n\sum_m \langle C_m|B(o)C_n\rangle\langle C_n|A(o)|C_m\rangle e^{i(E_n-E_m)-\beta E_m} \tag{27}$$

Because of the similar forms of (26) and (27) it is possible to write

$$F_{AB}(t) = \int_{-\infty}^{\infty} J(\omega)\, e^{\beta\omega} e^{-i\omega t}\, d\omega \tag{28}$$

$$F_{BA}(t) = \int_{-\infty}^{\infty} J(\omega)\, e^{-i\omega t}\, d\omega$$

where the spectral function, $J(\omega)$, is given by

$$J(\omega) = Z^{-1}\sum_n\sum_m \langle C_n|A(o)|C_m\rangle\langle C_m|B(o)|C_n\rangle e^{-\beta E_m}\delta(E_n-E_m-\omega) \tag{29}$$

The Fourier representation for the retarded Green function is given by

$$G_r(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} G_r(E)\, e^{-iEt}\, dE \tag{30}$$

$$G_r(E) = \int_{-\infty}^{\infty} G_r(t)\, e^{iEt}\, dt \tag{31}$$

Substituting $G_r(t)$, given by Eq. (17), into Eq. (31) gives

$$G_r(E) = -i\int_{-\infty}^{\infty} (F_{AB} - \eta F_{BA})\, e^{iEt}\, \Theta(t)\, dt \tag{32}$$

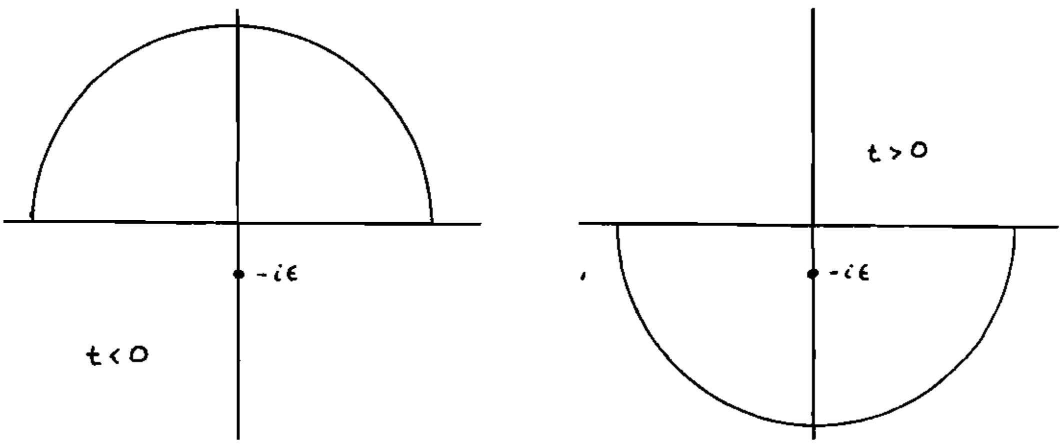
or

$$G_r(E) = -i\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} J(\omega)\, [\, e^{\beta\omega} - \eta\,]\, e^{i[E-\omega]t}\, \Theta(t)\, d\omega\, dt \tag{33}$$

The step function $\Theta(t)$ can be represented by

$$\Theta(t) = \lim_{\epsilon \to 0^+} \frac{i}{2\pi} \int_{-\infty}^{\infty} \frac{e^{-ixt}}{x + i\epsilon} \, dx \tag{34}$$

The evaluation of this integral is done by extending x to be a complex variable. The integral (34) is taken over the contours



Then by the Cauchy Integral Theorem the right hand side of (34) gives zero for $t < 0$ and unity for $t > 0$, thus giving a valid representation for $\theta(t)$. Then (33) becomes

$$G_r(E) = \lim_{\epsilon \to 0^+} \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} J(\omega) \, [e^{\beta\omega} - \eta] \, \frac{e^{i(E - x - \omega)t}}{x + i\epsilon} \, dt \, d\omega \, dx \tag{35}$$

Since

$$\delta(E - \omega - x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i(E - \omega - x)t} \, dt \tag{36}$$

Eq. (33) reduces to

$$G_r(E) = \lim_{\epsilon \to 0^+} \int_{-\infty}^{\infty} J(\omega) \, \frac{e^{\beta\omega} - \eta}{E - \omega + i\epsilon} \, d\omega \tag{37}$$

Similarly for the advanced Green function

$$G_a(E) = \lim_{\epsilon \to 0^+} \int_{-\infty}^{\infty} J(\omega) \frac{e^{\beta\omega} - \eta}{E - \omega - i\epsilon} d\omega \tag{38}$$

Until now E has been considered to be a real variable. Bogolyubov and Parasyuk[12] have proved that Eqs. (37) and (38) can be analytically extended into the complex E plane. Thus the function

$$G(E) = \int_{-\infty}^{\infty} J(\omega) \frac{e^{\beta\omega} - \eta}{E - \omega} d\omega \tag{39}$$

is an analytic function in the complex E plane. Then G(E) is the analytic continuation of $G_a(E)$ for Im $E > 0$ and of $G_r(E)$ for Im $E < 0$.

The discontinuity of $G(\omega')$ across the real axis is, for ω' real,

$$\lim_{\epsilon \to 0^+} [G(\omega' + i\epsilon) - G(\omega' - i\epsilon)] = \lim_{\epsilon \to 0^+} \int_{-\infty}^{\infty} J(\omega)[e^{\beta\omega} - \eta]\left\{\frac{1}{-\omega + \omega' + i\epsilon} - \frac{1}{\omega' - \omega - i\epsilon}\right\} d\omega \tag{40}$$

$$= -2\pi i\, [e^{\beta\omega'} - \eta]\, J(\omega')$$

since

$$\lim_{\epsilon \to 0^+} \left\{ \frac{1}{\omega' - \omega + i\epsilon} - \frac{1}{\omega' - \omega - i\epsilon} \right\} = -2\pi i\, \delta(\omega - \omega') \tag{41}$$

The time correlation function $F_{AB}(t)$ is then given by

$$F_{AB}(t) = \langle A(t) B(0) \rangle = \frac{i}{2\pi} \lim_{\epsilon \to 0^+} \int_{-\infty}^{\infty} \frac{e^{-i\omega t}}{\eta - e^{\omega\beta}} [G(\omega + i\epsilon) - G(\omega - i\epsilon)] d\omega \tag{42}$$

In general $G_r(E)$ and $G_a(E)$ must be known to construct

G(E). However, $G_r(E)$ and $G_a(E)$ can be shown to obey identical equations of motion and thus knowledge of either function is enough to construct G(E).

The above argument can be extended to yield

$$\langle F(A(t),B(t))\,B(0)\rangle = \frac{i}{2\pi}\lim_{\epsilon\to 0^+}\int_{-\infty}^{\infty}\frac{e^{-i\omega t}}{\eta - e^{\beta\omega}}\left[G(\omega+i\epsilon) - G(\omega-i\epsilon)\right]d\omega \tag{43}$$

where F(A(t), B(t)) is any conceivable product of operators A(t) and B(t), and G(E) is the analytic extension of the Green function

$$G_r(t) = -i\,\theta(t)\,\langle[\,F(A(t),B(t)),\,B(0)]\rangle \tag{44}$$

since the actual construction of A(t) in that argument was of no consequence to the final result.

The Green functions are determined from their equations of motion. These equations are formed by

$$\begin{aligned} i\frac{d}{dt}G_r(t) = {} & \delta(t)\,\langle[\,F(A(t),B(t)),\,B(0)]\rangle \\ & + \theta(t)\,\langle[\,\frac{d}{dt}F(A(t),B(t),\,B(0)]\rangle \end{aligned} \tag{45}$$

where equations (34) and (36) have been used. The equations of motion for the Heisenberg operators are known to be

$$i\frac{d}{dt}A(t) = [\,A(t),\mathcal{H}] \tag{46}$$

which is consistent with (19).

For systems of bosons or fermions the choice of η is a simple one. However, for systems where the commutation or anti-commutation rules are not c-numbers the choice may not be as simple. It may be that over certain range of temperatures the commutation rules ($\eta = 1$) would give the easiest solutions while over other ranges the anti-commutation rules ($\eta = -1$) would give the easiest solutions.

The poles of the spectral function, $G_r(E)$, are connected to the energy states of the system. Using Eqs. (26), (27), and (32) it follows that

$$G_r(E) = \lim_{\epsilon \to 0^+} Z^{-1} \sum_n \sum_m \frac{\langle C_m | B(0) | C_n \rangle \langle C_n | A(0) | C_m \rangle \left(e^{-\beta E_n} - \eta e^{-\beta E_m} \right)}{E - (E_m - E_n) + i\epsilon} \qquad (47)$$

Thus the poles for $G_r(E)$ occur at $E = E_m - E_n$, which corresponds to the energy difference between states m and n.

CHAPTER III

THE COUPLED GREEN FUNCTION EQUATIONS FOR $S=\frac{1}{2}$

The thermodynamic behavior of this system will be determined by the use of the temperature-dependent double-time Green function defined by equation (17). The choice of the operators A and B is made to effect a quasi-particle description for the system. The retarded Green function, defined for the Hamiltonian (4), is given by

$$G_1(j,t) = -i\theta(t)\langle[S_j^-(t),\ S_0^+(0)]\rangle \tag{48}$$

The choice of the commutator $(\eta=1)$ here is based on the commutator (6). The spin deviation operators are not pure boson operators, since the commutator is not a c-number. However, at low temperatures this commutator approximates a boson character. Thus it might be expected that this system could be described in terms of boson quasi-particles with corrections made for the non-c-number commutator.

The equation of motion for $G_1(j,t)$ is given by Eq. (44).

$$i\frac{\partial}{\partial t}G_1(j,t) = \delta(t)\langle[S_j^-(t),S_0^+(0)]\rangle + \theta(t)\langle[\frac{\partial}{\partial t}S_j^-(t),\ S_0^+(0)]\rangle \tag{49}$$

The function $\delta(t)$ is the Dirac delta function.

The derivative with respect to time of the spin deviation operators obeys Eq. (45). Using the Hamiltonian (4) and the commutation rules (6) it is easily established that

$$i \frac{\partial}{\partial t} S_j^-(t) = -\mu H S_j^-(t) + 2J \sum_\rho [S_j^z(t) S_{j+\rho}^-(t) - S_j^-(t) S_{j+\rho}^z(t)] \tag{50}$$

$$i \frac{\partial}{\partial t} S_j^+(t) = \mu H S_j^+(t) + 2J \sum_\rho [S_j^+(t) S_{j+\rho}^z(t) - S_j^z(t) S_{j+\rho}^+(t)] \tag{51}$$

Then Eq. (49) becomes

$$\left(i \frac{\partial}{\partial t} + \mu H\right) G_1(j,t) = -2\langle S^z\rangle \delta(t)\delta_{j,0} + 2Ji\theta(t) \sum_\rho \langle [S_j^-(t) S_{j+\rho}^z - S_j^z(t) S_{j+\rho}^-(t), S_0^+(0)]\rangle \tag{52}$$

As a result of the commutation rule (6) the terms in the sum are not all G_1 functions. These terms couple the G_1 function to a higher order Green function, G_2. This coupling is based on the identity between S_j^z and the operator $S_j^- S_j^+$, which can be verified from Eqs. (5), (6), and (7).

$$S_j^-(t) S_j^+(t) = (S - S_j^z)(S + S_j^z + 1) \tag{53}$$

For $S=\frac{1}{2}$ (53) reduces to

$$S_j^z = S - S_j^- S_j^+ \tag{54}$$

From here on the equations are restricted to the case $S=\frac{1}{2}$ because of the explicit use of (54). The G_1 equation becomes

$$\left(i \frac{\partial}{\partial t} + \mu H\right) G_1(j,t) + 2JS \sum_\rho [G_1(j,t) - G_1(j+\rho,t)] = -2\langle S^z\rangle \delta(t)\delta_{j,0} + 2J \sum_\rho [G_2(j, j+\rho, j+\rho, t) - G_2(j+\rho, j, j, t)] \tag{55}$$

where G_2 is defined by

$$G_2(1,2,3,t) = -i\,\theta(t)\langle[\,S_1^-(t)\,S_2^-(t)\,S_3^+(t),\ S_0^+(0)]\rangle \tag{56}$$

The numerals 1, 2, 3 will henceforth represent the lattice vectors j_1, j_2, j_3.

The equation of motion for G_2 is then

$$i\frac{\partial}{\partial t}G_2(1,2,3,t) = \delta(t)\langle[\,S_1^-S_2^-S_3^+,\ S_0^+]\rangle - i\,\theta(t)\langle[\,A(t),\ S_0^+(0)]\rangle \tag{57}$$

where

$$A(t) = [\,S_1^-(t),\mathcal{H}]\,S_2^-(t)S_3^+(t) + S_1^-(t)\,[S_2^-(t),\mathcal{H}]\,S_3^+(t) + S_1^-(t)S_2^-(t)\,[\,S_3^+(t),\mathcal{H}\,] \tag{58}$$

Then using Eqs. (50) and (51) the equation of motion for the G_2 function is

$$\begin{aligned}
\left(i\frac{\partial}{\partial t}+\mu H\right)G_2(1,2,3,t) &= -2\,\delta(t)\,[\,\delta_{1,0}\,S\langle S_2^-S_3^+\rangle + \delta_{2,0}\,S\langle S_1^-S_3^+\rangle \\
&\quad -\delta_{1,0}\delta_{2,0}\langle S_1^-S_3^+\rangle - \delta_{1,0}\langle S_2^-S_0^-S_0^+S_3^+\rangle - \delta_{2,0}\langle S_1^-S_0^-S_0^+S_3^+\rangle\,] \\
&\quad + 2Ji\,\theta(t)\sum_\rho\langle[\,(S_1^-(t)S_{1+\rho}^3(t) - S_1^3(t)S_{1+\rho}^-(t))\,S_2^-(t)\,S_3^+(t),\ S_0^+(0)\,]\rangle \\
&\quad + 2Ji\,\theta(t)\sum_\rho\langle[\,S_1^-(t)\,(S_2^-(t)S_{2+\rho}^3(t) - S_2^3(t)S_{2+\rho}^-(t))\,S_3^+(t),\ S_0^+(0)\,]\rangle \\
&\quad - 2Ji\,\theta(t)\sum_\rho\langle[\,S_1^-(t)S_2^-(t)\,(S_{3+\rho}^3(t)S_3^+(t) - S_{3+\rho}^+(t)S_3^3(t)),\ S_0^+(0)]\rangle
\end{aligned} \tag{59}$$

Again because of the commutation rule (6) G_2 is coupled to a higher order Green function. Using Eq. (54), the above equation becomes

$$\left(i\frac{\partial}{\partial t}+\mu H\right)G_2(1,2,3,t) + 2JS\sum_\rho[\,G_2(1,2,3,t)\,\{1-2\delta_{2,1+\rho}\} - G_2(1+\rho,2,3,t)\,\{1-2\delta_{1,2}\} \tag{60}$$

$$- G_2(1,2+\rho,3,t) + G_2(1,2,3+\rho,t)] = -2\delta(t)\{\delta_{1,0} S\langle S_2^- S_3^+\rangle + \delta_{2,0} S\langle S_1^- S_3^+\rangle$$

$$- \delta_{1,0}\delta_{2,0}\langle S_1^- S_3^+\rangle - \delta_{1,0}\langle S_2^- S_0^- S_0^+ S_3^+\rangle - \delta_{2,0}\langle S_1^- S_0^- S_0^+ S_3^+\rangle]$$

$$+ 2J\sum_\rho [\, G_3(1,2,1+\rho,1+\rho,3,t) - G_3(1+\rho,2,1,1,3,t) + G_3(1,2,2+\rho,2+\rho,3,t)$$

$$- G_3(1,2+\rho,2,2,3,t) + G_3(1,2,3,3,3+\rho,t) - G_3(1,2,3+\rho,3+\rho,3,t)]$$

where

$$G_3(1,2,3,4,5,t) = -i\,\theta(t)\langle[\, S_1^-(t) S_2^-(t) S_3^-(t) S_4^+(t) S_5^+(t), S_0^+(0)]\rangle \tag{61}$$

The equation of motion for G_3 can be derived by the same method used above to obtain the equations of motion for G_1 and G_2. The result is

$$(i\frac{\partial}{\partial t} + 4H)\, G_3(1,2,3,4,5,t) + 2JS\sum_\rho [\, G_3(1,2,3,4,5,t)\{1 - 2[\delta_{2,1+\rho} + \delta_{3,1+\rho} \tag{62}$$

$$+ \delta_{3,2+\rho} - \delta_{4,5+\rho}]\} - G_3(1+\rho,2,3,4,5,t)\{1 - 2[\delta_{1,3} + \delta_{2,3}]\} - G_3(1,2+\rho,3,4,5,t)\times$$

$$\times\{1 - 2\delta_{2,3}\} - G_3(1,2,3+\rho,4,5,t) + G_3(1,2,3,4+\rho,5,t) + G_3(1,2,3,4,5+\rho,t)\{1 -$$

$$2\delta_{4,5}\}] = -2\delta(t)[\,\delta_{1,0} S\langle S_2^- S_3^- S_4^+ S_5^+\rangle + \delta_{2,0} S\langle S_1^- S_3^- S_4^+ S_5^+\rangle$$

$$+ \delta_{3,0} S\langle S_1^- S_2^- S_4^+ S_5^+\rangle - \delta_{1,0}\delta_{3,0}\langle S_2^- S_3^- S_4^+ S_5^+\rangle - \delta_{2,0}\delta_{3,0}\langle S_2^- S_3^- S_4^+ S_5^+\rangle$$

$$- \delta_{1,0}\delta_{3,0}\langle S_1^- S_3^- S_4^+ S_5^+\rangle - \delta_{1,0}\langle S_2^- S_3^- S_0^- S_0^+ S_4^+ S_5^+\rangle - \delta_{2,0}\langle S_1^- S_3^- S_0^- S_0^+ S_4^+ S_5^+\rangle$$

$$- \delta_{3,0}\langle S_1^- S_2^- S_0^- S_0^+ S_4^+ S_5^+\rangle \quad + 2J\sum_\rho [\, G_4(1,2,3,1+\rho,1+\rho,4,5,t)$$

$$- G_4(1+\rho,2,3,1,1,4,5,t) + G_4(1,2,3,2+\rho,2+\rho,4,5,t) - G_4(1,2+\rho,3,2,2,4,5,t)$$

$$G_4(1,2,3,3+\rho,3+\rho,4,5,t) - G_4(1,2,3+\rho,3,3,4,5,t) + G_4(1,2,3,4,4,4+\rho,5,t)$$

$$-G_4(1,2,3,4+\rho,4+\rho,4,5,t) + G_4(1,2,3,5,5,4,5,t) - G_4(1,2,3,5+\rho,5+\rho,4,5,t)\Big]$$

where

$$G_4(1,2,3,4,5,6,7,t) = -i\,\theta(t)\langle[S_1^-(t)\,S_2^-(t)\,S_3^-(t)\,S_4^-(t)\,S_5^+(t)\,S_6^+(t)\,S_7^+(t),\ S_0^+(0)]\rangle \qquad (63)$$

It is clear that by continuing this process an infinite set of coupled differential equations will be generated. In order to determine G_i the Green function G_{i+1} must be known. This set of differential equations is restricted to the case $S=\frac{1}{2}$ since Eq. (54) was used to produce the coupling.

CHAPTER IV

THE FIRST ORDER SOLUTION

The first order results for this problem are obtained by setting $G_i=0$ for $i>1$. Attempts have been made to improve on this solution by expanding the G_2 function in terms of the G_1 function and thus obtaining renormalized results.[9, 13, 14] However, in general this approach is not guaranteed to give results which are consistent with the set of coupled equations. The present work is concerned with a solution of the G_2 equation with $G_3=0$, giving a solution, G_2, which will be used to obtain a second order result for G_1.

Consider first the approximation generated by $G_i=0$ for $i>1$. The G_1 equation then reads

$$\left(i\frac{\partial}{\partial t}+\mu H\right)G_1^{\circ}(j,t)+2JS\sum_{\rho}\left[G_1^{\circ}(j,t)-G_1^{\circ}(j+\rho,t)\right]=-2\langle S^z\rangle\,\delta(t)\,\delta_{j,0} \tag{64}$$

This equation is easily solved by Fourier inversion. Using Eqs. (13) and (30), $G_1(j,t)$ may be expressed by

$$G_1(j,t)=\frac{1}{2\pi N}\sum_{p}\int_{-\infty}^{\infty}G_1(p,\omega)e^{-i\omega t}e^{i\vec{p}\cdot\vec{j}}\,d\omega \tag{65}$$

Then Eq. (64) becomes

$$[\omega+\mu H+2JS(\gamma_0-\gamma_p)]\,G_1^{\circ}(p,\omega)=-2\langle S^z\rangle \tag{66}$$

or

$$G_1^{\circ}(p,\omega) = -\frac{2\langle S^3\rangle}{\omega + \eta H + zJS(\gamma_0 - \gamma_p)} \tag{67}$$

In order to understand this result and the meaning of the poles of G_1^{o}, consider Eq. (47)

$$G_1(j,\omega) = \lim_{\epsilon\to 0^+} Z^{-1}\sum_n\sum_m \frac{\langle C_n|S_0^+(0)|C_m\rangle\langle C_m|S_j^-(0)|C_n\rangle\,(e^{-\beta E_n} - e^{-\beta E_m})}{\omega + E_n - E_m + i\epsilon} \tag{68}$$

where $G_1(j,\omega)$ is the analytic extension of G_1. Then

$$G_1(p,\omega) = \lim_{\epsilon\to 0} \frac{Z^{-1}}{\sqrt{N}}\sum_n\sum_m \frac{\langle C_n|S_0^+(0)|C_m\rangle\langle C_m|S_p^-(0)|C_n\rangle\,(e^{-\beta E_n} - e^{-\beta E_m})}{\omega + E_n - E_m + i\epsilon} \tag{69}$$

where S_p^- is defined by (12).

At low enough temperatures the system should be described by the set of states $\{|0\rangle, |p\rangle\}$. The matrix elements are non-zero only if the states involved differ by one magnon of momentum p. Thus using (14)

$$G_1(p,\omega) = -\frac{2\langle S^3\rangle}{\omega + \eta H + zJS(\gamma_0 - \gamma_p)} \tag{70}$$

which agrees in form with (67). Thus the poles of G_1 give the first order single particle energies for the magnons. It is clear then that the first order Green function theory agrees with Bloch's spinwave theory.

The time dependent correlation functions can be written in terms of $G_1(p,\omega)$ by substituting (65) into Eq. (42).

$$\langle S_j^-(t)\, S_0^+(0)\rangle = \frac{i}{2\pi N}\lim_{\epsilon\to 0}\sum_p\int_{-\infty}^{\infty}\frac{e^{i\vec{p}\cdot\vec{j}}\, e^{-i\omega t}}{1-e^{-\beta\omega}}\left[G_1(p,\omega+i\epsilon) - G_1(p,\omega-i\epsilon)\right]d\omega \tag{71}$$

Using Eqs. (67) and (41) the first order time dependent correlation function is

$$\langle S_j^-(t)\, S_0^+(0)\rangle = \frac{2\langle S^z\rangle}{N}\sum_p \langle n\rangle_p^0\, e^{i\vec{p}\cdot\vec{j}}\, e^{iE_p^0 t} \tag{72}$$

where

$$\langle n\rangle_p^0 = \frac{1}{e^{\beta E_p^0}-1} \tag{73}$$

$$E_p^0 = \mu H + 2JS(\gamma_0-\gamma_p) \tag{74}$$

This result will be needed in later chapters.

CHAPTER V

THE SECOND ORDER CALCULATION

The second order calculation begins with solving for G_2 as given by Eq. (60) with $G_3=0$. That is

$$\left(i\frac{\partial}{\partial t}+\mu H\right)G_2(1,2,3,t) + 2JS\sum_{\rho}\Big[G_2(1,2,3,t)\left[1-2\delta_{2,1+\rho}\right] - G_2(1+\rho,2,3,t)\left[1-2\delta_{1,2}\right] \tag{75}$$

$$- G_2(1,2+\rho,3,t) + G_2(1,2,3+\rho,t)\Big] = -2\delta(t)\left[\delta_{1,0}\, S\langle S_2^- S_3^+\rangle + \delta_{2,0}\, S\langle S_1^- S_3^+\rangle\right.$$

$$\left. - \delta_{1,0}\,\delta_{2,0}\langle S_1^- S_3^+\rangle\right]$$

The four-product terms in the inhomogeneous term on the right hand side of (75) have been dropped in comparison to the two-product terms. This can be done without destroying the property that if 1=2 the total equation reduces to zero as it should, since $S_j^{\pm}\, S_j^{\pm}=0$ for the spin one-half system.

This equation is Fourier inverted to obtain a solution. Using Eq. (13) $G_2(1,2,3,t)$ may be represented by

$$G_2(1,2,3,t) = \frac{1}{2\pi N^3}\sum_{P_1}\sum_{P_2}\sum_{P_3}\int_{-\infty}^{\infty} G_2(P_1,P_2,P_3,\omega)\, e^{-i\omega t}\, e^{i[\vec{P}_1\cdot\vec{j}_1+\vec{P}_2\cdot\vec{j}_2+\vec{P}_3\cdot\vec{j}_3]}\,d\omega \tag{76}$$

Then Eq. (55) becomes

$$[\omega+\mu H+2JS(\gamma_0-\gamma_P)]\,G_1(P,\omega) = -2\langle S^3\rangle + \frac{2J}{N^2}\sum_{P_1}\sum_{P_2} G_2(P_1,P_2,P-P_1-P_2,\omega)\left[\gamma_{P-P_1}-\gamma_{P_2}\right] \tag{77}$$

and (75) becomes

$$[\omega + \mu H + zJS(\gamma_0 - \gamma_{p_1} - \gamma_{p_2} + \gamma_{p_3})]\, G_2(p_1, p_2, p_3, \omega) = -\, S_{p_3}[\, N(\delta_{p_1-p_3} + \tag{78}$$

$$\delta_{p_2-p_3}) - 2\,] + \frac{2J}{N}\sum_{p'} G_2(p', p_1+p_2-p', p_3, \omega)\,[\,\gamma_{p_1-p'} - \gamma_{p'}\,]$$

where

$$S_p = \sum_n \langle s_0^- s_n^+\rangle\, e^{-i\vec{p}\cdot\vec{n}} \tag{79}$$

The Nearest Neighbor Approximation

The solution of (78) for this approximation is obtained in Appendix I. The inversion of this solution, given by equation (I-23), to space-time co-ordinates gives

$$G_2(1,2,3,t) = \langle s_1^- s_3^+\rangle\, G_1(2,t) + \langle s_2^- s_3^+\rangle\, G_1(1,t) + U(1,2,3,t) \tag{80}$$

If the last term in this equation is neglected (80) reduces to the well known Hartree-Fock approximation of the G_2 function. The function U is thus a correction term to the Hartree-Fock terms which hopefully contains the dynamical interactions of the magnons.

The function $G_2(p_1, p_2, p_3, \omega)$ which is to be substituted into the G_1 equation is given by the substitution $p_3 = p - p_1 - p_2$ in (I-23). The result is

$$G_2(p_1, p_2, p-p_1-p_2, \omega) = \Big\{ \frac{(2\pi)^3}{U} S_{p-p_1-p_2}\,[\,\delta(p_1-p) + \delta(p_2-p)\,] + \frac{D_0}{D}\, 4JS\, S_{p-p_1-p_2} \times \tag{81}$$

$$\times\ \frac{\gamma_{p-p_1} + \gamma_{p-p_2} - \gamma_p - \gamma_{p-p_1-p_2}}{\omega + \epsilon^0_{p_1} + \epsilon^0_{p_2} - \epsilon^0_{p-p_1-p_2}} \Big\}\, G_1(p,\omega) + \frac{2\, S_{p-p_1-p_2}}{\omega + \epsilon^0_{p_1} + \epsilon^0_{p_2} - \epsilon^0_{p-p_1-p_2}} + \frac{\frac{4JU}{(2\pi)^3}\,(D_0/D)}{\omega + \epsilon^0_{p_1} + \epsilon^0_{p_2} - \epsilon^0_{p-p_1-p_2}} \times$$

$$\times \int \frac{S_{p-p_1-p_2}\,[\gamma_{p_1-p'} - \gamma_{p'}]}{\omega + E^{o}_{p'} + E^{o}_{p_1+p_2-p'} - E^{o}_{p-p_1-p_2}}\, d^3p' \;-\; \frac{2\langle S_o^- S_o^+\rangle (2\pi)^3}{v(\omega + E_p)} S_{p-p_1-p_2}\,[\delta(p-p_1) + \delta(p-p_2)]$$

Substitution of (81) into (77) and solving for G_1 gives

$$(\omega + E_p)\, G_1(p,\omega) = -2\langle S^3\rangle - \frac{4J\langle S_o^- S_o^+\rangle (\Gamma_o' - \Gamma_p')}{\omega + E_p} + V(p,\omega) \tag{82}$$

where

$$V(p,\omega) = \frac{4Jv^2}{(2\pi)^6} \iint S_{p-p_1-p_2} \frac{\gamma_{p-p_1} - \gamma_{p_2}}{\omega + E^o_{p_1} + E^o_{p_2} - E^o_{p-p_1-p_2}}\, d^3p_1\, d^3p_2 \tag{83}$$

$$+ \frac{(2J)^2 v^3}{(2\pi)^9} \frac{2D_o}{D} \iiint \frac{S_{p-p_1-p_2}\,[\gamma_{p_1-p'} - \gamma_{p'}][\gamma_{p-p_1} - \gamma_{p_2}]}{[\omega + E^o_{p'} + E^o_{p_1+p_2-p'} - E^o_{p-p_1-p_2}][\omega + E^o_{p_1} + E^o_{p_2} - E^o_{p-p_1-p_2}]}\, d^3p'\, d^3p_1\, d^3p_2$$

and the renormalized magnon energy is

$$E_p = \mu H + 2J(\Gamma_o - \Gamma_p) + W(p,\omega) \tag{84}$$

$$W(p,\omega) = \frac{(2J)^2 v^2 D_o}{2(2\pi)^6 D} \iint S_{p-p_1-p_2} \frac{[\gamma_p - \gamma_{p-p_1} - \gamma_{p-p_2} + \gamma_{p-p_1-p_2}][\gamma_{p-p_1} - \gamma_{p_2}]}{\omega + E^o_{p_1} + E^o_{p_2} - E^o_{p-p_1-p_2}}\, d^3p_1\, d^3p_2 \tag{85}$$

$$\Gamma_p' = \frac{v}{(2\pi)^3} \int S_{p'}[\gamma_o - \gamma_p - \gamma_{p'} + \gamma_{p-p'}]\, d^3p' = \sum_f [\langle S_o^- S_o^+\rangle - \langle S_o^- S_f^+\rangle]\, e^{i\vec{p}\cdot\vec{f}} \tag{86}$$

$$\Gamma_p = S(\gamma_o - \gamma_p) - \Gamma_p' = \sum_f [S - \langle S_o^- S_o^+\rangle + \langle S_o^- S_f^+\rangle]\, e^{i\vec{p}\cdot\vec{f}} \tag{87}$$

The analytic continuation of $G_1(p,\omega)$ off the real axis gives

$$[\omega + \mu H + 2J(\Gamma_o - \Gamma_p) + \mathrm{Re}(W(p,\omega)) \pm i\,\tfrac{\tau^{-1}}{2}]\, G_1(p, \omega \pm i\epsilon) = -2\langle S^3\rangle \tag{88}$$

$$- \frac{4J\langle S_o^- S_o^+\rangle (\Gamma_o' - \Gamma_p')}{\omega + \mu H + 2J(\Gamma_o - \Gamma_p) + \mathrm{Re}(W(p,\omega)) \pm i\,\frac{\tau^{-1}}{2}} + V(p, \omega \pm i\epsilon)$$

Re $(W) = P(W(p,\omega))$, where P is the principal value function.

$$\frac{\tau^{-1}(P,\omega)}{2} = -\pi\frac{(2J)^2 v^2 D_0}{2(2\pi)^6 D}\iint S_{P-P_1-P_2}[\gamma_P - \gamma_{P-P_1} - \gamma_{P-P_2} + \gamma_{P-P_1-P_2}][\gamma_{P-P_1} - \gamma_{P_2}] \times \tag{89}$$

$$\times\ \delta(\omega + E^0_{P_1} + E^0_{P_2} - E^0_{P-P_1-P_2})\, d^3P_1\, d^3P_2$$

since

$$\frac{1}{\omega-\omega'+i\epsilon} = P\left(\frac{1}{\omega-\omega'}\right) - \pi i\,\delta(\omega-\omega') \tag{90}$$

The poles of G_1 are given by the equation

$$\omega + \mu H + 2J(\Gamma_0 - \Gamma_P) + \mathrm{Re}\,(W(P,\omega)) \pm \frac{\tau^{-1}(P,\omega)}{2} = 0 \tag{91}$$

The low temperature solution is clearly

$$\omega = -\,\mathcal{E}(P) \mp i\,\frac{\tau^{-1}(P)}{2} \tag{92}$$

$$\mathcal{E}(P) = \mu H + 2J(\Gamma_0 - \Gamma_P) + \textstyle\sum_1(P) \tag{93}$$

$$\textstyle\sum_1(P) = P\left(\frac{(2J)^2 v^2 D_0}{2(2\pi)^6 D}\iint S_{P-P_1-P_2}\frac{[\gamma_P - \gamma_{P-P_1} - \gamma_{P-P_2} + \gamma_{P-P_1-P_2}][\gamma_{P-P_1} - \gamma_{P_2}]}{E^0_{P_1} + E^0_{P_2} - E^0_P - E^0_{P-P_1-P_2}}\, d^3P_1\, d^3P_2\right.$$

$$\frac{\tau^{-1}(P)}{2} = -\pi\frac{(2J)^2 v^2 D_0}{2(2\pi)^6 D}\iint S_{P-P_1-P_2}[\gamma_P - \gamma_{P-P_1} - \gamma_{P-P_2} + \gamma_{P-P_1-P_2}][\gamma_{P-P_1} - \gamma_{P_2}] \times \tag{94}$$

$$\times\ \delta(E^0_{P_1} + E^0_{P_2} - E^0_P - E^0_{P-P_1-P_2})\, d^3P_1\, d^3P_2$$

These results are of a quite general nature.[15] The poles of G_1 have real and imaginary parts. The real part is interpreted as being the renormalized magnon energy $\mathcal{E}(p)$. It is composed of three terms.

$$\mathcal{E}(P) = E^0_P - 2J(\Gamma_0' - \Gamma_P') + \textstyle\sum_1(P) \tag{95}$$

The first term is the first order energy term. The second term is generated by the Hartree-Fock terms in (80), and is called the Hartree-Fock energy correction term. It represents a decrease in the energy of the magnon due to its moving independently through an average potential field, and therefore does not represent an energy correction due to magnon-magnon interactions.

The last term in (95) represents the energy contribution due to magnon-magnon interactions. This term is the average energy gained by a magnon of momentum p as a result of its correlations with all the other magnons in the system.

The function, $\tau^{-1}(p)$, which is twice the imaginary part of the G_1 pole, is the lifetime of the single-particle excited state with momentum p.

The analytic extension of the second order solution for G_1 (p,ω) is then

$$G_1(p,\omega \pm i\epsilon) = -\frac{2\langle S^3\rangle}{\omega + \varepsilon(p) \pm \tau^{-1}/2} - \frac{4J\langle S_0^- S_0^+\rangle(\Gamma_0' - \Gamma_p')}{[\omega + \varepsilon(p) \pm \tau^{-1}/2]^2} + \frac{V(p,\omega \pm i\epsilon)}{\omega + \varepsilon(p) \pm \tau^{-1}/2} \tag{96}$$

The Infinite Range Approximation

The equation for G_2 given by (78) was obtained from (60) by setting $G_3 = 0$ and neglecting the four-product terms. In this approximation it is possible to incorporate these terms without further complicating the problem. To see how this is done consider these four-products as they appear in the G_2 equation of motion.

$$-\delta_{1,0}\langle S_2^- S_0^- S_0^+ S_3^+\rangle - \delta_{2,0}\langle S_1^- S_0^- S_0^+ S_3^+\rangle \tag{97}$$

These terms can be approximated at low temperatures by using

$$\langle S_1^- S_2^- S_3^+ S_4^+\rangle \cong \langle S_2^- S_3^+\rangle\langle S_1^- S_4^+\rangle + \langle S_1^- S_3^+\rangle\langle S_2^- S_4^+\rangle \tag{98}$$

This approximation can be established by using the Hartree-Fock approximation for G_2, given by equation (80) with U=0, and Eq. (43). It will be indicated later that this approximation of G_2 in this problem is valid at low temperatures. Then (97) becomes

$$-\delta_{1,0}\left[\langle S_2^- S_3^+\rangle\langle S_0^- S_0^+\rangle + \langle S_2^- S_0^+\rangle\langle S_0^- S_3^+\rangle\right] \tag{99}$$

$$-\delta_{2,0}\left[\langle S_1^- S_3^+\rangle\langle S_0^- S_0^+\rangle + \langle S_1^- S_0^+\rangle\langle S_0^- S_3^+\rangle\right]$$

At these low temperatures the correlation function $\langle S_g^- S_0^+\rangle$ is given by (72). This result is especially simple here since

$$\gamma_p = \sum_g e^{i\vec{p}\vec{g}} = N\delta_{p,0} - 1 \tag{100}$$

Therefore the first order energy is

$$E_p^0 = \mu H + 2JSN\left[1 - \delta_{p,0}\right] \tag{101}$$

Substitution of this into (72) gives

$$\langle S_0^- S_m^+\rangle = 2\langle S^z\rangle\langle n\rangle\delta_{m,0} \tag{102}$$

for N large, and $\langle n \rangle$ is given by

$$\langle n \rangle = 1/(e^{\beta[\mu H + 2JSN]} - 1) \tag{103}$$

Then the terms (99) become

$$- \delta_{1,0}[\langle S_2^- S_3^+ \rangle \langle S_0^- S_0^+ \rangle + 4\langle S^3 \rangle^2 \delta_{2,0}\delta_{3,0}] \tag{104}$$

$$- \delta_{2,0}[\langle S_1^- S_3^+ \rangle \langle S_0^- S_0^+ \rangle + 4\langle S^3 \rangle^2 \delta_{1,0}\delta_{3,0}]$$

The second term in the $\delta_{1,0}$ term can be put equal to zero since if 2=0 and 3=0 the four-product $\langle S_2^- S_0^- S_0^+ S_3^+ \rangle = 0$, and these terms are absent for that reason. The same is true for $4\langle S^3 \rangle^2 \delta_{1,0}\delta_{3,0}$ in the $\delta_{2,0}$ term. Thus using (104) the G_2 equation equivalent to (78) but with the four-product terms included is

$$[\omega + \mu H + 2JS(1 - \delta_{P_1,0} - \delta_{P_2,0} + \delta_{P_3,0})] G_2(P_1, P_2, P_3, \omega) = -2\langle S^3 \rangle S_{P_3} [N\{ \tag{105}$$

$$\delta_{P_1,-P_3} + \delta_{P_2,-P_3}\} - 2] + 2J\sum_{P'} G_2(P', P_1+P_2-P', P_3, \omega)[\delta_{P',P_1} - \delta_{P'}]$$

or

$$[\omega + \mu H + 2JS(1 - \delta_{P_1,0} - \delta_{P_2,0} + \delta_{P_3,0}) + 4JS] G_2(P_1, P_2, P_3, \omega) - 4JS \times \tag{106}$$

$$\times G_2(0, P_1+P_2, P_3, \omega) = -2\langle S^3 \rangle S_{P_3} [N\{\delta_{P_1,-P_3} + \delta_{P_2,-P_3}\} - 2]$$

Making the substitution of variables

$$P_1 = 0 \quad , \quad P_2 = P_1' + P_2' \tag{107}$$

in (106) and solving for $G_2(0, P_1'+P_2', P_3, \omega)$, the solution of (106) is then

$$G_2(p_1,p_2,p_3,\omega) = -\frac{2\langle S^3\rangle N\delta_{p_2-p_3}\, S_{p_3}}{\omega+\mu H+2JSN[1-\delta_{p_1,0}]+4JS} - \frac{2\langle S^3\rangle N\delta_{p_1-p_3}\, S_{p_3}}{\omega+\mu H+2JSN[1-\delta_{p_2,0}]+4JS} \tag{108}$$

$$+\frac{2\, S_{p_3}}{\omega+\mu H+2JSN[1-\delta_{p_1,0}-\delta_{p_2,0}+\delta_{p_3,0}]} - \frac{4JS\, S_{p_3}}{\omega+\mu H+2JSN[1-\delta_{p_1,0}-\delta_{p_2,0}+\delta_{p_3,0}]+4JS} \times$$

$$\times\left\{\frac{N\delta_{p_3,0}}{\omega+\mu H+2JSN[1-\delta_{p_1+p_2,0}]} + \frac{N\delta_{p_1+p_2+p_3,0}}{\omega+\mu H} - \frac{2}{\omega+\mu H+2JSN[\delta_{p_3,0}-\delta_{p_1+p_2,0}]}\right\}$$

In the limit

$$N\to\infty \qquad J\to 0 \qquad NJ = \text{constant} \tag{109}$$

it is clear that the first two terms on the right hand side of (108) can be written in terms of G_1 functions. The replacement of these G_1 functions by G_1 follows from the same argument that was used in the nearest neighbor approximation.

Substitution of these results into the G_1 equation gives, in the limit $N\to\infty$, $J\to 0$, and NJ=constant

$$\{\omega+\mu H+2JSN[1-\delta_{p,0}]\}\, G_1(p,\omega) = -2\langle S^3\rangle + 2\langle S_0^- S_0^+\rangle NJ[1-\delta_{p,0}]\, G_1(p,\omega) \tag{110}$$

or

$$\{\omega+\mu H+2JN\langle S^3\rangle[1-\delta_{p,0}]\}\, G_1(p,\omega) = -2\langle S^3\rangle \tag{111}$$

since $S-\langle S_0^- S_0^+\rangle = \langle S^3\rangle$.

Here again the energy has been renormalized by the Hartree-Fock terms in the G_2 equation. The energy is a

Hartree-Fock energy correction and therefore contains no interaction terms which, indeed, should be the case for the infinite range interaction.

The G_3 Termination

From an examination of the G_2 calculation it appears that to first order (low temperatures) an expansion of G_i in terms of G_{i-1} is possible. The expansion is determined by the inhomogeneous terms in the $\delta(t)$ term of the G_i equation. The approximation of G_3 functions in terms of G_2 functions can be carried out in this manner.

First of all the four-product terms in the G_3 equation are approximated using (98). Neglecting the G_4 terms, the six-products, and the sum over the G_3 functions Eq. (62) becomes

$$\left(i\frac{\partial}{\partial t}+\mu H\right) G_3(1,2,3,4,5,t) \cong -2\,\delta(t)\Big\{ \delta_{1,0}\, S\left[\langle S_2^- S_4^+\rangle\langle S_3^- S_5^+\rangle + \langle S_2^- S_5^+\rangle\langle S_3^- S_4^+\rangle\right] \tag{112}$$

$$+\,\delta_{2,0}\, S\left[\langle S_1^- S_4^+\rangle\langle S_3^- S_5^+\rangle + \langle S_1^- S_5^+\rangle\langle S_3^- S_4^+\rangle\right] + \delta_{3,0}\, S\left[\langle S_1^- S_4^+\rangle\langle S_2^- S_5^+\rangle + \langle S_2^- S_4^+\rangle\langle S_1^- S_5^+\rangle\right]$$

$$-\,\delta_{1,0}\delta_{3,0}\langle S_2^- S_3^- S_4^+ S_5^+\rangle - \delta_{2,0}\delta_{1,0}\langle S_2^- S_3^- S_4^+ S_5^+\rangle - \delta_{2,0}\delta_{3,0}\langle S_1^- S_3^- S_4^+ S_5^+\rangle \Big\}$$

Fourier inversion of this equation gives

$$\left[\omega+\mu H+2JS(\gamma_0-\gamma_{P_1}-\gamma_{P_2}-\gamma_{P_3}+\gamma_{P_4}+\gamma_{P_5})\right] G_3(P_1,P_2,P_3,P_4,P_5,\omega) = -2SN\Big\{ S_{P_1} S_{P_3} \times \tag{113}$$

$$\times\left[\delta_{P_1+P_4}\delta_{P_3+P_5} + \delta_{P_1+P_5}\delta_{P_3+P_4}\right] + S_{P_2} S_{P_3}\left[\delta_{P_2+P_4}\delta_{P_3+P_5} + \delta_{P_3+P_4}\delta_{P_2+P_5}\right]$$

$$+\, S_{P_1} S_{P_2}\left[+\delta_{P_2+P_4}\delta_{P_1+P_5} + \delta_{P_1+P_4}\delta_{P_2+P_5}\right]\Big\}$$

where the last three terms in (112) have been dropped since they do not give rise to G_1 functions. Solving for G_3 gives

$$G_3(p_1,p_2,p_3,p_4,p_5,\omega) \cong -\frac{2SN\,S_{p_1}S_{p_2}[\delta_{p_2+p_4}\delta_{p_1+p_5}+\delta_{p_1+p_4}\delta_{p_2+p_5}]}{\omega+4H+2JS[\gamma_0-\gamma_{p_3}]} \tag{114}$$

$$-\frac{2SN\,S_{p_1}S_{p_3}[\delta_{p_1+p_4}\delta_{p_3+p_5}+\delta_{p_1+p_5}\delta_{p_3+p_4}]}{\omega+4H+2JS[\gamma_0-\gamma_{p_2}]}-\frac{2SN\,S_{p_2}S_{p_3}[\delta_{p_2+p_4}\delta_{p_3+p_5}+\delta_{p_3+p_4}\delta_{p_2+p_5}]}{\omega+4H+2JS[\gamma_0-\gamma_{p_1}]}$$

$$\cong N S_{p_1}S_{p_3}[\delta_{p_1+p_4}\delta_{p_3+p_5}+\delta_{p_3+p_4}\delta_{p_1+p_5}]\,G_1^{\circ}(p_2,\omega) \tag{115}$$

$$+N S_{p_2}S_{p_3}[\delta_{p_2+p_4}\delta_{p_3+p_5}+\delta_{p_3+p_4}\delta_{p_2+p_5}]\,G_1^{\circ}(p_1,\omega)$$

$$+N S_{p_1}S_{p_2}[\delta_{p_2+p_4}\delta_{p_1+p_5}+\delta_{p_1+p_4}\delta_{p_2+p_5}]\,G_1^{\circ}(p_3,\omega)$$

The G_1° functions now are replaced by G_1 functions and (115) is Fourier inverted to space-time co-ordinates giving

$$G_3(1,2,3,4,5,t) \cong G_1(2,t)[\langle S_1^-S_4^+\rangle\langle S_3^-S_5^+\rangle+\langle S_3^-S_4^+\rangle\langle S_1^-S_5^+\rangle] \tag{116}$$

$$+G_1(1,t)[\langle S_2^-S_4^+\rangle\langle S_3^-S_5^+\rangle+\langle S_3^-S_4^+\rangle\langle S_2^-S_5^+\rangle]$$

$$+G_1(3,t)[\langle S_1^-S_4^+\rangle\langle S_2^-S_5^+\rangle+\langle S_2^-S_4^+\rangle\langle S_1^-S_5^+\rangle]$$

or using the Hartree-Fock expansion of G_2 in terms of G_1

$$G_3(1,2,3,4,5,t) \cong \langle S_1^-S_4^+\rangle G_2(2,3,5,t)+\langle S_2^-S_4^+\rangle G_2(1,3,5,t) \tag{117}$$

$$+\langle S_3^-S_4^+\rangle G_2(1,2,5,t)$$

Substitution of (117) into (60), Fourier inverting to momentum space, and regrouping the terms gives a renormalized coefficient for G_2. The coefficient now reads

$$\{\omega + [4H + 2J(\Gamma_0 - \Gamma_{P_1})] + [4H + 2J[\Gamma_0 - \Gamma_{P_2}]] - [4H + 2J(\Gamma_0 - \Gamma_{P_3})]\} G_2(P_1, P_2, P_3, \omega) \qquad (118)$$

Therefore the replacement of E_p^0 by E_p in the G_2 equation (I-17) seems to be consistent with the effect that the G_3 functions have on this equation. The proof is not complete, however, since the energies in (118) and E_p differ by the function $W(P,\omega)$. This was the magnon-magnon interaction term and it was generated by a detailed solution of the G_2 equation. Such a term would enter the renormalized G_2 coefficient if a more detailed representation of G_3 were made in this equation.

CHAPTER VI

THE CORRELATION FUNCTIONS AND MAGNETIZATION

The Nearest Neighbor Approximation

The correlation function $\langle S_n^-(t) S_0^+(0)\rangle$ can be calculated from the knowledge of the Fourier transform of the G_1 function. Substitution of equation (65) into (42) gives (in the limit $N \to \infty$)

$$\langle S_n^-(t) S_0^+(0)\rangle = \lim_{\epsilon\to 0^+} \frac{i v}{(2\pi)^4}\int d^3p \int_{-\infty}^{\infty} d\omega \; \frac{e^{i\vec{p}\cdot\vec{n}}\, e^{-i\omega t}}{1-e^{-\beta\omega}} \left[G_1(p,\omega+i\epsilon) - G_1(p,\omega-i\epsilon)\right] \tag{119}$$

Using equation (96)

$$G_1(p,\omega+i\epsilon) - G_1(p,\omega-i\epsilon) = -\frac{2\langle S^3\rangle}{\omega+E_p^+} + \frac{2\langle S^3\rangle}{\omega+E_p^-} \tag{120}$$

$$-\frac{4J\langle S_0^- S_0^+\rangle(\Gamma_0'-\Gamma_p')}{[\omega+E_p^+]^2} + \frac{4J\langle S_0^- S_0^+\rangle(\Gamma_0'-\Gamma_p')}{[\omega+E_p^-]^2}$$

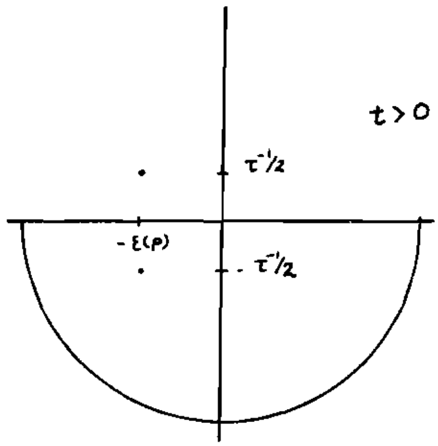
$$+\frac{4Jv^2}{(2\pi)^6}\iint S_{p-p_1-p_2}\,\frac{\gamma_{p-p_1}-\gamma_{p_2}}{[\omega+E_{p_1}^0+E_{p_2}^0-E_{p-p_1-p_2}^0+i\epsilon][\omega+E_p^+]}\,d^3p_1\,d^3p_2$$

$$-\frac{4Jv^2}{(2\pi)^6}\iint S_{p-p_1-p_2}\,\frac{\gamma_{p-p_1}-\gamma_{p_2}}{[\omega+E_{p_1}^0+E_{p_2}^0-E_{p-p_1-p_2}^0-i\epsilon][\omega+E_p^-]}\,d^3p_1\,d^3p_2$$

where the notation $E_p^\pm$ has been used to represent

$$E_p^\pm = \varepsilon(p) \pm \tau^{-1}(p)/2 \tag{121}$$

In order to evaluate (119), ω is extended to a complex variable. The contour chosen for $t>0$ is one which is closed in the lower half complex ω plane.



If $t<0$, the contour is closed in the upper half plane. In either case the contribution to the integral from the semicircles is zero. Therefore substitution of (120) into (119) gives

$$\langle S_m^-(t)\, S_0^+(0)\rangle = \frac{2\langle S^z\rangle v}{(2\pi)^3}\int \langle n\rangle_p\, e^{i\vec{p}\cdot\vec{m}}\, e^{-\frac{\tau^{-1}}{2}|t|}\, e^{i\varepsilon(p)t}\, d^3p \tag{122}$$

$$+\ \frac{4J^2\langle S_0^- S_0^+\rangle \beta v}{(2\pi)^3 J}\int \langle n\rangle_p^2\,(\Gamma_0'-\Gamma_p')\, e^{\beta\varepsilon(p)}\, e^{i\vec{p}\cdot\vec{m}}\, e^{-\frac{\tau^{-1}}{2}|t|}\, e^{i\varepsilon(p)t}\, d^3p$$

$$-\ \frac{4v^3}{(2\pi)^9}\iiint \frac{S_{p-p_1-p_2}\,[\gamma_{p-p_1}-\gamma_{p_1}]}{\gamma_p-\gamma_{p_1}-\gamma_{p_2}+\gamma_{p-p_1-p_2}}\, e^{i\vec{p}\cdot\vec{m}}\Big[\langle n\rangle_p\, e^{i\varepsilon(p)t}\, e^{-\frac{\tau^{-1}}{2}|t|} - \langle n\rangle_{p,p_1,p_2}\, e^{i(\varepsilon^0_{p_1}+\varepsilon^0_{p_2}-\varepsilon^0_{p-p_1-p_2})t}\Big]\, d^3p_1\, d^3p_2\, d^3p$$

$$\langle n\rangle_p = 1/(e^{\beta\varepsilon(p)}-1) \tag{123}$$

$$\langle n\rangle_{p,p_1,p_2} = 1/(e^{\beta[\varepsilon^0_{p_1}+\varepsilon^0_{p_2}-\varepsilon^0_{p-p_1-p_2}]}-1) \tag{124}$$

The second term in the definition of V, equation (83), has been dropped since it will give rise to higher order terms than those contributed by the first term.

The first term on the right hand side of (122) is just the second order correction to the similar term in the first order result (Eq. (72)). The second term represents a correction term due to the introduction of the G_1 functions into the G_2 equation. This term can be simplified by making the replacement

$$e^{\beta \varepsilon(p)} = \frac{1}{\langle n\rangle_p} + 1 \qquad (125)$$

Then the second term in (122) reads

$$\frac{4J\beta v}{(2\pi)^3}\int [\langle n\rangle_p + \langle n\rangle_p^2][\Gamma_0' - \Gamma_p'] e^{i\vec{p}\cdot\vec{m}} e^{-\frac{\Sigma}{2}^{-1}|t|} e^{i\varepsilon(p)t}\, d^3p \qquad (126)$$

The last term in (122) is generated by the term $\delta_{1,0}\delta_{2,0}\times$ $\times\langle S_1^- S_3^+\rangle$ in the G_2 equation, which guarantees the exact solution of this equation to be zero if 1=2, as it should be. This term is a sum of two terms, the first involving $\langle n\rangle_p$, the other $\langle n\rangle_{p,p_1,p_2}$. Making the substitution $p_2 = p_4 + p - p_1$, expanding the integrand for small p_a and p, and using Eq. (79) in the first of these terms gives,

$$-\frac{2v^2}{(2\pi)^6}\langle S_0^- S_0^+\rangle \iint \langle n\rangle_p \frac{\gamma_{p-p_1} - \gamma_{p_1}}{\gamma_0 - \gamma_{p_1}} e^{i\vec{p}\cdot\vec{m}} e^{-\frac{\Sigma}{2}^{-1}|t|} e^{i\varepsilon(p)t}\, d^3p_1\, d^3p \qquad (127)$$

Now

$$\frac{v}{(2\pi)^3}\int \frac{\gamma_{p-p_1} - \gamma_{p_1}}{\gamma_0 - \gamma_{p_1}}\, d^3p_1 = \frac{\gamma_0 - \gamma_p}{\gamma_0}\, Q_0 \qquad (128)$$

where a_o is defined in terms of the Watson integrals.

$$a_o = \frac{v}{(2\pi)^3}\int \frac{\gamma_{p_1}}{\gamma_o - \gamma_{p_1}}\, d^3p_1 = \frac{v}{(2\pi)^3}\int \frac{\gamma_o}{\gamma_o - \gamma_{p_1}}\, d^3p_1 - 1 \tag{129}$$

Then (127) becomes

$$-\frac{2 v a_o \langle S_o^- S_o^+\rangle}{\gamma_o}\int \langle n\rangle_p [\gamma_o - \gamma_p]\, e^{i\vec{p}\cdot\vec{m}}\, e^{-\xi^{-1}|t|}\, e^{i\varepsilon(p)t}\, d^3p \tag{130}$$

The second term in the last term in (122) reads

$$\frac{4v^3}{(2\pi)^9}\iiint S_{p-p_1-p_2}\,\frac{[\gamma_{p-p_1} - \gamma_{p_1}]\, e^{i\vec{p}\cdot\vec{m}}}{\gamma_p - \gamma_{p_1} - \gamma_{p_2} + \gamma_{p-p_1-p_2}}\,\langle n\rangle_{p,p_1,p_2}\, e^{i[E^o_{p_1} + E^o_{p_2} - E^o_{p-p_1-p_2}]t}\, d^3p_1\, d^3p_2\, d^3p \tag{131}$$

This term, as it stands, diverges in the limit $H \to 0$. In order to get around this divergence $\langle n\rangle_{p,p_1,p_2}$ is approximated by

$$\langle n\rangle_{p,p_1,p_2} \cong e^{-\beta E^o_{p_1}}\, e^{-\beta E^o_{p_2}}\, e^{\beta E^o_{p-p_1-p_2}} \cong \langle n\rangle^o_{p_1}\,\langle n\rangle^o_{p_2}\, e^{\beta E_{p-p_1-p_2}} \qquad (H \neq 0) \tag{132}$$

and $S_{p-p_1-p_2}$ is approximated by

$$S_{p-p_1-p_2} \cong \langle n\rangle^o_{p-p_1-p_2} \cong e^{-\beta E^o_{p-p_1-p_2}} \qquad (H \neq 0) \tag{133}$$

Using (132) and (133), and expanding the remainder of the integrand in (131) for small p_1 and p_2, (131) becomes

$$\frac{2v^3}{(2\pi)^9}\iiint \langle n\rangle^o_{p_1}\,\langle n\rangle^o_{p_2}\, e^{i\vec{p}\cdot\vec{m}}\, e^{i[E^o_{p_1} + E^o_{p_2} - E^o_{p-p_1-p_2}]t}\, d^3p_1\, d^3p_2\, d^3p \tag{134}$$

It is clear that this is the only term in the equation for the time-dependent correlation function which does not contain a damping factor, $e^{-\alpha|t|}$. This kind of a factor would come from an inclusion of the G_3 functions into the theory.

Using (126), (130), and (134) Eq. (122) becomes

$$\langle S_{\ell}^{-}(t)\,S_{0}^{+}(0)\rangle = \frac{v}{(2\pi)^3}\left[1-2\langle S_0^- S_0^+\rangle\right]\int \langle n\rangle_p\, e^{i\vec{p}\cdot\vec{\ell}}\, e^{-\Gamma_p^{-1}|t|}\, e^{i\epsilon(p)t}\, d^3p \tag{135}$$

$$+\frac{4J\beta\langle S_0^- S_0^+\rangle v}{(2\pi)^3}\int\left[\langle n\rangle_p+\langle n\rangle_p^2\right] e^{i\vec{p}\cdot\vec{\ell}}\left[\Gamma_0'-\Gamma_p'\right] e^{-\Gamma_p^{-1}|t|}\, e^{i\epsilon(p)t}\, d^3p$$

$$+\frac{2v}{(2\pi)^3}\iiint \langle n\rangle_{p_1}^{0}\,\langle n\rangle_{p_2}^{0}\, e^{i\vec{p}\cdot\vec{\ell}}\, e^{i\left[\epsilon_{p_1}^{0}+\epsilon_{p_2}^{0}-\epsilon_{p-p_1-p_2}^{0}\right]t}\, d^3p_1\, d^3p_2\, d^3p$$

$$+\frac{2v\langle S_0^- S_0^+\rangle a_0}{(2\pi)^3\gamma_0}\int \langle n\rangle_p\left[\gamma_0-\gamma_p\right] e^{-\Gamma_p^{-1}|t|}\, e^{i\epsilon(p)t}\, e^{i\vec{p}\cdot\vec{\ell}}\, d^3p$$

where $\langle S^3\rangle$ has been replaced by $S-\langle S_0^- S_0^+\rangle$.

The time-independent correlation function is then given by

$$\langle S_{\ell}^{-}(0)\,S_0^{+}(0)\rangle = \langle S_{\ell}^{-}(t)\,S_0^{+}(t)\rangle = \left[1-2\langle S_0^- S_0^+\rangle\right]\frac{v}{(2\pi)^3}\int \langle n\rangle_p\, e^{i\vec{p}\cdot\vec{\ell}}\, d^3p \tag{136}$$

$$+\frac{4J\beta\langle S_0^- S_0^+\rangle v}{(2\pi)^3}\int\left[\langle n\rangle_p+\langle n\rangle_p^2\right]\left[\Gamma_0'-\Gamma_p'\right] e^{i\vec{p}\cdot\vec{\ell}}\, d^3p$$

$$+\,2\left[\frac{v}{(2\pi)^3}\int \langle n\rangle_{p_1}^{0}\, d^3p_1\right]^2\delta_{\ell,0}+\frac{2\langle S_0^- S_0^+\rangle a_0 v}{(2\pi)^3\gamma_0}\int \langle n\rangle_p\left(\gamma_0-\gamma_p\right) e^{i\vec{p}\cdot\vec{\ell}}\, d^3p$$

Putting $\ell=0$ and solving for $\langle S_0^- S_0^+\rangle$, the leading terms are

$$\langle S_0^-(0)\,S_0^+(0)\rangle = 2\langle S^3\rangle\,\eta_0(\theta)\left[1+\frac{2a_0}{\gamma_0}\eta_1(\theta)+\eta_2(\theta)\right]+2\left(\eta_0^{0}(\theta)\right)^2\left[1+\frac{2a_0}{\gamma_0}\eta_1(\theta)\right] \tag{137}$$

$$\eta_0^{0}(\theta) = \frac{v}{(2\pi)^3}\int \langle n\rangle_p^{0}\, d^3p \quad ; \quad \theta = k_B T/J \tag{138}$$

$$\eta_0(\theta) = \frac{v}{(2\pi)^3}\int \langle n\rangle_p\, d^3p \tag{139}$$

$$\eta_1(\theta) = \frac{v}{(2\pi)^3} \int \langle n \rangle_p [\gamma_0 - \gamma_p] \, d^3p \tag{140}$$

$$\eta_2(\theta) = \frac{4v}{(2\pi)^3 \theta} \int [\langle n \rangle_p + \langle n \rangle_p^2][\Gamma_0' - \Gamma_p'] \, d^3p \tag{141}$$

Substitution of (137) into (135) gives the second order result for the time-dependent correlation function in terms of integrals over the boson distribution functions $\langle n \rangle_p$ and $\langle n \rangle_p^o$.

The magnetization per spin, M, is defined by

$$M = \frac{\langle S^3 \rangle}{S} = 1 - 2 \langle S_0^- S_0^+ \rangle \qquad (S=\tfrac{1}{2}) \tag{142}$$

Substituting (137) into (142) and solving for M, the leading terms are

$$M = 1 - 2\eta_0(\theta)\left[1 + \frac{2a_0}{\gamma_0}\eta_1(\theta) + \eta_2(\theta)\right] - 4\left[(\eta_0^o(\theta))^2 - (\eta_0(\theta))^2\right] \tag{143}$$

$$+ \frac{16a_0}{\gamma_0}\eta_1(\theta)\left[(\eta_0(\theta))^2 - (\eta_0^o(\theta))^2\right]$$

In order to evaluate M the renormalized energies $\varepsilon(p)$ must be known. These energies are functions of the S_p functions, given by Eq. (79). Using Eqs. (79) and (136),

$$S_p = 2\langle S^3 \rangle \langle n \rangle_p + 2\left(\eta_0^o(\theta)\right)^2 + \frac{2a_0}{\gamma_0}\eta_0(\theta)\langle n \rangle_p [\gamma_0 - \gamma_p] \tag{144}$$

$$+ \text{ higher order terms}$$

Then

$$\varepsilon(p) = E_p^o - 2J\frac{[\gamma_0 - \gamma_p]\,v}{\gamma_0 (2\pi)^3}\int S_p [\gamma_0 - \gamma_p] \, d^3p + \Sigma(p) \tag{145}$$

$$\cong E_p^o - 4J\langle S^3 \rangle \frac{\gamma_0 - \gamma_p}{\gamma_0}\eta_1(\theta) - 4J[\gamma_0 - \gamma_p](\eta_0^o(\theta))^2 + \Sigma(p) \tag{146}$$

Substitution of $\Sigma(p)$ given by (II-15) into (146) gives

$$\varepsilon(p) = E_p^o - 4J\langle S^3\rangle \frac{\gamma_o-\gamma_p}{\gamma_o}\eta_1(\theta) - \frac{8J\langle S^3\rangle A_o D_o}{\gamma_o D}\eta_1(\theta)\, p^2 + O(\theta^3) \qquad (147)$$

Using (147) the eta functions become, to order θ^4

$$\eta_o^o(\theta) = \zeta(\tfrac{3}{2})\left(\frac{3\theta}{2\pi\gamma_o\nu}\right)^{3/2} + \tfrac{3}{4}\pi\nu\zeta(\tfrac{5}{2})\left(\frac{3\theta}{2\pi\gamma_o\nu}\right)^{5/2} + \pi^2\omega_o^2\nu^2\zeta(\tfrac{7}{2})\left(\frac{3\theta}{2\pi\gamma_o\nu}\right)^{\frac{7}{2}} \qquad (148)$$

$$\eta_o(\theta) = \zeta(\tfrac{3}{2})\left(\frac{3\theta f(\theta)}{2\pi\gamma_o\nu}\right)^{3/2} + \tfrac{3}{4}\pi\nu\zeta(\tfrac{5}{2})\left(\frac{3\theta}{2\pi\gamma_o\nu}\right)^{5/2} + \pi^2\omega_o^2\nu^2\zeta(\tfrac{7}{2})\left(\frac{3\theta}{2\pi\gamma_o\nu}\right)^{\frac{7}{2}} \qquad (149)$$

$$\eta_1(\theta) = \gamma_o\pi\nu\zeta(\tfrac{5}{2})\left(\frac{3\theta}{2\pi\gamma_o\nu}\right)^{5/2} + \tfrac{5}{4}\gamma_o\pi^2\omega_o^2\nu^2\zeta(\tfrac{7}{2})\left(\frac{3\theta}{2\pi\gamma_o\nu}\right)^{\frac{7}{2}} \qquad (150)$$

$$\eta_2(\theta) = 4\gamma_o\pi^2\nu^2\zeta(\tfrac{5}{2})^2\left(\frac{3}{2\pi\gamma_o\nu}\right)^5\theta^4 \qquad (151)$$

where

$$f^{-1}(\theta) = 1 - \frac{4\langle S^3\rangle}{\gamma_o}\eta_1(\theta)\left[1 + 2A_oD_o/D\right] + O(\theta^3) \qquad (152)$$

and the constants ω_o^2, $\zeta(x)$, and ν are given in Appendix III. Using (150) and (152), $\eta_o(\theta)$ becomes, to order θ^4

$$\eta_o(\theta) = \zeta(\tfrac{3}{2})\left(\frac{3\theta}{2\pi\gamma_o\nu}\right)^{3/2} + \tfrac{3}{4}\pi\nu\zeta(\tfrac{5}{2})\left(\frac{3\theta}{2\pi\gamma_o\nu}\right)^{\frac{5}{2}} + \pi^2\omega_o^2\nu^2\zeta(\tfrac{7}{2})\left(\frac{3\theta}{2\pi\gamma_o\nu}\right)^{\frac{7}{2}} \qquad (153)$$

$$+ 3\pi\nu\zeta(\tfrac{3}{2})\zeta(\tfrac{5}{2})\left[1 + 2A_oD_o/D\right]\left(\frac{3\theta}{2\pi\gamma_o\nu}\right)^4$$

Substitution of the eta functions into (143) gives

$$M = 1 - 2\zeta(\tfrac{3}{2})\left(\frac{3\theta}{2\pi\gamma_o\nu}\right)^{3/2} - \tfrac{3}{2}\pi\nu\zeta(\tfrac{5}{2})\left(\frac{3\theta}{2\pi\gamma_o\nu}\right)^{5/2} - \qquad (154)$$

$$(+)\,2\pi^2\omega_o^2\nu^2\zeta(\tfrac{7}{2})\left(\frac{3\theta}{2\pi\gamma_o\nu}\right)^{7/2} - 6\pi\nu Q\zeta(\tfrac{3}{2})\zeta(\tfrac{5}{2})\left(\frac{3\theta}{2\pi\gamma_o\nu}\right)^4$$

where

$$Q = 1 + 2A_oD_o/D + 2a_o/3 \qquad (155)$$

For the simple cubic lattice (See Appendix III)

$$a_0 = .5162 \tag{156}$$
$$A_0 = .140$$
$$D_0/D = 1.20$$

and therefore

$$Q = 1.680 \tag{157}$$

which is the exact result obtained by Dyson. For the other cubic lattices the agreement should also be exact since this was found to be the case for the simple cubic lattice. The values given by Dyson for Q can therefore be used to calculate the middle term in (155). That is

$$2A_0D_0/D = Q - 1 - 2a_0/3 = C_0 \tag{158}$$

where

$$Q = \begin{cases} 1.68 & \text{s.c.} \\ 1.35 & \text{f.c.c.} \\ 1.45 & \text{b.c.c.} \end{cases} \tag{159}$$

are Dyson's values for Q. The values of C_0 are important because they appear in the proportionality constant in the magnon-magnon interaction energy.

The anomalous T^3 term which is present in the first order theory has been canceled out in the second order result. The cancellation can be seen in the third term of Eq. (143).

$$4\left[(\eta_0^{\circ}(\theta))^2 - (\eta_0(\theta))^2\right] \cong 4\left[\zeta(\tfrac{3}{2})^2\left(\frac{3\theta}{2\pi\gamma_0\nu}\right)^3 + \tfrac{3}{2}\pi\nu\,\zeta(\tfrac{3}{2})\,\zeta(\tfrac{5}{2})\left(\frac{3\theta}{2\pi\gamma_0\nu}\right)^4 + \cdots\right] \tag{160}$$

$$- 4 \left[\zeta\left(\tfrac{3}{2}\right)^2 \left(\frac{3\theta}{2\pi\delta_0\nu}\right)^3 + \tfrac{3}{2}\pi\nu\,\zeta\left(\tfrac{3}{2}\right)\zeta\left(\tfrac{5}{2}\right)\left(\frac{3\theta}{2\pi\delta_0\nu}\right)^4 + \cdots \right]$$

It is also noted that the T^4 terms contributed by these terms exactly cancel.

The Infinite Range Approximation

The solution of the G_1 equation in the limit $N \to \infty$, $J \to 0$, such that NJ=constant, in the second order theory is very simple.

$$G_1(\rho, \omega) = - \frac{2\langle S^z \rangle}{\omega + \mu H + 2JN\langle S^z \rangle [1 - \delta_{\rho,0}]} \tag{161}$$

The time-dependent correlation function is obtained by substituting (161) into (42) giving

$$\langle S_n^-(t)\, S_0^+(0) \rangle = 2\langle S^z \rangle \langle n \rangle\, \delta_{n,0}\, e^{i[\mu H + \varepsilon_0]t} \qquad ; \quad H = 0 \tag{162}$$

$$\langle n \rangle = \frac{1}{e^{2\beta\varepsilon_0\langle S^z \rangle} - 1} \tag{163}$$

$$\varepsilon_0 = NJ \tag{164}$$

The magnetization defined by

$$M = \frac{\langle S^z \rangle}{S} = 1 - 2\langle S_0^- S_0^+ \rangle \tag{165}$$

is obtained from the time-independent correlation function $\langle S_0^- S_0^+ \rangle$. Using (162)

$$\langle S_0^- S_0^+ \rangle = 2\langle S^z \rangle \langle n \rangle \tag{166}$$

Then

$$\frac{\langle S^3 \rangle}{S} = 1 - \frac{2}{S}\langle S^3 \rangle \langle n \rangle \tag{167}$$

Solving (167) for M gives

$$M = 1/(1 + 2\langle n \rangle) \tag{168}$$

$$\langle n \rangle = 1/(e^{\beta \varepsilon_0 M} - 1) \tag{169}$$

Substitution of (169) into (168) and solving for M gives

$$M \varepsilon_0 \beta = \ln\left(\frac{1+M}{1-M}\right) \tag{170}$$

which is the exact result given by Kittel and Shore.[4]

It is not too suprising that this is the case since the second order result for G_1 given by (161) can be obtained by a simple Hartree-Fock termination of the G_2 functions in the G_1 equation. That is

$$G_2(1,2,3,t) = \langle S_1^- S_3^+ \rangle G_1(2,t) + \langle S_2^- S_3^+ \rangle G_1(1,t) \tag{171}$$

Substitution of this into the G_1 equation, using the result $\langle S_0^- S_n^+ \rangle = 0$ for $n \neq 0$, and Fourier inversion of the result gives exactly the G_1 function (161). Since this is an infinite range interaction problem the Hartree-Fock should give very good results and, indeed, it gives the exact result.

If no attempt had been made to write the G_2 results in terms of the $\dot{G}_1$, and hence the G_1 functions, the result (170) would not have been obtained. In this case substitution of (108) into (77) and taking the prescribed limits gives

$$(\omega+\varepsilon_o)G_1(P,\omega) = -2\langle S^3\rangle - 2\langle S^3\rangle \frac{\langle S_o^- S_o^+\rangle}{\omega+\varepsilon_o} \quad ; \quad H=0 \tag{172}$$

Substitution of this result into (42) gives

$$\langle S_o^- S_o^+\rangle = 2\langle S^3\rangle\langle n\rangle^o + 2\,\varepsilon_o\beta\langle S^3\rangle\langle S_o^- S_o^+\rangle[\langle n\rangle^o]^2 e^{\beta\varepsilon_o} \tag{173}$$

$$\langle n\rangle^o = 1/(e^{\beta\varepsilon_o}-1) \tag{174}$$

Solving (174) for $e^{\beta\varepsilon_o}$ and substituting this result into (173) gives

$$\langle S_o^- S_o^+\rangle = 2\langle S^3\rangle\langle n\rangle + 2\langle S_o^- S_o^+\rangle\beta\varepsilon_o[\langle n\rangle^o + [\langle n\rangle^o]^2] \tag{175}$$

or

$$\langle S_o^- S_o^+\rangle = \frac{2\langle S^3\rangle\langle n\rangle^o}{1-2\beta\varepsilon_o[\langle n\rangle^o + (\langle n\rangle^o)^2]} \tag{176}$$

Then M is obtained by the substitution of (176) into (165).

$$M = 1 - \frac{2M\langle n\rangle^o}{1-2\beta\varepsilon_o[\langle n\rangle^o + (\langle n\rangle^o)^2]} \tag{177}$$

or

$$M = 1\Big/\left(1 + \frac{2\langle n\rangle^o}{1-2\beta\varepsilon_o[\langle n\rangle^o + (\langle n\rangle^o)^2]}\right) \tag{178}$$

which is not the same result as that given by (170). However, this result does agree with (170) in the limit of very low temperatures. As the temperature increases (178) will differ drastically from the exact solution (170). See Figure 4.

CHAPTER VII

GENERAL RESULTS

Renormalized Magnon Energies

The second order calculation has produced a renormalization of the first order magnon energy

$$E_p^0 = \mu H + 2JS[\gamma_0 - \gamma_p] \tag{179}$$

in terms of temperature-dependent corrections. The second order energy expression at low temperatures is given by

$$\begin{aligned} \varepsilon(p) = \mu H + 2JS[\gamma_0 - \gamma_p] - 2J[\Gamma_0' - \Gamma_p'] \\ + P\left(\frac{2JD_0 v^2}{D(2\pi)^6} \iint S_{p-p_1-p_2} \frac{[\gamma_p - \gamma_{p-p_1} - \gamma_{p-p_2} + \gamma_{p-p_1-p_2}][\gamma_{p-p_1} - \gamma_{p_2}]}{\gamma_p - \gamma_{p_1} - \gamma_{p_2} + \gamma_{p-p_1-p_2}} d^3p_1 d^3p_2 \right) \end{aligned} \tag{180}$$

The third term in this expression represents a net decrease in the energy of the magnons as they move through an average potential field, while the last term represents a net decrease in the energy due to the interaction of a magnon with all of the other magnons. At low temperatures and momenta (180) reduces to Eq. (147). The leading temperature terms are

$$\varepsilon(p) = E_p^0 - 2J[\gamma_0 - \gamma_p]\,\eta_1(\theta)/\gamma_0 - 4JA_0 D_0\, p^2 \eta_1(\theta)/D\gamma_0 \tag{181}$$

If the higher order momentum terms in $\Sigma'(p)$ are neglected

$$\eta_1(\theta) = \eta_1^{H.F.}(\theta) \tag{182}$$

where

$$\eta_1^{H.F.}(\theta) = 1/\left(e^{\beta \epsilon_p^{H.F.}} - 1\right) \tag{183}$$

$$\epsilon_p^{H.F.} = \epsilon_p^{\circ} - 2J[\Gamma_0' - \Gamma_p'] \tag{184}$$

which is the Hartree-Fock energy. Substitution of $\eta_1(\theta)$ into (181) gives

$$\mathcal{E}(\rho) = -\mu H + J\left\{1 - 2\left[Q - \tfrac{2}{3}a_0\right]\pi\nu\,\zeta\!\left(\tfrac{5}{2}\right)\left(\frac{3\theta}{2\pi\gamma_0\nu}\right)^{5/2} + O(\theta^3)\right\}\rho^2 \tag{185}$$

The constant Q is given by Eq. (155).

$$Q = 1 + 2A_0D_0/D + \tfrac{2}{3}a_0 \tag{186}$$

or

$$Q - \tfrac{2}{3}a_0 = 1 + 2A_0D_0/D \tag{187}$$

The factor $2A_0D_0/D$ represents the contribution to the energy due to magnon-magnon interactions. The number one in (187) represents the Hartree-Fock energy contribution. The $\theta^{5/2}$ term in (185) gives a θ^4 contribution to the magnetization while the term of order θ^3 gives a $\theta^{9/2}$ contribution. Thus the lowest temperature contribution produced by dynamical interactions is θ^4, which agrees with Dyson's results.

This renormalization of the energy can be thought of as producing an effective temperature-dependent exchange constant for small momenta. In this range

$$\mathcal{E}(p) = \mu H + J_{eff.}\, p^2 \tag{188}$$

Using Eq. (184)

$$\frac{J_{eff.}}{J} = 1 - 2\,\eta_1^{H.F.}(\theta)\left[1 + 2A_0 D_0 / D\right]/\gamma_0 + O(\theta^3) \tag{189}$$

$$= 1 - 2\,\eta_1^{H.F.}(\theta)\left[Q - \tfrac{2}{3}a_0\right]/\gamma_0 + O(\theta^3)$$

The ratio $J_{eff.}/J$ can be measured by inelastic neutron diffraction.[15] Figure 1 shows a plot of Eq. (189) for a face-centered-cubic lattice. A value of $\Theta_c = 4$ was used in the plot against Θ/Θ_c. This value for the normalized Curie point, Θ_c, will be discussed later on in this chapter. Figure 1 also shows the results from experiments on nickel, which is a face-centered-cubic ferromagnetic solid with S close to one-half, which were reported by Lowde.[16]

Lifetimes

The imaginary part of the renormalized energy given by (94) is interpreted as the lifetime of a single particle state. To see this consider the correlation function $\langle S_0^+(0) S_n^-(t)\rangle$. Substitution of the second order G_1 solution, (96), into (40), using Eq. (28), and retaining the lowest temperature term gives

$$\langle S_0^+(0) S_n^-(t)\rangle = \frac{1}{N}\sum_p e^{i\vec{p}\cdot\vec{n}}\, e^{i\mathcal{E}(p)t}\, e^{-\tau^{-1}|t|} \tag{190}$$

The Fourier inversion of the $S_j^{\pm}$ operators is given by

$$S_j^{\pm} = \frac{1}{\sqrt{N}} \sum_p S_p^{\pm} e^{i\vec{p}\cdot\vec{j}} \tag{191}$$

when S_p^- is the creation operator for a magnon, given by (12), and S_p^+ is the destruction operator for a magnon. Using (190) and (191) it is easily shown that

$$\sum_{p'} \langle S_{p'}^+(0) S_p^-(t)\rangle = e^{i\varepsilon(p)t} e^{-\xi^{-1}|t|} \tag{192}$$

It is assumed now that the set of states used to calculate (190) can be replaced by a set of orthogonal single particle magnon states. In other words it is assumed that the low temperature behavior of this system can be entirely explained by using a set of one-particle "wave functions", $|p,T\rangle$ which are temperature dependent and which describe the state of a magnon with a renormalized temperature dependent energy, $\varepsilon(p)$, and momentum p. Then

$$\langle S_{p'}^+(0) S_p^-(t)\rangle = \sum_{p''} \langle p'',T| S_{p'}^+(0) S_p^-(t) |p'',T\rangle \tag{193}$$

Since the states $|p,T\rangle$ are assumed to be orthogonal

$$\langle S_{p'}^+(0) S_p^-(t)\rangle = \delta_{p,p'} \langle p,T| S_p^+(0) S_p^-(t) |p,T\rangle \tag{194}$$

Then (192) becomes

$$\langle p,T| S_p^+(0) S_p^-(t) |p,T\rangle = e^{i\varepsilon(p)t} e^{-\xi^{-1}|t|} \tag{195}$$

or

$$|\langle p,T|\, S_p^+(0)\, S_p^-(t)\,|p,T\rangle|^2 = e^{-\tau^{-1}|t|} \tag{196}$$

Equation (196) then gives the probability that one could add a magnon with momentum p to the system at time $t=-t_0$, remove a magnon with momentum p at t=0, and come back to the original state. However, if the magnon that was added to the system at $t=-t_0$ interacts with another magnon before t=0 then it is impossible for the system to return to the original state simply by destruction of a magnon with momentum p. Therefore it should be expected that the probability (196) should decrease as $|t|$ increases. Hence τ^{-1} is a measure of the "interaction rate" and is called the lifetime for these single particle states.

The lifetime $\tau^{-1}(p)$ is given by Eq. (94). The low temperature expansion of (94) is obtained by using (144) for S_p. After one integration the leading term is

$$\tau^{-1}(p) = \frac{J v^2 p^2 D_0}{(2\pi)^4 D} \int_0^\infty \int_0^\pi \int_0^{2\pi} \langle n\rangle_{p'}\, |\vec{p}'-\vec{p}|\, |\vec{p}'|^2 \cos\theta \, d^3p' \tag{197}$$

where θ is the angle between $\vec{p}$ and $\vec{p}'$. The leading term of (197) is then

$$\tau^{-1}(p) = \left(\frac{6}{\gamma_0 \nu}\right)^3 \frac{\sqrt{\pi}\, J D_0 a}{32\, \pi^3 D}\, \zeta\!\left(\tfrac{5}{2}\right) p^3 \theta^{5/2} \qquad pa \ll \theta^{1/2} \tag{198}$$

$$\tau^{-1}(p) = \left(\frac{6}{\gamma_0 \nu}\right)^3 \frac{J D_0}{12\, \pi^2 D}\, \zeta(3)\, p^2 \theta^3 \qquad pa \gg \theta^{1/2} \tag{199}$$

where a is the lattice constant.

Equation (198) differs by the factor D_0/D from the lifetime calculated by Pincus, Sparks, and LeCraw[17] which was obtained using Dyson's[7] mean free path, after Eq. (111) of Reference (7) has been corrected by replacing $\zeta(\frac{3}{2})$ by $\frac{1}{2}\,\zeta(\frac{5}{2})$.

The Magnetization

The magnetization formula (154) for the nearest neighbor approximation is in exact agreement with Dyson's results up to order θ^4 in the temperature. The anomalous T^3 term is missing in this second order expression due to its cancellation by terms generated by the $\delta_{1,0}\delta_{2,0}\langle s_1^- s_2^+\rangle$ term in the G_2 equation. Thus G_2 being zero if 1=2 is a necessary condition for the removal of this anomalous T^3 term.

In order to make an extension of these results to higher temperatures consider the leading terms in Eq. (144).

$$M = 1 - 2\eta_0(\theta)\left[1 + 2a_0\eta_1(\theta)/\gamma_0 + \eta_2(\theta)\right] \tag{200}$$

The function $\eta_2(\theta)$ was introduced into the theory as a result of the introduction of the G_1 function into the solution of the G_2 equation. Eq. (200) gives the correct low temperature expansion of the magnetization up to order θ^4.

Suppose (200) is extended to higher temperatures. The interaction energy is known only to order p^2 in the momentum and therefore higher momentum contributions are neglected. The temperature dependence of the p^2 term is known exactly to order $\theta^{5/2}$. Higher order temperature corrections can be neglected here since their numerical contributions to (200) are small. Then in this approximation η_0 reduces to

$$\eta_0(\theta) = \eta_0^{H.F.}(\theta)\left[1 + \frac{[Q-1-\frac{2}{3}a_0]\,\Phi(\theta)}{1-[Q-\frac{2}{3}a_0]\,\Phi(\theta)}\right]^{\frac{3}{2}} \tag{201}$$

where

$$\Phi(\theta) = 2\,\eta_1^{H.F.}(\theta)/\gamma_0 \tag{202}$$

$$\eta_1^{H.F.}(\theta) = \frac{v}{(2\pi)^3}\int \langle n\rangle_p^{H.F.}\,[\gamma_0-\gamma_p]\,d^3p \tag{203}$$

$$\eta_0^{H.F.}(\theta) = \frac{v}{(2\pi)^3}\int \langle n\rangle_p^{H.F.}\,d^3p \tag{204}$$

$$\langle n\rangle_p^{H.F.} = \frac{1}{e^{\beta E_p^{H.F.}}-1} \tag{205}$$

$$E_p^{H.F.} = J[\gamma_0-\gamma_p][1-\Phi(\theta)] \quad ; \quad H=0 \tag{206}$$

The energy E_p is the Hartree-Fock energy. Only the first term in the definition of η_2 has been retained since the other term can be neglected for temperatures up to the Curie point. Then the magnetization formula becomes

$$M = 1-2\,\eta_0(\theta)\left[1+\frac{[Q-1-\frac{2}{3}a_0]\;\Phi(\theta)}{1-[Q-\frac{2}{3}a_0]\,\Phi(\theta)}\right]^{\frac{3}{2}}\left(1+a_0\,\Phi(\theta)+\gamma_0\,\Phi^2(\theta)/\theta\right) \tag{207}$$

Eq. (207) is plotted in Figure 2 for a simple cubic lattice. The Curie point is found to be

$$\theta_c = 1.92 \tag{208}$$

This value is about four per cent off the theoretical value of $\theta_c = 2.0$ given by Domb and Sykes[18] from a high temperature series.

Figure 3 represents a plot of Eq. (207) for a face-centered-cubic lattice and for the experimental points for Nickel. The Curie point given by this theory is found to be

$$\theta_c = 4.00 \tag{213}$$

This represents exact agreement with the value $\theta_c = 4.0$ given by Domb and Sykes. The relatively poor agreement at temperatures up to about eighty per cent of the Curie point may be due to the existence of conduction electrons in Nickel and to the existence of an internal crystalline field.[19, 20] However, at temperatures above this range this approximation gives agreement with the Nickel data, indicating that the Heisenberg model may give an adequate mathematical representation of Nickel in this temperature range.

The magnetization formulas (170) and (178) are plotted in Figure 4. Eq. (170) is exact and was obtained by expressing terms in the G_2 equation in terms of G_1 functions and thus forcing a renormalization of the coefficient of G_1 in the G_1 equation. Eq. (178) was derived in the same manner as (170) but no attempt was made to express G_2 in terms of G_1 functions.

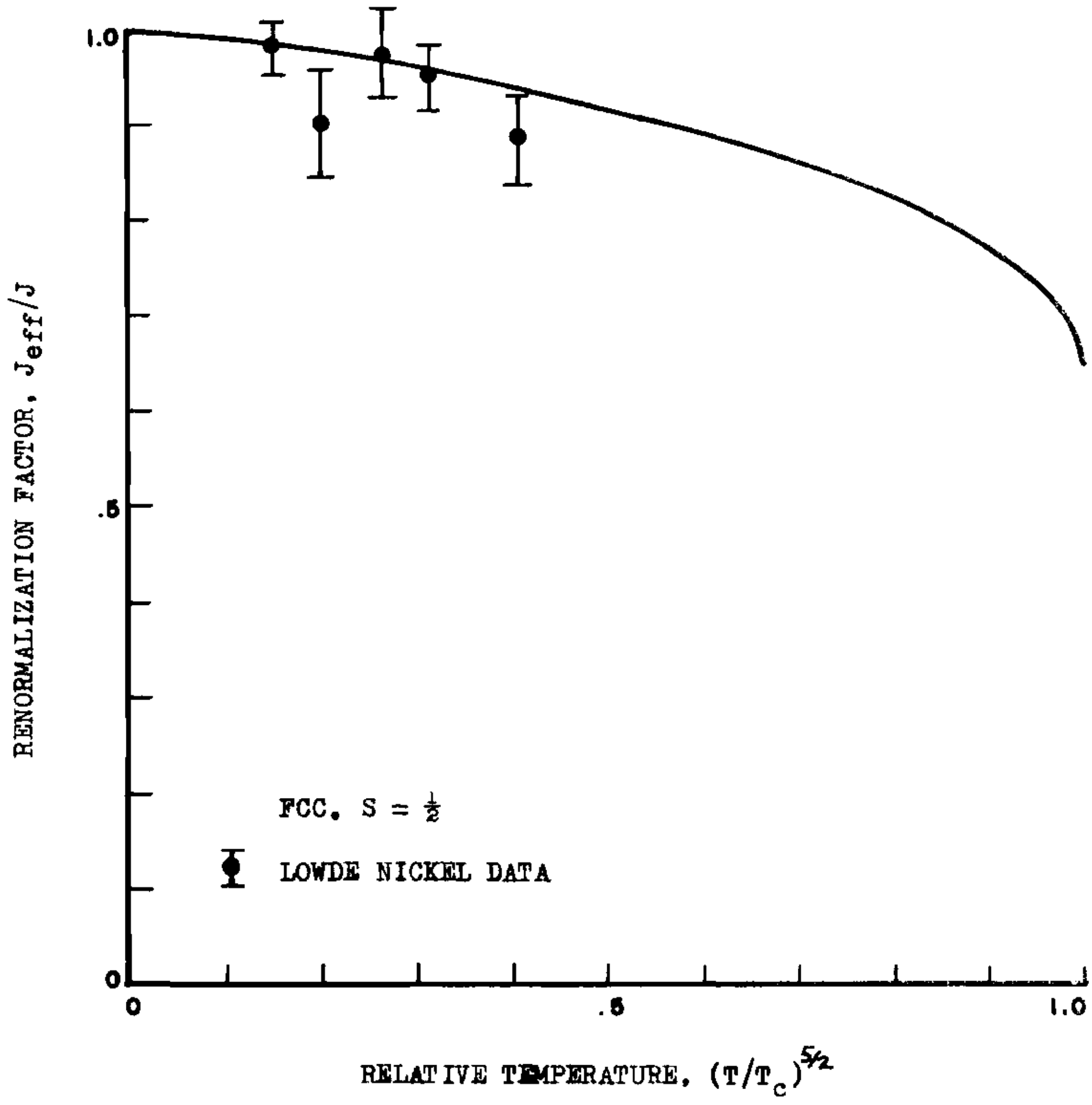


Figure 1. The Renormalization Factor for a Face-Centered-Cubic Lattice.

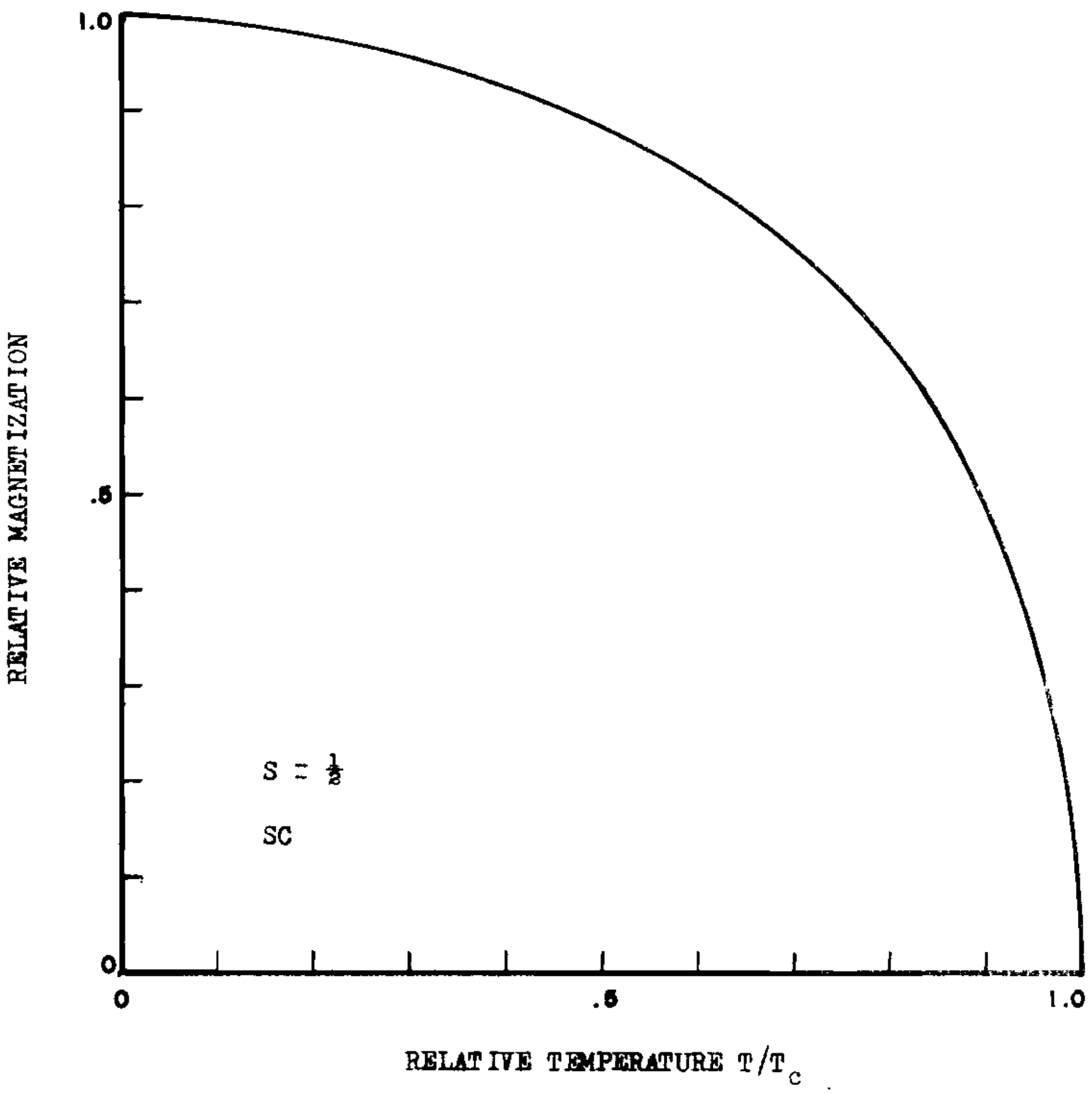


Figure 2. Theoretical Magnetization Curve for a Simple Cubic Lattice.

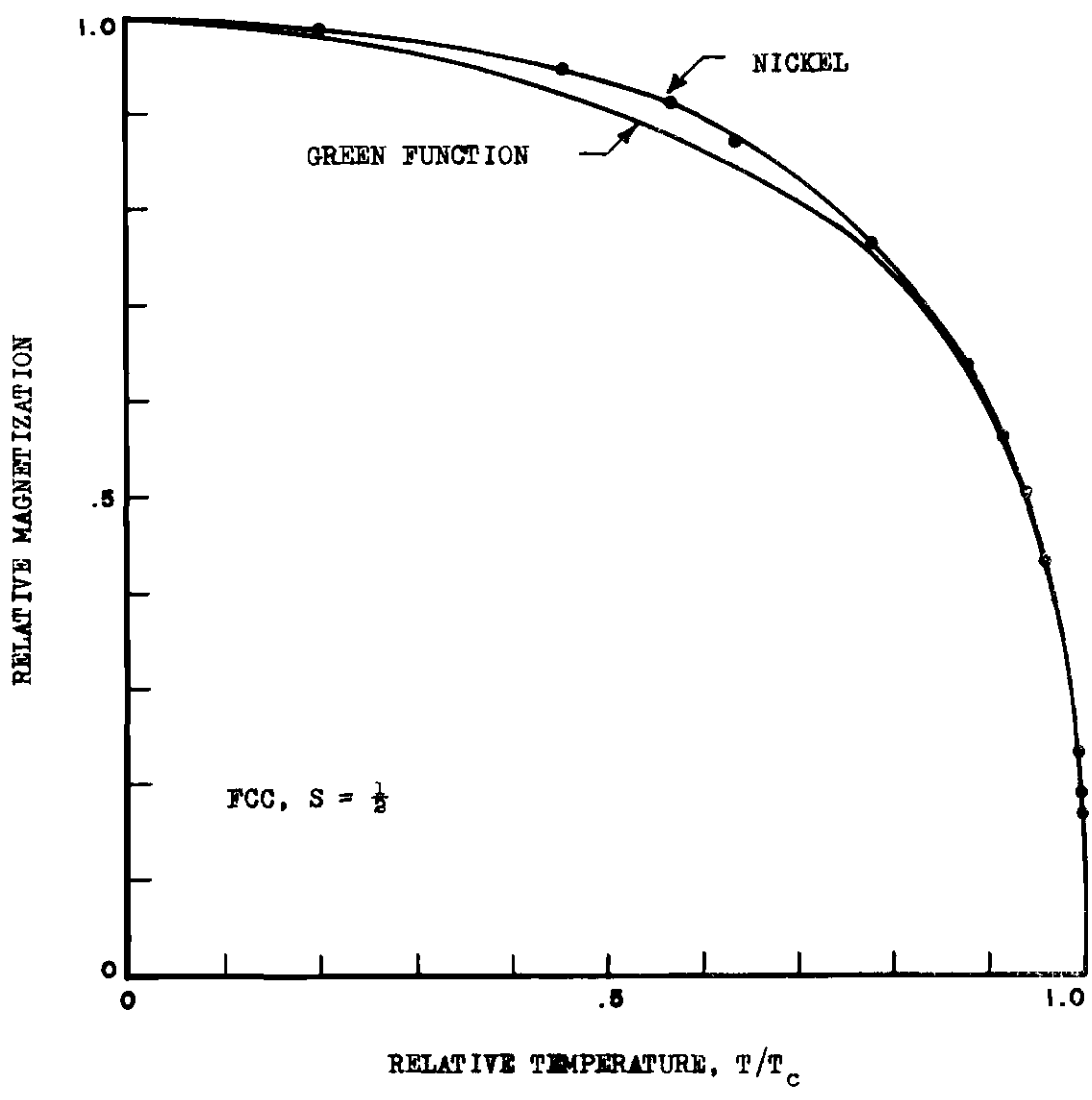


Figure 3. The Magnetization Curve for Nickel Compared with the Theoretical Curve.

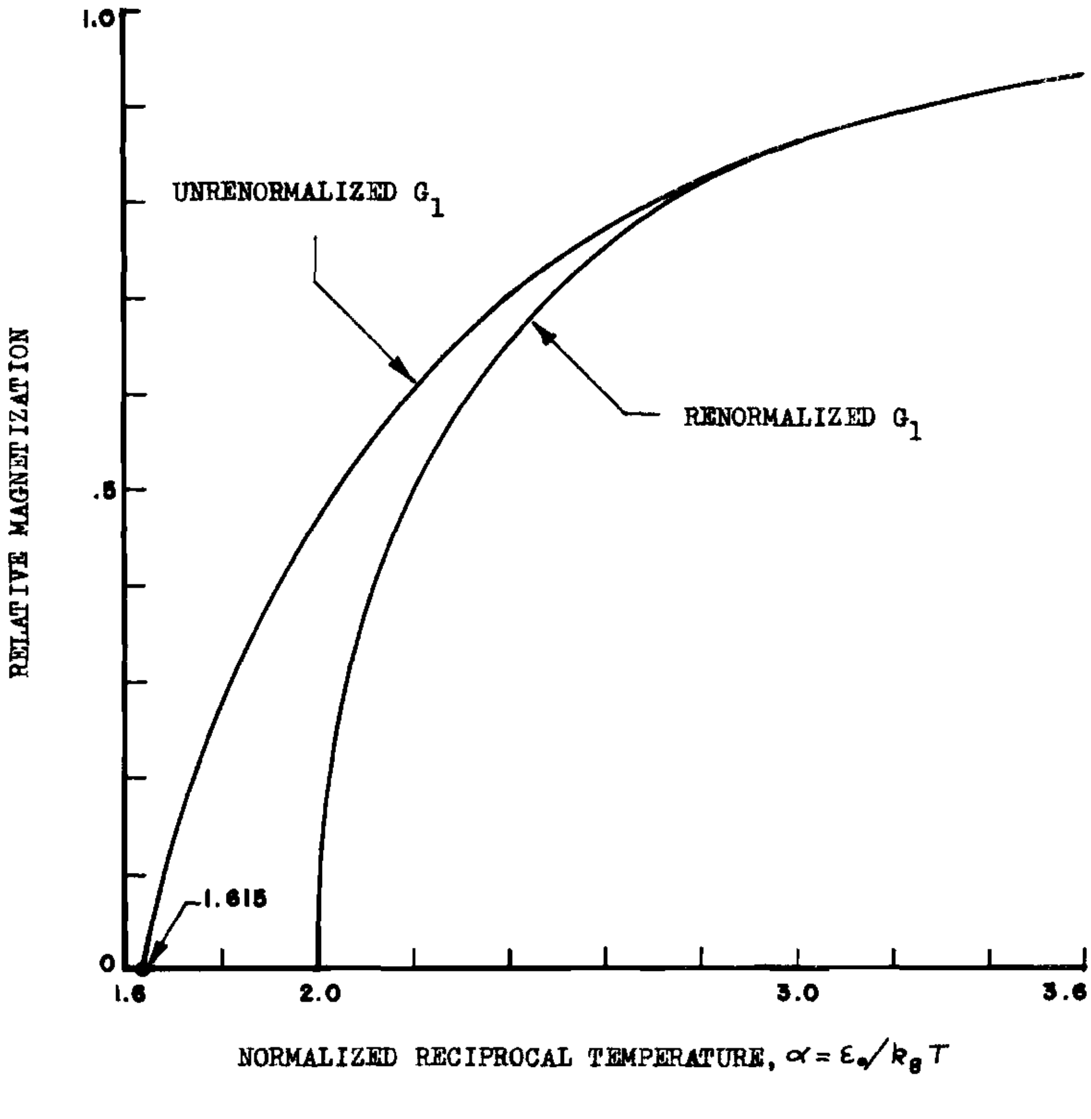


Figure 4. The Magnetization for a Uniformly Interacting Spin System.

CHAPTER VIII

CONCLUSIONS

This work shows that it is possible to solve the second order Green function equations defined for the Heisenberg Hamiltonian within an energy renormalization framework, providing in the case of the nearest neighbor approximation expressions for the magnon-magnon interaction energy and lifetimes for single particle excited states. These expressions are generated by the G_2 equation and are not introduced into the theory from external arguments.

This theory also shows that when interactions are not neglected an expansion of the G_2 function in terms of G_1 functions is in general impossible for double-time Green functions. However, an energy renormalization can be effected by a proper treatment of the terms in the G_2 equation which gives rise to these interaction terms.

Because of the agreement of the results obtained in this work with Dyson's results, it is concluded that the Green function theory is providing a well ordered scheme for calculation of the physical properties for the Heisenberg ferromagnet.

APPENDIX I

CALCULATION OF G_2 FOR NEAREST NEIGHBOR APPROXIMATION

Equation (75) is solved by letting $N \to \infty$. In this limit p becomes a continuous variable and

$$\frac{1}{N}\sum_{p} \to \frac{v}{(2\pi)^3}\int d^3p \qquad \text{(I-1)}$$

where the integration is taken over the first Brillouin zone. The symbol v denotes the number of particles per unit volume. In terms of the lattice constant "a" for cubic structures

$$v = a^3/n = \begin{cases} a^3 & \text{s.c.} \\ a^3/2 & \text{b.c.c.} \\ a^3/4 & \text{f.c.c.} \end{cases} \qquad \text{(I-2)}$$

In this limit (75) converts to a Fredholm Integral equation.[21] Using (I-1) and making the substitution

$$\left\{\omega + \mu H + 2JS\left[\gamma_0 - \gamma_{p_1} - \gamma_{p_2} + \gamma_{p_3}\right]\right\} G_2(p_1, p_2, p_3, \omega) = F(p_1, p_2, p_3, \omega) \qquad \text{(I-3)}$$

equation (75) becomes

$$F(p_1, p_2, p_3, \omega) - \frac{2Jv}{(2\pi)^3}\int F(p', p_1+p_2-p', p_3, \omega)\frac{[\gamma_{p_1-p'} - \gamma_{p'}]}{\omega + \mu H + J[\gamma_0 - \gamma_{p'} - \gamma_{p_1+p_2-p'} + \gamma_{p_3}]}\, d^3p' \qquad \text{(I-4)}$$

$$= \frac{2S(2\pi)^3 S_{p_3}}{v}\left[\delta(p_1+p_3) + \delta(p_2+p_3)\right] + 2S_{p_3}$$

where $\delta(x)$ is the Dirac delta function.

Let

$$\alpha_\rho(x) = \frac{2JU}{(2\pi)^3}\left[e^{i\vec{x}\cdot\vec{\rho}} - 1\right] \tag{I-5}$$

$$\beta_\rho(x) = \frac{e^{-i\vec{x}\cdot\vec{\rho}}}{\omega + \mu H + J[\gamma_0 - \gamma_x - \gamma_{p_1+p_2-x} + \gamma_{p_3}} \tag{I-6}$$

Then (I-4) becomes

$$F(x, p_1+p_2-x, p_3, \omega) - \int F(x', p_1+p_2-x', p_3, \omega) \sum_\rho \alpha_\rho(x)\beta_\rho(x')\, d^3x' \tag{I-7}$$

$$= \frac{-2S(2\pi)^3 S_{p_3}}{U}\left[\delta(x+p_3) + \delta(p_1+p_2+p_3-x)\right] + 2S_{p_3} \equiv I(x)$$

This is a Fredholm Integral equation of the second kind. The solution is obtained by a direct application of the Fredholm theory. Let

$$c_{\rho,\rho'} = \int \alpha_\rho(x)\,\beta_{\rho'}(x)\; d^3x \tag{I-8}$$

$$f_\rho = \int I(x)\,\beta_\rho(x)\; d^3x \tag{I-9}$$

Then the solution of (I-4) is

$$F(x, p_1+p_2-x, p_3, \omega) = I(x) + \sum_\rho X_\rho\, \alpha_\rho(x) \tag{I-10}$$

where the X_ρ are solutions of the matrix equation

$$[I - C]X = f \tag{I-11}$$

where I is the unit matrix.

Assuming p_1+p_2, p and p_3 small

$$C_{\rho,\rho'} = C_{\rho',\rho} \cong \frac{v}{(2\pi)^3}\int \frac{e^{i\vec{x}\cdot(\vec{\rho}-\vec{\rho}')} - e^{-i\vec{x}\cdot\vec{\rho}}}{\gamma_0-\gamma_x}\, d^3x \tag{I-12}$$

For a simple cubic structure C is a 6 x 6 matrix. The solution of (I-11) can be written in the form

$$X_\rho = \frac{1}{D}\sum_{\rho'} D^{\rho}_{\rho'} f_{\rho'} \tag{I-13}$$

where the f_ρ are given by (I-9) and D is the determinant of the matrix [I-C]. The $D^{\rho}_{\rho'}$ are minors of the matrix [I-C] which arise naturally in the solution of (I-11) by Cramer's method. Then

$$F(x, P_1+P_2-x, P_3, \omega) = I(x) + \frac{1}{D}\sum_{\rho}\sum_{\rho'} \alpha_\rho(x)\, D^{\rho}_{\rho'} f_{\rho'} \tag{I-14}$$

The determinants D^{ρ}_{ρ} have the special property of being equal. Let $D^{\rho}_{\rho} = D_0$. Then

$$F(x, P_1+P_2-x, P_3, \omega) = I(x) + \frac{D_0}{D}\sum_{\rho}\alpha_\rho(x) f_\rho + \frac{1}{D}\sum_{\substack{\rho\ \rho' \\ \rho\neq\rho'}}\sum \alpha_\rho(x)\, D^{\rho}_{\rho'} f_{\rho'} \tag{I-15}$$

The double sum in (I-15) will be neglected since it appears to be a higher order term than the single sum term although a proof of this is lacking.

The functions f_ρ are given by (I-9).

$$\frac{v}{S(2\pi)^3} f_\rho = -4JSS_{P_3}\, \frac{e^{i\vec{P}_3\cdot\vec{\rho}} + e^{-i[\vec{P}_1+\vec{P}_2+\vec{P}_3]\cdot\vec{\rho}}}{\omega+4H+2JS[\gamma_0-\gamma_{P_1+P_2+P_3}]}$$
$$+ \frac{4Jv S_{P_3}}{(2\pi)^3}\int \frac{e^{-i\vec{p}'\cdot\vec{\rho}}}{\omega+4H+2JS[\gamma_0-\gamma_{p'}-\gamma_{P_1+P_2-p'}+\gamma_{P_3}]}\, d^3p' \tag{I-16}$$

Using equations (I-16), (I-15), (I-5), and (I-3)

$$G_2(p_1,p_2,p_3,\omega) = -\frac{2S(2\pi)^3 S_{p_3}\,\delta(p_1+p_3)}{v[\omega+E^\circ_{p_2}]} - \frac{2S(2\pi)^3 S_{p_3}\,\delta(p_2+p_3)}{v[\omega+E^\circ_{p_1}]} \tag{I-17}$$

$$-4JSS_{p_3}\frac{D_o}{D}\frac{\gamma_{p_1+p_3}+\gamma_{p_2+p_3}-\gamma_{p_1+p_2+p_3}-\gamma_{p_3}}{[\omega+E^\circ_{p_1}+E^\circ_{p_2}-E^\circ_{p_3}][\omega+E^\circ_{p_1+p_2+p_3}]} + \frac{2S_{p_3}}{\omega+E^\circ_{p_1}+E^\circ_{p_2}-E^\circ_{p_3}}$$

$$+\frac{4JS_{p_3}D_o v}{D(2\pi)^3}\int \frac{-\gamma_{p_1'}+\gamma_{p_1'-p_1}}{[\omega+E^\circ_{p_1'}+E^\circ_{p_1+p_2-p_1'}-E^\circ_{p_3}][\omega+E^\circ_{p_1}+E^\circ_{p_2}-E^\circ_{p_3}]}\,d^3p_1'$$

where E°_p is the first order magnon energy

$$E^\circ_p = \mu H + 2JS[\gamma_o - \gamma_p] \tag{I-18}$$

Replacing S by $\langle s^z\rangle + \langle s_o^- s_o^+\rangle$, and using equation (67) the first three terms on the right hand side of (I-17) can be written in terms of G_1° functions. In order to obtain renormalized energies for the magnons these G_1° functions must be replaced by the G_1 functions which are solutions of (77).

Suppose for the moment that this replacement is made. Then the coefficient of the G_1 would be renormalized by the G_1 terms in the G_2 solution, giving a temperature-dependent renormalized energy, E_p. There is however, a more fundamental problem here. The $G_1(p,\omega)$ function has poles which correspond to energies of single particle states. The $G_2(p_1,p_2,p_3,\omega)$ function has poles which correspond to two particle states. The Kronecker delta functions in (I-17) reduce the poles of the G_2 function to ones which correspond to single particle states as long as magnon-magnon interactions are absent. This second order calculation contains the interactions and therefore some adjustment must be made if G_2 functions are to be expressed by G_1 functions.

Let $E(P_1,P_2)$ be the interaction energy between particles of momentum p_1 and p_2 respectively. Then the total interaction energy of a particle with momentum p_1 due to all of the other particles is

$$E_1 = \sum_{\substack{P_2 \\ P_2 \neq P_1}} \langle n \rangle_{P_2} E(P_1, P_2) \tag{I-19}$$

where $\langle n \rangle_{P_2}$ is the number of particles with momentum p_2. If the particles are indistinguishable then certainly

$$E(P_1,P_2) = E(P_2,P_1) \tag{I-20}$$

and the total interaction energy between pairs of particles with one of these particles having a momentum p_1 is

$$E_2 = 2 \sum_{\substack{P_2 \\ P_2 \neq P_1}} \langle n \rangle_{P_2} E(P_1, P_2) \tag{I-21}$$

The interaction energy which occurs in the poles of G_1 is given by (I-19) while the interaction energy which occurs in the poles of G_2 is given by (I-21). Therefore it is clear that G_1 functions cannot be substituted on the right hand side of Eq. (I-17). However, if a function G_1' is defined to be equal to G_1 except that it contains (I-21) instead of (I-19) then (77) will give a self consistent solution for G_1'.

After the G_1' function has been found the replacement of (I-21) by (I-19) in the solution would give G_1.

A procedure which will give the same results is to find the term in the G_2 equation which will give rise to this interaction term in the G_1 solution and divide it by two. This is the approach that will be used here.

It is shown in Chapter V that the term in (I-17) which gives rise to the interaction energy is the third term in Eq. (I-17). Thus this term is divided by two and

$$- \frac{2S}{\omega + E_p^\circ} = \frac{-2\left[\langle S^z\rangle + \langle S_o^- S_o^+\rangle\right]}{\omega + E_p^\circ} \rightarrow G_1(p,\omega) - \frac{2\langle S_o^- S_o^+\rangle}{\omega + E_p} \tag{I-22}$$

where E_p is the renormalized single particle energy and G_1 is the solution of Eq. (77). Then Eq. (I-17) becomes

$$\begin{aligned} G_2(p_1,p_2,p_3,\omega) &= \frac{(2\pi)^3}{v} S_{p_3}\left[\delta(p_1+p_3)\, G_1(p_2,\omega) + \delta(p_2+p_3)\, G_1(p_1,\omega)\right] \\ &+ 2JS\, S_{p_3} \frac{D_o}{D} \frac{\gamma_{p_1+p_3} + \gamma_{p_2+p_3} - \gamma_{p_3} - \gamma_{p_1+p_2+p_3}}{\omega + E_{p_1}^\circ + E_{p_2}^\circ - E_{p_3}^\circ}\, G_1(p_1+p_2+p_3,\omega) \\ &+ \frac{4JS_{p_3} D_o v}{(2\pi)^3 D} \int \frac{\gamma_{p_1-p'} - \gamma_{p'}}{\left[\omega + E_{p_1}^\circ + E_{p_2}^\circ - E_{p_3}^\circ\right]\left[\omega + E_{p'}^\circ + E_{p_1+p_2-p'}^\circ - E_{p_3}^\circ\right]}\, d^3p' \\ &+ \frac{2S_{p_3}}{\omega + 4H + J\left[\gamma_o - \gamma_{p_1} - \gamma_{p_2} + \gamma_{p_3}\right]} - \frac{2\langle S_o^- S_o^+\rangle (2\pi)^3}{v} S_{p_3}\left[\frac{\delta(p_1+p_3)}{\omega + E_{p_2}} + \frac{\delta(p_2+p_3)}{\omega + E_{p_1}}\right] \end{aligned} \tag{I-23}$$

APPENDIX II

THE MAGNON-MAGNON INTERACTION ENERGY

The interaction energy $\Sigma(p)$ is in general a very complicated function of the temperature.

$$\Sigma(p) = P\left(\frac{2JU^2 D_0}{(2\pi)^6 D} \iint S_{p-p_1-p_2} \frac{[\gamma_p - \gamma_{p-p_1} - \gamma_{p-p_2} + \gamma_{p-p_1-p_2}][\gamma_{p-p_1} - \gamma_{p_2}]}{\gamma_p - \gamma_{p_1} - \gamma_{p_2} + \gamma_{p-p_1-p_2}} \, d^3 p_1 \, d^3 p_2 \right) \tag{II-1}$$

The function $S_{p-p_1-p_2}$ is given by (144). After making the change of variables

$$\begin{aligned} \vec{p}_2 &= \vec{x} + \vec{p} - \vec{p}_1 \\ \vec{p}_1 &= \vec{y} + \tfrac{1}{2}(\vec{x} + \vec{p}) \end{aligned} \tag{II-2}$$

Eq. (II-1) becomes, after some simplification

$$\Sigma(p) = - P\left(\frac{32 J D_0 U^2}{D(2\pi)^6} \iint [\langle S^z \rangle \langle n \rangle_x + (\eta_0^0(\theta))^2] \otimes \right. \tag{II-3}$$

$$\left. \otimes \sum_{\rho} \sum_{\rho'} \sin \vec{p} \cdot \frac{\vec{\rho}}{2} \sin \vec{p} \cdot \frac{\vec{\rho}'}{2} \frac{\sin \vec{x} \cdot \frac{\vec{\rho}}{2} \sin \vec{x} \cdot \vec{\rho}'/2 \cos \vec{y} \cdot \vec{\rho} \cos \vec{y} \cdot \vec{\rho}'}{\gamma_0 - \gamma_{y + \frac{1}{2}(x+p)} - \gamma_{y - \frac{1}{2}(x+p)} + \gamma_x} \, d^3x \, d^3y \right)$$

In order to obtain the low temperature and momenta approximation of this integral the integrand is expanded in powers of $\vec{x}$ and $\vec{p}$. The leading term of the expansion gives

$$\Sigma(p) = - 2J \langle S^z \rangle \frac{D_0}{D} \sum_{\rho} \sum_{\rho'} (\vec{p} \cdot \vec{\rho})(\vec{p} \cdot \vec{\rho}') \, \alpha_{\rho,\rho'} \, \beta_{\rho,\rho'} \tag{II-4}$$

$$- 2J[\eta_0^o(\theta)]^2 \frac{D_o}{D} \sum_{\rho}\sum_{\rho'} (\vec{P}\cdot\vec{\rho})(\vec{P}\cdot\vec{\rho}')\alpha_{\rho,\rho'}\beta^o_{\rho,\rho'}$$

$$\alpha_{\rho,\rho'} = \frac{v}{(2\pi)^3}\int \frac{\cos\vec{y}\cdot\vec{\rho}\,\cos\vec{y}\cdot\vec{\rho}'}{\gamma_o - \gamma_y}\, d^3y \tag{II-5}$$

$$\beta_{\rho,\rho'} = \frac{v}{2(2\pi)^3}\int \langle n\rangle_x (\vec{x}\cdot\vec{\rho})(\vec{x}\cdot\vec{\rho}')\, d^3x \tag{II-6}$$

$$\beta^o_{\rho,\rho'} = \frac{2v}{(2\pi)^3}\int \sin\tfrac{1}{2}\vec{x}\cdot\vec{\rho}\,\sin\tfrac{1}{2}\vec{x}\cdot\vec{\rho}'\, d^3x \tag{II-7}$$

$$\beta^o_{\rho,\rho} = 1 \tag{II-8}$$

These results are easy to evaluate for a simple cubic lattice. In this case

$$\beta_{\rho,\rho'} = \beta^o_{\rho,\rho'} = 0 \quad \text{if } \vec{\rho} \neq -\vec{\rho}', \vec{\rho}' \tag{II-9}$$

Since $\alpha_{\rho,\rho}$, $\beta_{\rho,\rho}$, and $\beta^o_{\rho,\rho}$, are independent of ρ , let

$$\alpha_{\rho,\rho} = \alpha_o \tag{II-10}$$

$$\beta_{\rho,\rho} = \beta_o$$

Then (II-4) becomes

$$\Sigma(P) = -8J\langle s^3\rangle \alpha_o \frac{D_o}{D}\beta_o P^2 + O(\theta^3) \tag{II-11}$$

Now at low temperatures

$$\beta_o = \frac{v}{2(2\pi)^3}\int \langle n\rangle_x (\vec{x}\cdot\vec{\rho})^2 d^3x \simeq \eta_1(\theta)/\gamma_o \tag{II-12}$$

where $\eta_1(\theta)$ is given by (140). Then

$$\Sigma(P) = -8J\langle s^3\rangle D_o A_o \eta_1(\theta) P^2/\gamma_o D + O(\theta^3) \tag{II-13}$$

It is easy to show that for a face-centered-cubic and body-centered-cubic lattices $\Sigma(P)$ can be written in the form

$$\Sigma(P) = -A\eta_1(\theta)P^2 + O(\theta^3) \qquad \text{(II-14)}$$

However, the constant A is much harder to obtain. Thus for the cubic lattices the interaction energy $\Sigma(P)$ can be written in the form

$$\Sigma(P) = -8J\langle S^3\rangle D_0 A_0 P^2 \eta_1(\theta)/\gamma_0 D + O(\theta^3) \qquad \text{(II-15)}$$

where A= α_0 for the simple cubic lattice.

APPENDIX III

NUMERICAL RESULTS

The integrals which must be evaluated in order to get numerical answers are in general too complicated to obtain in closed form for arbitrary temperatures. The procedure for evaluating these integrals involves the replacement

$$\frac{v}{(2\pi)^3}\int d^3p \rightarrow \frac{1}{N}\sum_p \tag{III-1}$$

(See I-1). Of course the limit to an infinite lattice must be taken in order for (III-1) to be valid. However, the integrals $\int \cdots d^3p$ can be approximated by taking N large and summing over the appropriate p vectors, the larger N the better the approximation.

For a simple cubic lattice the set of p vectors given in Chapter I is summed over for a given N. For the face-centered-cubic lattice additional p vectors must be added to the simple cubic set since there are now more lattice points for the same volume of the sample. This can be accomplished in two ways.

Suppose the set of p vectors chosen for the simple cubic lattice is given by

$$p_i = 2\pi n_i / N^{1/3} \tag{III-2}$$

$$0 \leq n_x < N^{1/3} \qquad \text{(III-3)}$$
$$0 \leq n_y < N^{1/3}$$
$$0 \leq n_z < N^{1/3}$$

In order to make $\{\vec{P}_i\}$ a complete set of vectors for the face-centered-cubic lattice the additional points

$$N^{1/3} \leq n_x < 2N^{1/3} \qquad \text{(III-4)}$$
$$0 \leq n_y < N^{1/3}$$
$$0 \leq n_z < N^{1/3}$$

or any cyclic permutation of the variables x, y, and z, must be added to those listed in (III-3).

Another way of accomplishing the same thing is that instead of adding more vectors p to the set (III-3) additional sets of energies are assigned to the basic set of vectors.[16] For a simple cubic lattice with one lattice point per unit cell

$$\gamma_0 - \gamma_P = 6 - 2\cos P_x - 2\cos P_y - 2\cos P_z \qquad \text{(III-5)}$$

and for a face-centered-cubic lattice with four lattice points per unit cell

$$\gamma_0 - \gamma_P = 12 \mp 4\cos(P_x/2)\cos(P_y/2) \mp 4\cos(P_y/2)\cos(P_z/2) \qquad \text{(III-6)}$$
$$\mp 4\cos(P_z/2)\cos(P_x/2)$$

where in both cases the p vectors are given by (III-3). In the case of the face-centered-cubic lattice each of the sets of signs in (III-6) is summed over.

All of the sums were calculated using a Burrough's B-5500 computer using a method for summation over the p vectors outlined in Reference (10). It is faster from the standpoint of computer time to use (III-5) and (III-6) for the function $\gamma_0 - \gamma_p$ than to add additional p vectors to the set (III-3), and therefore this procedure was used in writing the Algol program for the computer.

The D_0/D Ratio

The numerical value of D_0/D is important since it appears as a factor in the magnon-magnon interaction energy, $\Sigma(p)$, the lifetime, $\tau^{-1}(p)$, and in the constant Q which determines the coefficient of the θ^4 term in the magnetization.

These determinants are relatively simple for the simple cubic lattice.

$$D = \begin{vmatrix} a & b & b & c & b & b \\ b & a & b & b & c & b \\ b & b & a & b & b & c \\ c & b & b & a & b & b \\ b & c & b & b & a & b \\ b & b & c & b & b & a \end{vmatrix} \qquad \text{(III-7)}$$

$$D_o = \begin{vmatrix} a & b & b & c & b \\ b & a & b & b & c \\ b & b & a & b & b \\ c & b & b & a & b \\ b & c & b & b & a \end{vmatrix} \tag{III-8}$$

where

$$a \cong 1 - \frac{v}{(2\pi)^3} \int \frac{1 - \cos \vec{p}\cdot\vec{\rho}}{\gamma_o - \gamma_p}\, d^3p \tag{III-9}$$

$$b \cong \frac{v}{(2\pi)^3} \int \frac{\cos \vec{p}\cdot(\vec{\rho}-\vec{\rho}\,') - \cos \vec{p}\cdot\vec{\rho}\,'}{\gamma_o - \gamma_p}\, d^3p \tag{III-10}$$

$$c \cong \frac{v}{(2\pi)^3} \int \frac{\cos 2\vec{p}\cdot\vec{\rho} - \cos \vec{p}\cdot\vec{\rho}}{\gamma_o - \gamma_p}\, d^3p \tag{III-11}$$

The constants a, b, and c are independent of nearest neighbor distances $\vec{\rho}$. The computer results for the simple cubic lattice are

$$a = 0.833 \tag{III-12}$$

$$b = 0.0309$$

$$c = 0.0354$$

Substitution of these values into (III-7) and (III-8) gives

$$D = (.798)^3(.650) \tag{III-13}$$

$$D_o = (.798)^2(.625)$$

Thus, for a simple cubic lattice

$$D_o/D = 1.20 \tag{III-14}$$

It is estimated that this figure is correct to within an accuracy of about four per cent.

The Value of A_o for the Simple Cubic Lattice

The constant A_o defined by Eq. (II-15) is

$$A_o = \frac{v}{(2\pi)^3}\int \frac{\cos^2(\vec{p}\cdot\vec{\rho})}{\gamma_o - \gamma_p}\, d^3p \tag{III-15}$$

The computer calculation gives

$$A_o = 0.140 \tag{III-16}$$

Values of Constants Used in the Text

$$\nu = \begin{cases} 1 & \text{s.c.} \\ 2^{1/3} & \text{f.c.c.} \\ 3\times 2^{-4/3} & \text{b.c.c.} \end{cases} \tag{III-17}$$

$$\omega_o^2 = \begin{cases} \frac{33}{32} & \text{s.c.} \\ \frac{15}{16} & \text{f.c.c.} \\ \frac{281}{288} & \text{b.c.c.} \end{cases} \tag{III-18}$$

$$Q = \begin{cases} 1.68 & \text{s.c.} \\ 1.35 & \text{f.c.c.} \\ 1.45 & \text{b.c.c.} \end{cases} \tag{III-19}$$

The Watson integrals are

$$\lambda_0 = \frac{v}{(2\pi)^3}\int \frac{\gamma_0}{\gamma_0 - \gamma_p}\, d^3p = \begin{cases} 1.5164 & \text{s.c.} \\ 1.3447 & \text{f.c.c.} \\ 1.3932 & \text{b.c.c.} \end{cases} \qquad \text{(III-20)}$$

The Riemann-zeta functions have the values

$$\zeta(\tfrac{3}{2}) = 2.612 \qquad \text{(III-21)}$$

$$\zeta(\tfrac{5}{2}) = 1.341 \qquad \text{(III-22)}$$

$$\zeta(\tfrac{7}{2}) = 1.127 \qquad \text{(III-23)}$$

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