SPIN COMPLEXES IN FERROMAGNETISM

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ABSTRACT

The spin-wave theory in Heisenberg model of ferromagnetism is investigated with the Holstein - Primakoff transformation and with emphasis on the spin wave interactions. The temperature T_o below which the concept of magnons is valid is determined. By a special expansion formalism of operator $(1-a^+a/2S)^{\frac{1}{2}}$ which yields $1+(1-(1-\frac{1}{2S})^{\frac{1}{2}})a^+a$ it is shown that quantized spin waves which behave like spin 1 quasi-particles (with dispersion relation $\omega \sim k^2$) called magnons at temperatures $T < T_o$, are Bosons with an effective (negative) electrochemical potential μ that varies as T in the wave-wave interaction approximation. The various coefficients of T^ν in the expression of the spontaneous magnetization $M(T)/M(o) \equiv 1-(C_1T^{3/2}+C_2T^{5/2}+C_3T^{7/2}+C_4T^4)$ as well as the specific heat for some ferromagnets are calculated. The results are remarkably close to the experimental values obtained by other investigators. The method used enables one to deal especially with regimes of small spin values S for which μ differs substantially from zero. The influence of the chemical potential on some thermodynamic quantities are found for ferromagnets with Hexagonal-close-packed structures, as well as for cubic crystals. The existence of the spin wave interactions and hence of non-zero effective chemical potential is shown to give rise to a lowering of the thermodynamic internal energy with the implication that spin waves, on the average, form bound states called spin complexes. The kinematical as well as the dynamical interactions on the thermodynamic quantities are also found for some ferromagnets, by subjecting the magnons to intermediate statistics. The influence of the spin-wave-spin-wave-spin-wave interactions on the coefficients of T^{ν} in the expression of the spontaneous magnetization of some ferromagnets are found to be negligible in comparison with wave-wave interactions. An attempt is made to extend the above calculations to spin complexes in antiferromagnetism, a phenomenon which seems to be relevant to high temperature superconductivity.

DEDICATION

This work is dedicated to the Lord God Almighty in whom lies the mystery of wisdom and understanding.

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CERTIFICATION

I certify that this work was carried out by Miss Ibiyinka Agboola Ademokun in the Department of Physics, University of Ibadan, Ibadan.

1/12/88

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CHAPTER I

FERROMAGNETISM

1.1 Introduction

Our aim is to elucidate new concepts and formalism that are germane to the subject of spin waves in low temperature ferromagnetism using the metals Iron, Cobalt, Nickel, Gadolinium and Dysprosium as concrete examples.

Magnetism is a phenomenon displayed by, or a macroscopic property possessed by some charge-neutral material bodies whereby one body physically attracts or repels another. In fact, in the modern parlance, magnetism is one of the oldest of the observed phenomena in the history of science. According to CHIKAZUMI (1964), scientific investigations were first made in the sixteenth century by Gilbert, who studied terrestrial magnetism and magnetic induction. He found that a magnet loses its magnetism at high temperature. The most fruitful period in the study of electricity and magnetism came at the end of the eighteenth century and continued through the nineteenth century, culminating in the great Maxwell's equations. The law of magnetic interaction between two magnetic poles was discovered at the end of the eighteenth century.

Magnetism due to electric currents was investigated by Oersted, Ampere, Biot and Savart at the beginning of the nineteenth century. Arago tried to magnetize a magnetic substance by using an electric current. Discoveries of diamagnetism by Faraday, of magnetostriction (a deformation due to magnetization) by Joule, of the curie law by Curie, of hysteresis by Ewing were all made during the beginning of the nineteenth century. Ewing perhaps was the first person to study magnetic phenomena from the atomistic point of view. He tried to explain the phenomenon of hysteresis in terms of the magnetic interaction between molecular magnets. He was followed by Langevin and Weiss, who gave the correct interpretations of paramagnetism and ferromagnetism respectively from the atomistic stand point. It is now known that magnetism is caused by moving electric charges.

To look for elementary sources of a magnetic field, we may consider a circular current I, enclosing an area S. The combination IS = M is the magnetic Dipole moment of the circular current. The circular current, also called the current loop, is a magnetic dipole and thus a source of a magnetic field. But do such current loops exist in nature? According to Ampere's hypothesis, electric currents flow inside molecules and atoms, which implies that atoms and molecules are current loops, and therefore are magnetic dipoles. In fact, Ampere's hypothesis was confirmed when the electron structure of the atom had been understood. It was confirmed in the sense that electrons moving around atomic nuclei produce electric currents, and current loops produce the magnetic field. However, if these words are interpreted literally, in terms of classical (non-quantum) concepts, since only classical concepts were known in Ampere's time, the inescapable conclusion is that nature has no elementary magnets, that is, no smallest sources of a magnetic field since the average classical radius of such loops is zero. But this conclusion is in contradiction with the reality. It is incorrect because it ignores the quantum nature of the motion of microscopic particles. Classical mechanics, often referred to as Newtonian mechanics to emphasize the role of its creator, provides an accurate description of the motion of macroscopic bodies, but the motion of electrons in atoms is governed by quantum, not classical mechanics. This radically changes all properties of the atom, including its magnetic properties.

Quantum mechanics does not reject the fact that the gyromagnetic ratio for the electron is

$$(\gamma = e/2m_e) \qquad \ldots(1.1\text{-}1)$$

where e is the charge and m_e is the mass of an electron. Hence an electron in a state with the projection of its angular momentum equal to m, where m = 0, ±1, ±2, ...,±ℓ (according to space quantization) in quantum mechanics has the projection of its magnetic moment

$$M_z = \frac{e\hbar m}{2m_e}, \; m = 0, \pm 1, \pm 2, \ldots, \pm \ell \qquad \ldots(1.1\text{-}2)$$

and ħ is planck's constant.

The conclusion that this suggests is that a moving electron can constitute an elementary magnet, provided it is in a state with non-zero angular momentum. On the other hand, an electron moving round the nucleus may be in the state with zero angular momentum, (the S-state) in which case $M_z = 0$, too.

With the observations of the experiment carried out by Stern and Gerlach while sending a beam of silver atoms through a non-uniform magnetic field as well as the suspicion borne from an analysis of atomic spectra, a quantum particle may possess an INTRINSIC ANGULAR momentum. This is inherent to the particle in addition to the orbital angular momentum caused by the motion of the particle in space. Therefore an electron in a state with zero orbital angular momentum possesses a non-zero value for the projection of its magnetic moment by virtue of its intrinsic angular momentum.

This intrinsic momentum is also called SPIN. The projection of the intrinsic momentum of a particle can assume not only integral values but half integral values as well.

The magnetic moment of a free atom basically has four principal sources:

(i) the spin with which electrons are endowed.

(ii) their orbital angular momentum about the nucleus,

(iii) the combination of both intrinsic and orbital angular momenta J, and

(iv) the change in the orbital moment induced by an applied magnetic field.

The first three effects give paramagnetic contributions to the magnetization, and the fourth gives a diamagnetic contribution.

The most natural way to classify the magnetic properties of a material is by its response to an applied magnetic field. The response is characterized by the susceptibility X, in the relation

$$M = XB_o \qquad \ldots (1.1\text{-}3)$$

where M is the magnetization, or magnetic moment per unit volume, and B_o is the applied field.

Diamagnetic materials have a small, negative temperature independent susceptibility X. The magnitude of X is of the order of 10^{-6} cm^3/mole. Since it is negative, the induced moment is directed oppositely to the magnetic field. This kind of magnetism is a direct consequence of Lenz's law applied to the motions of the elementary charges (generally electrons) of the system. All materials have diamagnetic contributions to their susceptibilities, but for most materials, the diamagnetic contribution to X is small compared to the total, and is usually neglected.

For Paramagnets, the susceptibility is positive and temperature dependent. It is of the order of $10^{-3}cm^3$/mole at room temperature and varies approximately as 1/T, where

T is temperature. (see fig. 1.1). This kind of magnetic behaviour can be explained as a consequence of two opposing effects: one, the tendency of the applied field to orient the moments in the direction of the field, and the other, the tendency of thermal agitation to randomize the orientations of magnetic moments. The paramagnetic susceptibility varies linearly with B_o for small fields and consequently vanishes for zero applied field.

However, it is also well known that some crystals containing magnetic atoms develop a macroscopic magnetic moment in the absence of an applied field, if they are cooled to sufficiently low temperatures. These are ferromagnetic materials or simply ferromagnetics.

Ferromagnetism does not exist at all temperatures. As temperature increases, the intrinsic spontaneous magnetic moment of a body decreases and vanishes at a certain temperature T_c called the Curie temperature (See fig. 1.2). This of course occurs if the external magnetic field is zero. Above the Curie temperature, ferromagnetic materials become paramagnetic. At high temperatures all ferromagnetic materials are paramagnetic but not all paramagnetic materials are ferromagnetic at low temperatures. Different materials

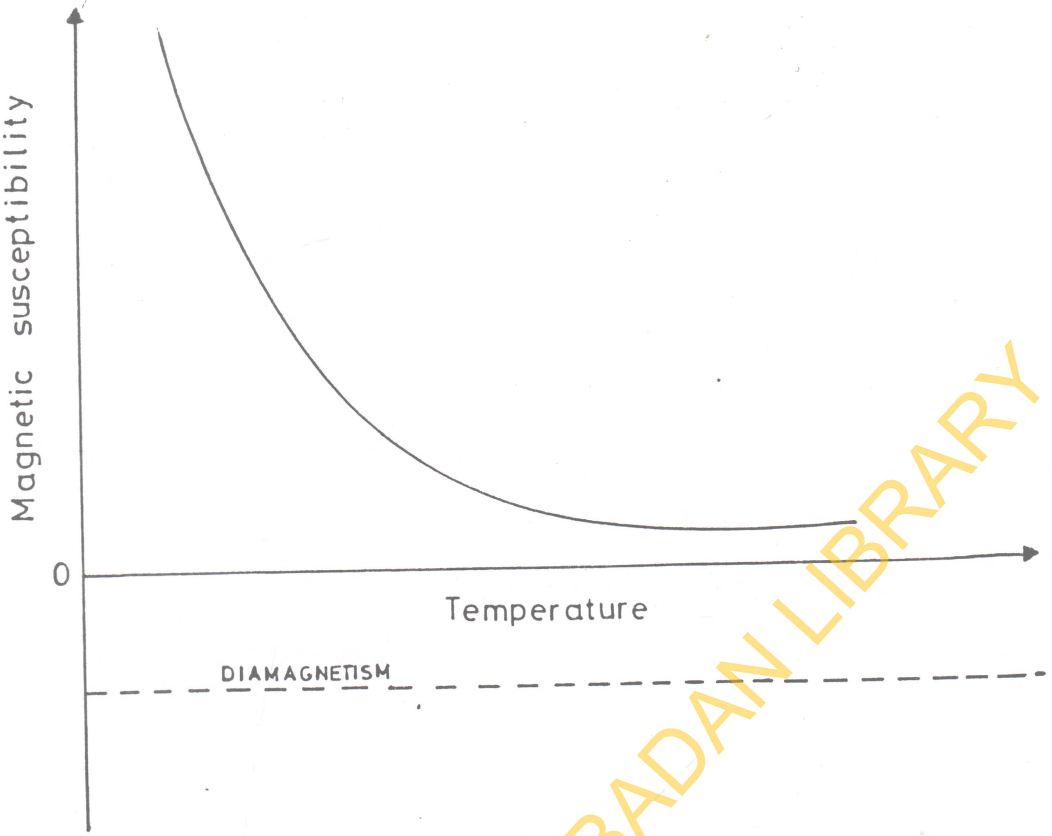


Fig.1.1 Characteristic magnetic susceptibility of diamagnetic and paramagnetic substances.

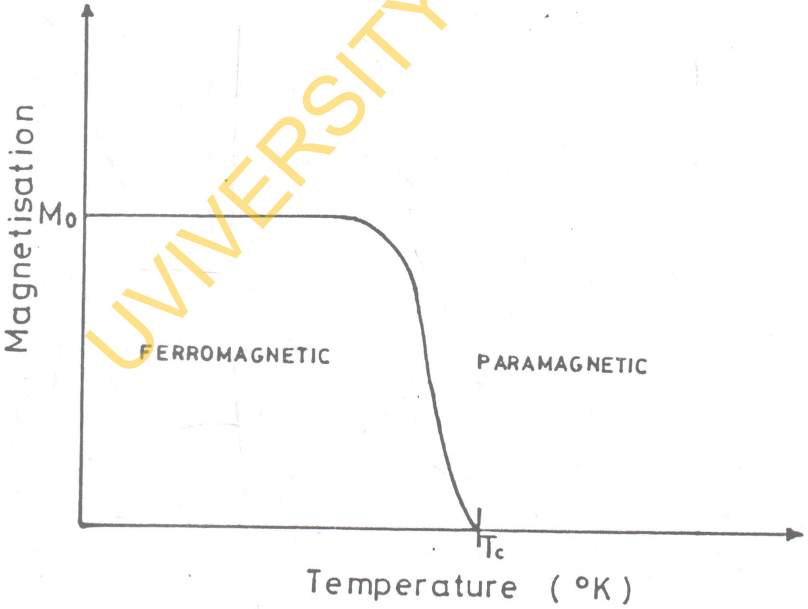


Fig. 1.2 Spontaneous magnetization as a function of temperature.

have different values of the curie temperature T_c and spontaneous magnetic moment density M_s at $T \to 0$.

Neel predicted the existence of another kind of cooperative magnetic phenomenon, which he called Antiferromagnetism. In the simplest form of an antiferromagnetic material, the lattice of magnetic atoms can be divided into two equivalent interpenetrating sublattices, A and B, such that A atoms have only B atoms as nearest neighbours, and vice versa. The magnetic interactions are such as to cause the sublattice magnetizations to be antiparallel. At absolute zero, each sublattice has its maximum saturation magnetization, and as the temperature increases, thermal agitation reduces the sublattice spontaneous magnetization in much the same way as for a ferromagnetic material. However, the net magnetic moment of the spontaneously magnetized antiferromagnet is zero at all temperatures, because of the exact cancellation of the spontaneous magnetization of the two equivalent sublattices.

The outstanding development in the phenomenological description of ferromagnetism is the theory of the molecular field by Weiss. Shortly before this, Langevin had developed his theory of paramagnetism based on the fundamental idea that the orientation of molecular dipole of moment $\underline{\mu}$ in a field $\underline{B}$ is governed by the Boltzmann's distribution law. Given N elementary dipoles per volume, each of magnetic dipole moment $\underline{\mu}$, in a magnetic field B, the kinetic energy E is given by

$$E = -\underline{\mu}\cdot\underline{B} = \mu B \text{ Cos } \theta ; \quad \mu = |\underline{\mu}|, \ B = |\underline{B}|, \qquad \ldots (1.1\text{-}4)$$

θ is the angle between $\underline{\mu}$ and $\underline{B}$. Writing

$$m = \frac{\langle \underline{\mu}\cdot\underline{B}\rangle}{|\underline{B}|} = \langle \mu \text{Cos}\theta \rangle \qquad \ldots (1.1\text{-}5)$$

$$m = \frac{\int_0^{\pi} \mu \text{Cos}\theta \ e^{\beta\mu B \text{Cos}\theta} 2\pi \text{Sin}\theta \ d\theta}{\int_0^{\pi} e^{\beta\mu B \text{Cos}\theta} 2\pi \text{Sin}\theta \ d\theta} \qquad \ldots (1.1\text{-}6)$$

$$M = Nm = N\mu \ \text{Cotanh}\beta\mu B - \frac{N}{\beta B} \qquad \ldots (1.1\text{-}7)$$

For small β (high temperature T) $\beta\mu B << 1$, for small x,

$$\tanh x = x - x^3/3, \quad \text{cotanh}x = (x - \frac{x^3}{3})^{-1} = \frac{1}{x(1-x^2/3)} = \frac{1}{x}(1 + \frac{x^2}{3})$$

$$m \simeq \mu(\frac{1}{\beta\mu B} + \frac{\beta\mu B}{3}) - \frac{1}{\beta B} \qquad \ldots (1.1\text{-}8)$$

$$M = \frac{N\mu^2\beta B}{3} = (\frac{N\mu^2}{3k})\frac{B}{T} \qquad \ldots (1.1\text{-}9)$$

The basic idea of the Weiss theory is that the effective field acting on an elementary magnet in a ferromagnetic medium is not to be identified with the applied field $\underline{B}$, but is rather to be taken as $\underline{B}+q\underline{M}$ where $\underline{M}$ is the intensity of magnetization and q is a proportionality factor independent of temperature. The portion qM is called the molecular field and is clearly a manifestation of the cooperative phenomenon by virtue of which the atomic magnets tend to be parallel. The Weiss theory has the merit of simplicity, for any phenomena can be explained by taking $B+qM$ instead of B in equation (1.1-7). With this modification with B replaced by $B+qM$, eqn. (1.1-7) becomes

$$M = N\mu\left[\left(\mathrm{Cotanh}\,\frac{\mu(B+qM)}{kT}\right) - \left(\frac{\mu(B+qM)}{kT}\right)^{-1}\right] \qquad ..(1.1\text{-}10)$$

If we neglect saturation effects, and so make the approximation

$$\mathrm{Cotanh}\,\mu\frac{(B+qM)}{kT} - \left(\mu\frac{(B+qM)}{kT}\right)^{-1} = \frac{1}{3}\mu\frac{(B+qM)}{kT}$$

approximate to small $\mu(B+qM)/kT$, then after solving for M, the relation (1.1-10) reduces to

$$\chi = \partial M/\partial B = N\mu^2/3k(T-T_c) \qquad ...\ (1.1\text{-}11)$$

Here X denotes the susceptibility and

$$T_c = N\mu^2 q/3k \qquad \ldots (1.1-12)$$

Equation (1.1-11) gives an infinite solution at $T = T_c$, and so the Weiss theory immediately gives us a critical point or CURIE TEMPERATURE. Below T_c it is no longer allowed to make the approximation above because the moment ceases to be linear in the field strength, enormous magnetization can be obtained without the necessity of corresponding applied fields, and the behaviour becomes ferromagnetic. This simple analysis furnishes a remarkably satisfactory description of the salient experimental facts. The two most important of the many successes of the Weiss theory are the following:

(i) The linear relation which is predicted by equation (1.1-11) between the reciprocal of the susceptibility and the temperature above the curie point. The linearity is on the whole quite well confirmed experimentally. As the temperature is lowered towards the curie point, the experimental curves begin to deviate more from linearity. The intercept on the axis $\frac{1}{X}$ i.e. $\frac{1}{X} = 0$, corresponds to infinite susceptibility, or in other words, to ferromagnetism. Usually it occurs at a lower temperature T_c', than the value T_c which is obtained by extrapolation from the linear behaviour at higher temperatures. The quantities T_c and T_c' are sometimes called the paramagnetic and ferromagnetic curie points, respectively. The difference between them is relatively small representing a second order effect.

(ii) The other success of the Weiss theory is its prediction concerning the variation of saturation magnetization with temperature below the curie point. The great mystery of the Weiss theory was how to explain the large molecular fields. They were supposed to be a manifestation of powerful coupling between elementary magnets. However, at the time, the only known interaction between them was the classical dipole - dipole coupling, whose potential is

$$V_{ij} = \frac{\mu_i \cdot \mu_j}{r_{ij}^3} - \frac{3(\mu_i \cdot r_{ij})(\mu_j \cdot r_{ij})}{r_{ij}^5} \quad \ldots (1.1\text{-}13)$$

where r_{ij} is the distance between the two dipoles.

However, this interaction is far too weak to yield the coupling required by the Weiss theory. It gives a maximum value 4π for the constant q in the molecular field qM, whereas the successful application of the Weiss theory requires that q be of the order 10^5.

The development of quantum mechanics was a great help in the understanding of ferromagnetic phenomena. In the first place it was accompanied by the Uhlenbeck - Goudsmit concept of electron spin. The latter has a ratio of magnetic moment to angular momentum equal to e/m instead of the classical $e/2m$. This behaviour is to be expected if most of the orbital angular momentum is largely destroyed by interatomic forces in the solid state leaving only the spin. The quantum theory of ferromagnetism is usually developed on the basis that the orbital contributions to the magnetic moment are negligible. Actually they cannot be forgotten entirely as evidenced by the fact that the gyromagnetic ratios of ferromagnetics are usually nearer 1.9 than 2.0.

One thing which quantum theory has obviously done is to introduce a discrete series of orientations rather than a continuous distribution as in the classical Langevin theory. That is, the kinetic energy E of each magnetic dipole μ in a magnetic field $\underset{\sim}{B}$, is given by

$$H = -\underline{\mu}\cdot\underline{B} = -\frac{e\hbar}{2m}\underline{L}\cdot\underline{B} = -\mu B.\underline{L} \qquad \ldots(1.1\text{-}14)$$

where L is the angular momentum operator with eigenvalues $\ell = -s, \; -s+1, \; \ldots, \; 0, \; 1, \; \ldots, \; s$

The partition function given by Trace $(\exp(-\beta H))$ is

$$Q_1 = \sum_{\ell=-s}^{s} e^{\beta\mu B\ell}$$

$$= e^{-\beta\mu Bs} \sum_{\ell=0}^{2s} e^{\beta\mu B\ell} \qquad \ldots(1.1\text{-}15)$$

If we put $\alpha = \beta\mu B$, then

$$Q_1 = e^{-\alpha s}(1-e^{(2s+1)\alpha})/(1-e^{\alpha})$$

$$= \frac{e^{-\alpha s} . e^{\frac{2s+1}{2}\alpha}(e^{-\frac{2s+1}{2}\alpha} - e^{\frac{2s+1}{2}\alpha})}{e^{\alpha/2}(e^{-\alpha/2} - e^{\alpha/2})} \qquad \ldots(1.1\text{-}15a)$$

$$Q_1 = \frac{\mathrm{Sinh}((2s+1)/2)\alpha}{\mathrm{Sinh}(\alpha/2)} \qquad \ldots(1.1\text{-}16)$$

$$m = \frac{1}{\beta}\frac{\partial}{\partial B}\ln Q_1 = \frac{\mu\partial}{\partial\alpha}\ln Q_1 \qquad \ldots(1.1\text{-}17)$$

$$m = \mu\{\frac{2s+1}{2}\,\mathrm{Cotanh}(\frac{2s+1}{2})\alpha - \frac{1}{2}\,\mathrm{Cotanh}\frac{\alpha}{2}\} \qquad \ldots(1.1\text{-}18)$$

The magnetization M is given by

$$M = Nm = N\mu\{\frac{2s+1}{2}\ \mathrm{Cotanh}(\frac{2s+1}{2})\alpha - \frac{1}{2}\mathrm{Cotanh}\frac{\alpha}{2}\} \qquad \ldots (1.1\text{-}19)$$

One important contribution of quantum mechanics is to unravel the mystery of the large Weiss molecular fields. The puzzle was solved by HEISENBERG (1926) who showed that the explanation is provided by the exchange forces characteristic of quantum mechanics. These interactions were a direct consequence of the restrictions placed on the wave functions by the Pauli Exclusion Principle. This principle requires that the electronic wave functions be antisymmetric with respect to exchange of space and spin coordinates of a pair of electrons, and it turns out that such a requirement makes the energy eigenvalues depend on the relative spin orientations of the electrons. This effect can then be interpreted in terms of an interaction which tends to orient the spin angular momenta (and consequently the magnetic moments) of the atoms.

This effect can be seen in the simplest case of the quantum mechanics of a two-electron system. Suppose that we have two electrons subject to fields derived from similar potential functions the Hamiltonian operator for the pair is then

$$H = \frac{-\hbar^2}{2m} \nabla_1^2 - \frac{\hbar^2}{2m} \nabla_2^2 + V(1)+V(2) + \frac{e^2}{r_{12}} = H^o + \frac{e^2}{r_{12}} \qquad \ldots (1.1\text{-}20)$$

where the numbers 1 and 2 refer to the spatial coordinates of the two electrons and r_{12} is the separation of the two electrons. If we begin by neglecting the interaction between the two electrons, we have a wave equation that satisfies

$$H^o\psi = E^o\psi \qquad \ldots (1.1\text{-}21)$$

which can be separated into independent wave equations involving each electron. There are then solutions

$$\psi = \psi_i(1)\psi_j(2), \quad E^o = E_i+E_j \qquad \ldots (1.1\text{-}22)$$

where ψ_i and ψ_j are solutions for a single electron moving in the potential V. If we apply first order perturbation theory to calculate the effect of the interaction, we find

$$E = E^o+\int \psi_i^*(1)\psi_j^*(2) \frac{e^2}{r_{12}} \psi_i(1)\psi_j(2)\, dr_1 dr_2 \qquad \ldots (1.1\text{-}23)$$

$$= E^o + C_{ij}$$

where C_{ij} has the physical interpretation as the average Coulomb interaction of two electrons in states i and j respectively. This result, however, was obtained without considering the Pauli principle, which requires that the total wave function be antisymmetric with respect to exchanging the space and spin coordinates of the two electrons. Quantum mechanics of electron spins shows that two spins of $s = \frac{1}{2}$ combine to give two states which may be characterized by the total spin S^1. The singlet s state $(S^1 = 0)$ is antisymmetric and the triplet t state $(S^1 = 1)$ is symmetric in the spin coordinates. The appropriate total wave functions are, (SMART 1966),

$$\psi_s = \frac{1}{\sqrt{2}}[\psi_i(1)\psi_j(2)+\psi_j(2)\psi_i(1)]\Phi \ , \ E_s^o = E_i+E_j$$

$$\psi_t = \frac{1}{\sqrt{2}}[\psi_i(1)\psi_j(2)-\psi_j(2)\psi_i(1)]\Phi \ , \ E_t^o = E_i+E_j \qquad \ldots(1.1\text{-}24)$$

where Φ is the spin function. These two functions are degenerate as they stand, but we now recalculate the first order perturbation contribution to the energy, we find

$$E_s = E^o+C_{ij}+J_{ij}$$

$$E_t = E^o+C_{ij}-J_{ij}$$

where

$$J_{ij} = \int \psi_i^*(1)\psi_j^*(2)\, \frac{e^2}{r_{12}}\, \psi_i(2)\psi_j(1)\, dr_1 dr_2 \qquad \ldots(1.1\text{-}25)$$

is the exchange energy of two electrons in states i and j.

DIRAC (1928) showed that for the special cases of localized electrons in orthogonal orbitals, the effect of the Pauli principle could be taken into account by adding to the Hamiltonian a term of the form

$$\sum_{i<j} -J_{ij}\,[\tfrac{1}{2} + 2S_i.S_j] \qquad \ldots\ (1.1\text{-}26)$$

This result suggests that the spin-dependent contributions to the energy arising from the Pauli Principle may for some purposes be regarded as caused by two body spin-spin interactions of the form

$$H = -2 \sum_{i<j} J_{ij} S_i \cdot S_j \qquad \ldots(1.1\text{-}27)$$

This operator is known as the Heisenberg Hamiltonian although its form was first deduced by Dirac and the first extensive use in magnetic theory by Van Vleck.

J_{ij} is called the exchange integral and in some situations super-exchange integral. The word exchange appeared because the symmetric and antisymmetric wave functions describe the state of electrons that are interchanged. The term exchange interaction emphasizes that the structure of the spin Hamiltonian is such that electrons are as if coupled through some specific interaction whose strength is a function of the relative orientation of the spins of electrons. In this sense the exchange interaction reminds us of the magnetic interaction. The exchange integral J_{ij} is a measure of interaction intensity. J_{ij} is predominantly negative, although cases of $J_{ij}>0$ do happen, and it is they that explain the most spectacular magnetic property, namely, ferromagnetism. For our work, we take $J_{ij}>0$, and our concern is not so much as to the origin of J, but on the consequence of the positive bond J in low temperature ferromagnetism.

1.2 The Heisenberg Model

The basic requirement of a fundamental theory in physics is that there must be a Hamiltonian. The question has always been: What Hamiltonian is appropriate to display spontaneous magnetisation? The Heisenberg model suggests that spontaneous magnetization arises from a coupling of the spin angular momenta, S_i rather than the total angular momenta J_i. This particular assumption is of course exact for atoms or ions with orbital angular momenta $L = 0$. It is a reasonable approximation for most of the transition metal series but is inappropriate for the rare earths like cesium, ytterbium, lutecium and others; since $L \neq 0$.

The crystal contains atoms with magnetic moments associated with their spin angular momenta. The magnetic atoms are assumed to interact in pairs according to (1.1-27) and to be subjected to an external applied field. In this case, neglecting the translational motion our starting model Hamiltonian for the crystal is

$$H = -2 \sum_{i<j} J_{ij} \underline{S}_i . \underline{S}_j - g\mu_B B_o \sum_i S_{i_z} \qquad \ldots (1.2\text{-}1)$$

where the first term on the right is the Heisenberg interaction energy and the second term is the Zeeman energy in an applied field B_o directed along the z axis. We introduce two additional restrictions on the Heisenberg model: we consider only cases in which all magnetic atoms are identical and all magnetic lattice sites are crystallographically equivalent. These restrictions are not arbitrary assumptions but rather are necessary conditions for the existence of ferromagnetism. It should be noted that this Hamiltonian neglects a number of factors which are important in determining the magnetic properties of real crystals. As mentioned previously we have not included possible orbital contributions to the magnetic moment. We have neglected the crystal field effects which give rise to magnetic anisotropy. We have also not included demagnetizing effects, which depend on the shape of the sample and may be quite important for systems near magnetic saturation. Moreover, the model is not sufficiently general to allow for anisotropic or antisymmetric exchange interactions. These neglected phenomena may have significant effects on the cooperative magnetic properties of particular crystals but in general they are of secondary importance compared to the terms in (1.2-1). To try to include everything simultaneously would result in a problem too cumbersome to handle by the techniques available. Rather we usually concentrate on the simple model (1.2-1) and try to show that it is capable of explaining the most important properties of ferromagnets.

If we consider only crystals with a single kind of magnetic atom and all magnetic lattice sites equivalent, then all nearest neighbour pairs have identical interactions. As exchange interactions are expected to fall rapidly with increasing distance it seems likely that only a few sets of interactions need be considered. So we restrict ourselves to the case of nearest neighbour only.

In principle, all the thermodynamic properties of the system described by this model with the above restrictions could be obtained by finding the eigenvalues of H, constructing the partition function and taking the appropriate partial derivatives. In practice this problem for a three-dimensional crystal is much too difficult to be solved by any frontal attack and various approximation methods of solution have been devised.

A way in which the Heisenberg model can be simplified is by changing the interaction potential. This is done in the so called Ising model.

1.3 The Lenz-Ising Model

The Lenz-Ising model is an attempt to simulate the structure of a physical ferromagnetic substance with high anisotropy. Its main virtues lies in the fact that a two-dimensional Ising model yields to an exact treatment in statistical mechanics. It is the only non-trivial example of phase transition that has been worked out with mathematical rigour (HUANG 1963).

In the Ising model, the system considered is an array of N fixed points called lattice sites that form an n-dimensional periodic lattice $(n = 1,2,3)$. The geometrical structure of the lattice may for example be cubic or hexagonal. Associated with each lattice is a spin variable $S_i (i = 1,...,N)$ which is a number that is either +1 or -1. There are no other variables. If $S_i = +1$, the i^{th} site is said to have spin up and if $S_i = -1$, it is said to have spin down. A given set of numbers $\{S_i\}$ specifies a configuration of the whole system.

The coupling energy is of the form $-2JS_{zi}S_{zj}$ rather than S as it is assumed that there is only one free spin per atom. In a certain sense the Ising model is a purely mathematical creation as it neglects the interactions $-2J(S_{xi}S_{xj} + S_{yi}S_{yj})$ between the components of spin perpendicular to the direction of the magnetic field, which are often important physically, except in highly anisotropic crystals.

The One-Dimensional Ising Model

The one-dimensional Ising model is a chain of N spins, each spin interacting only with its two nearest neighbours and with an external magnetic field B_o. The energy for the configuration specified by $\{S_1, S_2, \ldots, S_N\}$ is

$$E_I = -J\sum_{k=1}^{N} S_k S_{k+1} - B_o\sum_{k=1}^{N} S_k \qquad \ldots (1.3\text{-}1)$$

We impose the boundary condition,

$$S_{N+1} \equiv S_1 \qquad \ldots (1.3\text{-}2)$$

The partition function is

$$Q_I(B_o,T) = \sum_{S_1}\sum_{S_2},\ldots,\sum_{S_N} \exp[\beta\sum_{k=1}^{N}(JS_kS_{k+1}+B_oS_k)] \qquad \ldots (1.3\text{-}3)$$

where each S_k independently assumes the value ±1; we define,

$n_k = +1$ if $S_k = S_{k+1}$

$n_k = -1$ if $S_k = -S_{k+1}$

and note that $\sum_k S_k = \frac{1}{2}\sum_k(S_k+S_{k+1})$.

From the following,

S_k	S_{k+1}	n_k	$\sum_k S_k$
1	1	1	1
1	-1	-1	0
-1	1	-1	0
-1	-1	1	-1

the partition function is obtained as

$$Q_I = \sum_{\substack{\text{all} \\ \text{configuration}}} \sum_{n_k} \exp(\beta J n_k + \beta B_o S_k) \qquad \ldots (1.3\text{-}4)$$

$$= \prod_{k=1}^{N} \sum_{n_k} \exp(\beta J n_k + \beta B_o S_k) \qquad \ldots (1.3\text{-}5)$$

Then,

$$\ln Q_I = \sum_k \ln Q \, , \quad Q = \sum_{n_k} \exp(\beta J n_k + \beta B_o S_k)$$

$$Q = \exp(\beta J + \beta B_o) + \exp(\beta J - \beta B_o) + \exp(-\beta J) + \exp(-\beta J)$$

And,

$$m = \frac{1}{\beta} \frac{\partial}{\partial B_o} \ln Q \qquad \ldots (1.3\text{-}6)$$

or

$$Nm = N \frac{\exp(\beta J + \beta B_o) - \exp(\beta J - \beta B_o)}{\exp(\beta J + \beta B_o) + \exp(\beta J - \beta B_o) + 2e^{-\beta J}} \qquad \ldots . (1.3\text{-}7)$$

As $B_o \rightarrow 0$, $m \rightarrow 0$, and, there exists no spontaneous magnetization.

This result also holds for Heisenberg one dimensional model. Therefore the one-dimensional nearest neighbour Ising model does not exhibit ferromagnetism, although OJO,A. (1973) and others have shown that there exists ferromagnetism for a one-dimensional Ising model, with long- range interaction. There is a considerable literature on the calculation of crystalline characteristic values and curie points with the Ising model. Such treatments have the merit of being clear cut and rigorous for the assumed problem. However they have been confined primarily to one or two dimensional rather than three dimensional lattices. Even where a rigorous calculation with the Ising model is possible for the actual lattice pattern, the results should not be identified too closely with the actual magnetic behaviour of the material simply because of the inadequacy and arbitrariness of the model. This model of Ising and Lenz is too crude however to elucidate the low temperature thermodynamic properties of ordered magnetic systems. Fortunately another method, particularly adapted to the low temperature region was developed by Bloch (1930).

1.4 The Spin waves and Spin complexes

The starting point of Bloch's attack is Slater's observations that the characteristic values of the Heisenberg exchange coupling can be rigorously determined if the spins of all but one atom are parallel. The solutions can be interpreted as representing waves of disturbance in which the reversed spin is propagated through the crystal with various possible wavelengths. The fundamental hypothesis of the Bloch calculation is that if there are k reversed spins, the solution can be obtained by additive superposition of k solutions in which a single spin is reversed. This will be an allowable approximation only if k is small compared with N, so that the probability of two or more reversed spins being at the same point of the lattice is negligible. Hence the Bloch method of calculation with the Heisenberg model is only satisfactory in the immediate neighbourhood of complete saturation ($M = N\mu$) and consequently only at temperatures near absolute zero. This theory of Bloch explicitly assumes that the density of reversed spins is so small that the effects of obstruction and interaction between two or more Spin waves can be neglected. This is an approximation that will certainly be good at sufficiently low temperatures, less good at higher temperatures.

At higher temperatures, BETHE (1931) made a thorough study of the effects of Spin wave interactions in a one-dimensional chain of Spins. He showed that in addition to the elementary Bloch spin waves, there exist excitations in which a block of two or more reversed spins travel together through the chain to form a BOUND STATE called a SPIN COMPLEX. On the average, the energy of such a state is less than the sum of the energies of free spin waves.

1.5 Stoner's method

The Heisenberg theory which have discussed is based on the Heitler-London model. This model represents a non-polar approximation. It supposes that the electrons responsible for ferromagnetism always remain on the same atom and do not participate in electrical conduction. This is an idealization never completely realized in fact. Another limiting case is furnished by the model of ommerfeld. In this model of itinerant electrons, one supposes that the 3d electrons circulate independently and freely from one atom to another. The resulting momentary shortage or surplus of charge on any particular atom makes the crystal instantaneously polar. Theoretical calculations from this point of view have been made by Bloch, by Slater and especially by Stoner. Evidently, the truth is somewhere between the Heiter-London model and that of itinerant electrons.

The calculations of Stoner are based on a well defined, clear cut model. It is assumed that the electron energy levels are attributes of the whole crystal rather than the individual atom, and can be handled by the Fermi-Dirac Statistics. A molecular field is used to represent the exchange interaction. The Stoner procedure can hence be characterized as the superposition of the Weiss molecular field on the Sommerfeld theory of electronic conduction, and depicts what is called collective electron ferromagnetism.

One is apt to wonder whether from the agreement with experiment or other considerations, one can deduce whether the non polar Heisenberg model or the polar Stoner one comes closest to reality. It is impossible to say anything very definite on this subject.

The actual intermediate case which is between the Heitler-London model and that of itinerant electrons is what we have attempted to explain in our work. Instead of considering the individual spins of electrons, all the spins should be taken as a collective because each spin interacts with several other spins simultaneously, thereby causing some fluctuations in the spin values.

1.6 The motivation of our investigation

A new attack on the problem of Spin wave interactions was opened by HOLSTEIN AND PRIMAKOFF (1940). They considered the behaviour of a three dimensional ferromagnetic array of spins in an external magnetic field. They succeeded in defining a set of coordinates which describe accurately the quantum state of the system. In terms of these coordinates, the Hamiltonian of the system splits into two parts, one quadratic in the amplitudes and one of higher order. The quadratic part alone would give a theory of non-interacting spin waves. Identical with the linear approximation of Bloch, DYSON (1956) invented a general theory of spin wave interactions. In his theory, he defines two kinds of interactions. One is the kinematical interaction which arises from the fact that more than 2S+1 units of reversed spin (S is the magnitude of atomic spin in units of h) cannot be attached to the same atom. The other is the dynamical interaction which represents the non-diagonal part of the Hamiltonian in his basic set of states. Dyson critizes Holstein and Primakoff spin wave theory saying that although the kinematical interaction does not appear, the dynamical interaction is so strong in their treatment that one cannot get rid of mathematical difficulties.

Prior to Dyson's paper, several authors obtained correction terms in the expression of the spontaneous magnetization of ferromagnetism at low temperatures. Among these authors, SCHAFROTH (1954) and HEBERG (1954) followed the ideas of Holstein and Primakoff, they were neither in agreement with each other nor with Dyson. OGUCHI (1959) has shown that the origin of their incorrect results are not in Holstein-and-Primakoff's method itself, but in their poor approximations. Oguchi in his work, has shown that a careful treatment of Holstein and Primakoff's method gives the same results (to first order in 1/S) as Dyson's, Oguchi's treatment which is an expansion in 1/S is suitable for large S. We in our work study the interactions of spin waves in an Heisenberg model of a ferromagnet using Holstein and Primakoff's method. Our method as we shall show is very suitable for small S, that is for $\frac{1}{2} \leqslant S \leqslant 2$.

In chapter two, we outline the theory of spin waves and spin complexes, with emphasis on wave-wave interactions. Spin waves being essentially spin fluctuations, we examine the Temperature Limitation on the spin waves. The method of Holstein and Primakoff is outlined.

In chapter three, we introduce the spin wave-spin wave interactions. We realize magnons as ideal Bosons, with an effective electrochemical potential μ. We calculate the modification by μ of the Bloch coefficient of $T^{3/2}$ in the expressions for the spontaneous magnetization and of specific heat, in the cases of cubic ferromagnetic metals.

In chapter four, we apply our concept of effective chemical potential to the Hexagonal close packed ferromagnets and calculate the influence thereof. In Chapter five, we calculate the additional effects due to the dynamical and kinematical interactions. And chapter six gives the discussion, summary and conclusion of our investigations.

As usual in many-body problems, our investigations use the language of second-quantization in quantum mechanics and of quantum statistical mechanics. Let us give an outline of the language.

1.7 The Second Quantization Method

In a quantum-mechanical investigation of the system consisting of a large number of identical particles which interact weakly in an arbitrary manner we often use the the second quantization method. This method is particularly useful in a system where the number of particles is a variable quantity,

If we consider a system consisting of N identical non-interacting particles for example, the free electrons in a metal, or the phonons in a crystal, the Schrodinger equation for a stationary state in this system may be written

$$\sum_{i=1}^{N}\left[\frac{-\hbar^2}{2m}\Delta_i + V(r_i)\right]\psi(r_1,r_2,\ldots,r_N) = E\psi(r_1,r_2,\ldots,r_N) \quad \ldots (1.7\text{-}1)$$

where the first term refers to the kinetic energy in an operation form,

$$\Delta_i = \frac{\partial^2}{\partial x_i^2} + \frac{\partial^2}{\partial y_i^2} + \frac{\partial^2}{\partial z_i^2} \qquad \ldots (1.7\text{-}2)$$

m is the mass of each particle. The second term represents the potential energy as a function of the position vectors $r_i = \{x_i, y_i, z_i\}$ E denotes the binding energy of the whole system in a given stationary state. The solution to the above equation is usually taken in the form

$$\psi = \psi q_1(r_1)\psi q_2(r_2), \ldots, \psi q_N(r_N) \qquad \ldots (1.7\text{-}3)$$

where q_i labels a set of quantum numbers characterizing a given stationary state. Every q_i represents a full set of quantum numbers which describe the state as occupied by an individual particle. The functions ψq_i are the solutions to the Schrodinger equation for one particle,

$$\left[\frac{-\hbar^2}{2m}\Delta_i + V(r_i)\right]\psi q_i(r_i) = Eq_i\psi q_i(r_i) \qquad \ldots (1.7\text{-}4)$$

However, the wave function (1.7-3) does not satisfy the symmetry requirement. In general, it is neither symmetrical nor antisymmetrical with respect to the exchange of the coordinates of any two particles. Consider for instance, a system of two identical particles. Clearly the possible wave functions are given by a combination which is either symmetric or antisymmetric

$$\psi_{s,a} = \frac{1}{\sqrt{2}}[\psi_1(r_1)\psi_2(r_2) \pm \psi_2(r_1)\psi_1(r_2)] \qquad \ldots (1.7\text{-}5)$$

where s and a correspond to + and -, respectively. Each wave function is normalized to unity.

The above result can be generalized to a system having an arbitrarily large number of identical particles, N. In this case we require for the total wave function to be either symmetrical or antisymmetrical with respect to the permutation of the coordinates belonging to any pair of particles. In the former case we say that the particles obey Bose-Einstein statistics, whereas in the latter case we say that the particles obey Fermi-Dirac statistics. The former particles are called Bosons which according to Pauli's investigations have an integer spin in units $\hbar$ (e.g. photons, phonons, π-mesons). The latter particles are called fermions which according to the same Pauli's investigation have a half-integer spin in units $\hbar$ (e.g. electrons, nucleons, deuterons).

To expose the problem of second quantization in a complete form we start from the assumption that the system of N non-interacting particles, say bosons, is subjected to an external field. Then every boson occupies one state which belongs to the set of states whose energies are $E_o, E_1, E_2 \ldots$ Let us denote the corresponding wave functions with

$$\psi q_o(r),\ \psi q_1(r), \psi q_2(r) \ldots .$$

clearly the energy of such a general state is given by the matrix element of the single particle operator $H_1(r)$,

$$E_i = \int_{-\infty}^{\infty} \psi^* q_i(r_1)\, H_1(r_1)\, \psi q_i(r_1) d\tau_1 \qquad \ldots (1.7\text{-}6)$$

whereas the interaction between the particles is given by the matrix element of the two-particle operator $H_{12}(r_1,r_2)$

$$V_{ij} = \int d\tau_1 \int d\tau_2\, \psi^* q_i(r_1)\, \psi q^*_j(r_2) H_{12}(r_1,r_2) \psi q_j(r_2) \psi q_i(r_1) \quad \ldots (1.7\text{-}7)$$

$$W_{ij} = \int d\tau_1 \int d\tau_2\, \psi^* q_i(r_1)\, \psi^* q_j(r_2) H_{12}(r_1,r_2) \psi q_i(r_2) \psi q_j(r_2) \quad \ldots (1.7\text{-}8)$$

Let us assume that there are n_i identical bosons in a given state with the energy E_i. Clearly we must have $\Sigma n_i = N$, where the sum runs over all allowed states of the system, Since the Pauli exclusion principle does not apply to the boson system, any individual number n_i may be as large as possible provided that the total number of bosons N is sufficiently large.

Therefore instead of characterizing the system by giving the set of energies and the corresponding wave functions we may characterize it by giving the set of energies and the corresponding occupation numbers, n_i. Since the system is subject to an external field the particles are allowed in the course of time to change their positions in the configurational space and hence to make the transitions from one energy state to another. It is therefore desirable to introduce a specific operational formalism in order to account for the dynamical behaviour of the particles. For this purpose we consider the individual wave functions as the amplitudes of a field the absolute magnitude of which determines the probability of finding the particle in the state defined by a particular individual wave function. Hence we replace the wave functions $\psi q_i(r)$ and $\psi^* q_i(r)$ by a set of annihilation and creation operators as follows:

$$\begin{aligned} \psi q_i(r) &\rightarrow N^{\frac{1}{2}} \psi q_i(r) a_i , \\ \psi^* q_i(r) &\rightarrow N^{\frac{1}{2}} \psi^* q_i(r) a_i^+ , \end{aligned} \qquad \ldots (1.7\text{-}9)$$

where the operator a_i takes (annihilates) a boson from the state E_i to another state, and the operator a_i^+ brings (creates) to the state E_i a boson from another state.

The above operators satisfy the following commutation relations

$$[a_i, a_j^+] = \delta_{ij}$$

$$[a_i, a_j] = [a_i^+, a_j^+] = 0 \qquad \ldots (1,7\text{-}10)$$

the second relation embodies the fact that any two bosons may be interchanged without changing the sign of the wave functions.

To find a physical meaning for the first commutation relation in equation (1,7-10), we introduce the state vectors which characterize the given state completely. The state vectors are designated as

$$|n_o, n_1, n_2, \ldots\rangle \qquad \ldots (1.7\text{-}11)$$

to indicate that there are n_i identical bosons in a given state of energy E_i.

The matrix elements for the creation and annihilation operators are most conveniently defined by

$$a_i^+|n_o, n_1, \ldots, n_i, \ldots\rangle = (n_i+1)^{\frac{1}{2}}|n_o, n_1, \ldots, n_i+1 \ldots\rangle$$

$$a_i|n_o, n_1, \ldots, n_i, \ldots\rangle = (n_i)^{\frac{1}{2}}|n_o, n_1, \ldots, n_i-1 \ldots\rangle \qquad \ldots (1,7\text{-}12)$$

We may observe that the occupation number operator

$$N_i = a_i^+ a_i \qquad \text{... (1.7-13)}$$

has the following matrix element

$$N_i|n_o, n_1, \ldots, n_i \ldots\rangle = n_i|n_o, n_1, \ldots, n_i \ldots\rangle \qquad \text{... (1.7-14)}$$

Now the first commutation relation has a set of equivalent operational equations in the form

$$\begin{aligned}
a_i^+ N_i &= (N_i - 1)a_i^+ ,\\
a_i^{+2} a_i^2 &= a_i^+ N_i a_i = N_i(N_i-1)\\
a_i^{+3} a_i^3 &= a_i^{+2} N_i a_i^2 = N_i(N_i-1)(N_i-2)\\
&\cdot\\
&\cdot\\
&\cdot\\
a_i^{+k} a_i^k &= a_i^{+(k-1)} N_i a_i^{(k-1)} = N_i(N_i-1)\ldots(N_i-k+1)
\end{aligned} \qquad \text{...(1.7-15)}$$

Therefore the matrix elements of the above operational identities become

$$\langle n_o, n_1 \ldots n_i \ldots | a_i^{+k} a_i^k | n_o, n_1 \ldots n_i \ldots\rangle$$

$$= n_i(n_i-1)\ldots(n_i-k+1)\langle n_o, n_1, \ldots, n_i \ldots | n_o, n_1, \ldots, n_i \ldots\rangle$$

$$\text{... (1.7-16)}$$

Clearly the operator $a_i^{+k} a_i^k$ is a product of some operator and its hermitian conjugate, Therefore $n_i(n_i-1)\ldots(n_i-k+1)$ cannot be negative.

Using equation [(1.7-6 - (1.7-10)], we may write the total Hamiltonian in the form (see NOVAKOVIC (1975))

$$H = \sum_i E_i a_i^+ a_i + \frac{N}{2(N-1)} \sum_{i,j} (V_{ij}+W_{ij}) a_i^+ a_j^+ a_j a_i \quad \ldots (1.7\text{-}17)$$

where E_i, V_{ij} and W_{ij} denote the matrix elements of the single particle and two particle operators respectively. The summations are taken over all allowed states, so if N is sufficiently large then $N/(N-1)$ may be replaced by 1.

If we put $a_i^+ a_i = n_i$, $E_i = \hbar w_i$ and

$a_i^+ a_j^+ a_j a_i \equiv n_i n_j$, $V_{ij}+W_{ij} \equiv U_{ij}$,

we have

$$H = \sum_i \hbar w_i n_i + \frac{1}{2} \sum_{ij} U_{ij} n_i n_j \quad \ldots (1.7\text{-}18)$$

The first term on the right gives the Hamiltonian of an ideal gas of quantum harmonic oscillators. The second term depicts the mutual interactions among the oscillators. Hamiltonians of this type are very important in many-body systems. And in our investigations, as we shall see, such a Hamiltonian is the starting point in spin-wave theory.

CHAPTER II

SPIN WAVES AND SPIN COMPLEXES

In this chapter, we shall consider a collection of mutually interacting spin waves, and the existence of spin complexes.

2.1 Theory of Spin waves

One approach to the low-temperature thermodynamic behaviour of ferromagnets is provided by BLOCH (1930) theory of spin waves. In the ground state of the exchange Hamiltonian (1.2-1) which will be realized at zero degrees, each spin has the maximum allowable value of S_i^z, namely S.

A spin wave may be described as a sinusoidal disturbance of the spin system within simple cases, the amplitude at each magnetic ion site proportional to $S-S_i^z$.

Let us consider a linear chain, $S = \frac{1}{2}$ with periodic boundary conditions, The Hamiltonian will be written as

$$H = -\frac{1}{2}g\mu_B B_o \sum_i \sigma_i^z - \frac{1}{2}J\sum_{i,j}\left(\frac{1}{2}\sigma_i^+\sigma_j^- + \frac{1}{2}\sigma_i^-\sigma_j^+ + \sigma_i^z\sigma_j^z\right) \text{(See Fluggae (1966))} \quad \ldots (2.1\text{-}1)$$

(see Fluggae (1966)

where H has been expressed by means of the raising and lowering operators $S_i^{\pm} = S_{ix} \pm S_{iy}$ and of S_i^z, and for $S = \frac{1}{2}$, use has been made of the Pauli matrices σ_x, σ_y and σ_z where $\sigma^+ = \sigma_x + i\sigma_y, \sigma^- = \sigma_x - i\sigma_y$, $\underline{S}_i = \frac{\hbar}{2}\underline{\sigma}_i$ and

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

This Hamiltonian has the ground state eigenfunctions for N spins,

$$\psi_o = \alpha_1 \alpha_2 \alpha_3 \ldots \alpha_N \qquad (2.1\text{-}2)$$

where α is Spin-up state and β is spin-down state.

This is the state at zero degrees Kelvin. It represents the maximum alignment of spins or complete magnetization. As temperature increases the system will be excited out of the ground state. The next state may be thought of as one in which the i^{th} spin is reversed.

$$\phi_i = \alpha_1 \alpha_2 \ldots \alpha_{i-1} \beta_i \alpha_{i+1} \ldots \alpha_N \qquad \ldots(2.1\text{-}3)$$

However, this ϕ_i is not an eigenfunction of (2.1-1). An eigenfunction may be formed from a linear combination of ϕ_i, each member of the combination containing a reversal at a different magnetic ion site

$$\psi_k = \sum_i C_i^k \phi_i \qquad \ldots (2.1\text{-}4)$$

In a demonstration basic to Bloch's theory, SLATER showed that each such combination is equivalent to a wave like disturbance of wave number k, and that the allowed values of k can be determined from periodic boundary conditions.

The wave-like properties of the solutions (2.1-4) for the case of a linear chain are demonstrated as follows. Periodic boundary conditions are equivalent to bending the chain around in a ring so that the first spin is also the N+1 Spin. Each spin i has two nearest neighbours i+1 and i-1 with which it interacts through the exchange integral J. We then set out to evaluate the following inner product, obtained from the Schroedinger equation

$$\langle\phi_j|H|\psi_k\rangle = \langle\phi_j|E\;|\psi_k\rangle \qquad \ldots\;(2.1\text{-}4)$$

This yields

$$[E+\tfrac{1}{2}(N-2)g\mu_B B_o + \tfrac{1}{2}(N-4)J]C_j^k + J(C_{j+1}^k + C_{j-1}^k) = 0 \qquad \ldots(2.1\text{-}5)$$

We may assume solutions of the form

$$C_j^k = N^{-\frac{1}{2}}e^{ikja}, \qquad \ldots\;(2.1\text{-}6)$$

where a is the distance between spins. The periodic boundary conditions require C_j^k to equal C_{j+N}^k, and hence the allowed values of k are given by

$$kaN/2\pi = 0,1,2,\ldots,N-1 \qquad \ldots\;(2.1\text{-}7)$$

The wave like properties of the solutions (2.1-3) is shown by (2.1-6). When the latter is inserted into (2.1-5) there results an equation relating the energy E and the wave number k.

$$E+\tfrac{1}{2}(N-2)g\mu_B B_o + \tfrac{1}{2}(N-4)J+2J\text{Coska} = 0 \qquad \ldots (2.1\text{-}8)$$

which may be written as the following dispersion relation

$$E - E^o = \varepsilon_k = h\omega_k = g\mu_B B_o + 2J(1-\text{Coska}) \qquad \ldots (2.1\text{-}9)$$

where

$$E^o = -\tfrac{1}{2}Ng\mu_B B_o - \tfrac{1}{2}NJ \qquad \ldots (2.1\text{-}10)$$

is the ground state energy.

The energy ε_k is that required to excite the Spin wave. In three dimensions, the disperson relation according to BLOCH (1930) becomes

$$\varepsilon_k = g\mu_B B_o + 2SzJ(1-\gamma_k) \qquad \ldots (2.1\text{-}11)$$

where

$$\gamma_k = z^{-1}\Sigma_n \exp(-ik.r_n) \qquad \ldots (2.1\text{-}12)$$

Here $\underline{r}_n$ denotes the vectors to the z nearest neighbours.

We can with the above say that the dispersion law has been derived for a single spin wave in an otherwise perfectly aligned system of spin vectors. The question arises: Can a disturbance in a non-perfect system be pictured as a spin wave?

Bloch argued that this is reasonable at low temperatures and that the eigenstate of the ferromagnet should be very nearly a linear superposition of non-interacting spin waves of the form (2.1-4). Bloch's point was that the presence of one spin wave cannot seriously modify the derivation of the Dispersion law for a second spin wave, and similarly on up to n spin waves, provided n is much smaller than the number N of spins in the sample. Bloch's conjecture, if correct, furnishes the basis for a spin wave theory, and the thermodynamic properties of a ferromagnet can then be computed from statistical properties of superposed spin waves.

The first study of the validity of BLOCH's superposition conjecture was made by BETHE (1931) and limited to the linear chain with $S = \frac{1}{2}$.

2.2 Two-Spin-wave States

Consider, in analogy with (2.1-2), the functions

$$\phi_{j\ell} = \alpha_1\alpha_2 \ldots \beta_j \ldots \beta_\ell \ldots \alpha_n \qquad \ldots(2.2\text{-}1)$$

with two spin reversals, and form the combinations

$$\psi_k = \sum_{j,\ell} C^k_{j\ell}\, \phi_{j\ell} \qquad \ldots\ (2.2\text{-}2)$$

Here the possible combinations are classified by total momenta k, which are good quantum numbers since H is translationally invariant. In analogy with (2.1-4) we now form

$$<\phi_{j\ell}|H|\psi_k> = <\phi_{j\ell}|E|\psi_k> \qquad \ldots (2.2\text{-}3)$$

to obtain the characteristic equation for the $C^k_{j\ell}$:

$$(E-E^o-2g\mu_B B_o-4J)C^k_{j\ell}+J(C^k_{j,\ell-1}+C^k_{j,\ell+1,\ell}+C^k_{j-1,\ell})$$

$$= 0;\ j,\ell \text{ not neighbours} \qquad \ldots (2.2\text{-}4)$$

$$= J(C^k_{jj}+C^k_{\ell\ell}-C^k_{j\ell}-C^k_{\ell j}),\quad j,\ell \text{ neighbours}$$

We note that the right hand side of (2.2-4) is zero everywhere. If it were everywhere zero, a solution would be

$$C^k_{j\ell} = e^{iKR}\text{Cos } pr \qquad \ldots (2.2\text{-}5)$$

with

$$R = \tfrac{1}{2}(j+\ell)a;\quad r = (j-\ell)a \qquad \ldots (2.2\text{-}6)$$

This yields the energy

$$E-E^o = \varepsilon_k(p) = 2g\mu_B B_o+4J\,[1-\text{Cos}(\tfrac{1}{2}ka)\text{Cos}(pa)] \qquad \ldots (2.2\text{-}7)$$

With

$$K = k+k';\quad p = \tfrac{1}{2}(k-k') \qquad \ldots (2.2\text{-}8)$$

it is readily seen that this energy can be written

$$\varepsilon_k(p) = 2g\mu_B B_o+2J(1-\text{Cos } ka)+2J(1-\text{Cos } k'a) \qquad \ldots (2.2\text{-}9)$$

that is, the energy is simply the sum of the energies of two non-interacting spin waves of total momentum K and relative momentum p. The non-zero right hand terms in (2.2-4) thus account for interactions between the two spin waves.

These will mix states of different p, and hence the solutions are

$$C^{k}_{j\ell} = e^{iKR}\,[N^{-1}\Sigma_p e^{ipr} f(p)] = e^{ikR}F(r) \qquad \ldots (2.2\text{-}10)$$

with

$$f(p) = f(-p), \quad F(r) = F(-r) \qquad \ldots (2.2\text{-}11)$$

where $f(p) = \text{Cos } pr$.

In our investigation we are not interested in just two waves, but in a large collection of them. We shall show in chapter three that they constitute a system of spin complexes.

2.3 Temperature Limitation of Spin waves

The concept of spin waves and of magnons as quasi particles is not trivial, strictly speaking spin waves exist at absolute zero temperature. To clarify this AKIN OJO (1988), in his work on temperature limitation on spin waves has shown that instead of considering the individual spins of electrons, all the spins should be taken as a collective because each spin interacts with several other spins simultaneously, thereby causing some fluctuations in the spin values.

He has shown that the spin waves in a Heisenberg ferromagnet of curie temperature T_c, lattice constant a and nearest neighbour z have at temperature T the dispersion relation $\omega^2 = \omega_o^2 + CTk^2$. From this is inferred that spin waves (magnons) are well defined quasi-particles if $\pi/2a >> k >> k_A(T) \sim (z-1)T^{\frac{1}{2}}/T_c$ or equivalent if $T << T_o$ and $T_o \sim T_c^2/(z-1)^2$. We proceed to outline this work. The Heisenberg ferromagnet with the following Hamiltonian is considered

$$H = -J \sum_{j=1}^{N} \sum_{n} S_j . S_n, \qquad \ldots (2.3-1)$$

where $\{S_n\}$ are the z nearest-neighbour spins to spin j and J is the binary bond.

The dispersion relations of the spin waves are known to be

$$\omega_k = \frac{E_k}{\hbar} = \frac{4JS}{\hbar} \sum_{a} [1-\exp(ik.a)] = \omega_o \qquad \ldots (2.3-2)$$

where $|\underline{a}| = a$, the lattice constant.

The same dispersion relations are obtained if one uses the quantum dynamics

$$\frac{i\hbar dS_j}{dt} = [S_j,H[= [S_j,H_j], \qquad \ldots (2.3\text{-}3)$$

where

$$H_j = -J\sum_n S_j . S_n, \qquad \ldots (2.3\text{-}4)$$

and expand

$$S_j(t) = S_j^{(o)} + T_j(t) \qquad \ldots (2.3\text{-}5)$$

Under the approximation $S^o_{my} = S^o_{mx} = 0$, $S^o_{mz} = S$, for all m, and that $T_j \equiv T_{jx} + iT_{jy}$, $T_j \sim \exp(ik.R^o_j)$ where R_j is the position of spin S_j, one obtains

$$\frac{d}{dt}T_j = i\left(\frac{4JS}{\hbar}\right)F(k)T_j \equiv iG(k)T_j \qquad \ldots (2.3\text{-}6)$$

where the form factor is given by

$$F(k) = \sum_{\underline{a}}[1-\exp(i\underline{k}.\underline{a})] \qquad \ldots (2.3\text{-}7)$$

Instead of considering one spin, all the spins were taken as a collective, and use was therefore made of the Bohm-Pines collective coordinate method in PINES and BOHM (1952). AKIN OJO argued that the collective coordinate method is applicable because each spin interacts with several other spins simultaneously adding that the interactions are not of the binary collision type. At temperature $T>0$, the position R_j of S_j may differ from constant R_j^o.

The spin density at x is defined by

$$D(x) = \sum_{j=1}^{N} S_j \delta(x-R_j), \quad R_j = R_j(t) \qquad \ldots (2.3\text{-}8)$$

and

$$\delta D(x) = \sum_j T_j \delta(x-R_j)$$

is the spin deviation density. Then

$$\rho(k) = \int D(x)\exp(-ik.x)dx$$

$$= \sum_j S_j \exp(-ik.R_j) \qquad \ldots (2.3\text{-}9)$$

To first order,

$$\rho(k) = \rho^o(k) + \tau(k), \quad \text{with} \quad S_j = S_j^o + T_j,$$

$$\rho^o(k) = \sum_j S_j^o \exp(-ik.R_j), \qquad \ldots (2.3\text{-}10)$$

$$\tau(k) = \sum_j T_j \exp(-ik.R_j),$$

where

$$T_j = T_{jx} + iT_{jy}, \quad \tau(k) = \tau_x(k) + i\tau_y(k)$$

and define the expectation value of $\tau(k)$ by

$$L(k) = \langle\tau(k)\rangle \equiv \sum_j \langle T_j\rangle \exp(-ik.R_j) \qquad \ldots (2.3\text{-}11)$$

using equation (2.3-6) twice in the form

$$\frac{d}{dt}\langle T_j\rangle = iG(k)\langle T_j\rangle$$

we have

$$\frac{d^2L}{dt^2} = -G^2(k)L + \sum_j \langle T_j\rangle(-ik\cdot\dot{R}_j)^2\exp(-ik.R_j)$$

$$+ \sum_j -ik.[2iG(k)\dot{R}_j+\ddot{R}_j]\langle T_j\rangle\exp(-ik.R_j) \quad \ldots (2.3\text{-}12)$$

The second summation is zero if

$$2iG(k)\dot{R}_j+\ddot{R}_j = 0, \quad \text{for all } j, \quad \dot{R}_j \equiv \frac{dR_j}{dt} .$$

That is,

$$R_j(t) = R_j^0+r_j \exp(-i\Omega t), \Omega = 0 \text{ or } 2G \equiv 2\omega_o \quad \ldots (2.3\text{-}13)$$

This shows a fluctuation of the positions of the spins. We may use the Fermi-Dirac distribution at temperature T to average the velocities to obtain

$$(k\dot{R}_j)^2_{av} = k^2\langle V_j^2\rangle = k^2\theta/M \qquad \ldots (2.3\text{-}14)$$

where $\theta = k_BT$, k_B is the Boltzmann constant, and M is the mass of the collection of electrons that give rise to each spin S_j in which case if $|S_j| = S$, then $M = 2SM_e$,

M_e is the mass of an electron, and R_j is to be taken as the centre of charge or mass of such a collection. Consequently, equation (2.3-12) becomes

$$\frac{d^2L(k)}{dt^2} = [-G^2(k) - k^2\theta/M]L(k) \qquad \dots (2.3\text{-}15)$$

which gives the dispersion relation

$$\omega^2 = G^2+k^2(\theta/M) = \omega_o^2+(\theta/M)k^2 \qquad \dots (2.3\text{-}16)$$

It is well known that in the standard method, the temperature effects come in only when one determines the thermal average number of magnons, using the Bose-Einstein distribution at temperature T. But now, equation (2.3-13) shows that at $\theta > o$ the positions of the spins vibrate and equation (2.3-16) demonstrates that ω depends on θ. Equation (2.3-16) also enables one to estimate the value of k and of the temperature for which the quasi particles ($\omega \sim k^2$) called magnons are well defined. Obviously, $\omega \sim k^2$ provided in equation (2.3-16)

$$\omega_o^2 \gg (\theta/M)k^2 \qquad \dots (2.3\text{-}17)$$

In equation (2.3-7), $\omega_o = 2JSk^2a^2/\hbar$.

Hence,

$$\pi/2a >> k >> \hbar(\theta/M)^{\frac{1}{2}}/2JSa^2 \qquad \ldots (2.3\text{-}18)$$

and .. consequently,

$$k_BT = \theta << (2JSa/\hbar)^2M \doteq (2JSa/\hbar)^2/2SM_e \qquad \ldots (2.3\text{-}19)$$

are the conditions necessary to have magnons. These equivalent conditions are more concretely stated with the use of the RUSHBROOKE and WOOD (1958) expression

$$\frac{k_BT_c}{J} = \frac{5}{96}(z-1)(11x-1), \; x = S(S+1) \qquad \ldots (2.3\text{-}20)$$

for the cubic crystals, with

$k_B = 1.38\text{x}10^{-23}$, $M_e = 9.1\text{x}10^{-31}$ kg, $\hbar = 1.0546 \text{ x } 10^{-34}JS^{-1}$,
$a = 2.5\text{x}10^{-10}$ m and $S((S+1)^2) \leqslant \frac{1}{4}$.

We obtain the inequalities

$6\text{x}10^9 >> k >> k_A$ and $T<<T_o$, where

$$T_o = 2\text{x}10^{-3}[T_c/(z-1)]^2 \qquad \ldots (2.3.21)$$

Using these criteria, we compute the values of the temperature T_o, below which magnons are well-defined quasi-particles, for several metals. These values are displayed on Table 2.1

For the Hexagonal close packed crystals,

writing $\frac{k_BT_c}{J} = \theta_c$

we have

$$k_A = \hbar(\frac{k_B T}{m})^{\frac{1}{2}}/2SJa^2 = \hbar T^{\frac{1}{2}}\theta_c/(2SM_e)^{\frac{1}{2}}2Sa^2 k_B^{\frac{1}{2}}T_c$$

and

$$T_o = [\frac{6x10^9(2SM_e)^{\frac{1}{2}}x2Sa^2 k_B^{\frac{1}{2}}T_c}{\hbar\theta_c}]^2 = 1.23x10^{-3}(\frac{T_c}{\theta_c})^2 S^3$$

Table 2.1: Temperature T_o of some ferrometals

Ferrometals	Transition Temp T_c(k)	T_o(k)	Number of nearest neighbours z
IRON (BCC)	1040	44	8
COBALT (FCC)	1300	28	12
NICKEL (FCC)	630	7	12
GADOLINIUM (HCP)	292	0.4	12
DYSPROSIUM (HCP)	85	0.02	12

AKIN OJO showed that for iron (T_c = 1040K, z = 8), T_o = 44K; for f_{cc} cobalt (T_c = 1300K, z = 12), T_o= 28K; and for nickel (T_c = 630K, z = 12), T_o = 7K.

We have shown that for Gadolinium (T_c = 292K, z = 12), T_o = 0.4K, and for Dysprosium (T_c = 85K, z = 12), T_o = 0.02K.

For temperature $T >> T_o$, the second term in equation (2.3-16) dominates and then $\omega \sim k$, so that the spin waves are indeed waves. But then, the approximation $S_j = S_j^o + T_j$ is expected to be invalid, in which case the second order terms which feature wave-wave interactions must be included.

We can say that at $T >> T_o$, the wave-wave interactions becomes dominant and hence must not be neglected A way of accommodating them is by the method of Holstein and Primakoff, which we now outline.

2.4 The Method of Holstein and Primakoff

HOLSTEIN and PRIMAKOFF (1940) worked out a spin wave theory which includes the important dipolar and pseudo dipolar interactions. The general program is to treat spin waves as quantized particles subject to creation and annihilation operators. To this end, spin deviation operators are introduced,

$$N_\ell = S - S_\ell^z \qquad \ldots (2.4\text{-}1)$$

and the eigenstates ψ_E of the Hamiltonian are expanded in eigenstate ϕ of these operators

where

$$N_\ell \Phi_{n_1,\ldots,n_N} = N_\ell \Phi_{n_1,\ldots,n_N} \qquad \ldots (2.4\text{-}2)$$

Here N_ℓ, is the spin deviation of the ℓ^{th} atom, and n_ℓ is the eigenvalue.

The spin-raising and lowering operators have the following well known properties

$$S_\ell^+ \Phi_{n_\ell} = [(S-S_\ell{}^z)(S+S_\ell{}^z+1)]^{\frac{1}{2}} \Phi_{n_\ell -1} \qquad \ldots (2.4\text{-}3)$$

$$S_\ell^- \Phi_{n_\ell} = [(S+S_\ell^z)(S-S_\ell{}^z+1)]^{\frac{1}{2}} \Phi_{n_\ell +1} \qquad \ldots (2.4\text{-}4)$$

It is to be noted that the spin-raising operator lowers the number of spin deviations, and vice versa.

Creation and Annihilation operators, working directly on the spin deviations are now introduced.

$$a_\ell^+ \Phi_{n_\ell} = (n_\ell+1)^{\frac{1}{2}} \Phi_{n_\ell +1} \qquad \ldots (2.4\text{-}5)$$

$$a_\ell \Phi_{n_\ell} = (n_\ell)^{\frac{1}{2}} \Phi_{n_\ell -1} \qquad \ldots (2.4\text{-}6)$$

These operators have the property

$$a_\ell^+ a_\ell = N_\ell \qquad \ldots (2.4\text{-}7)$$

and satisfy the commutation relations

$$[a_\ell , a_m^+] = \delta_{\ell m}$$
$$[a_\ell^+ , a_m^+] = 0 = [a_\ell , a_m] \qquad \ldots(2.4\text{-}8)$$

From the above equations the following operator relations are easily deduced.

$$S_\ell^+ = (2S)^{\frac{1}{2}} f_\ell a_\ell \; ; \; S_\ell^- = (2S)^{\frac{1}{2}} a_\ell^+ f_\ell ; \; S_\ell^z = S - a_\ell^+ a_\ell \qquad \ldots (2.4\text{-}9)$$

where

$$f_\ell = [1-(a_\ell^+ a_\ell /2S)]^{\frac{1}{2}} \qquad \ldots (2.4\text{-}10)$$

These equations, when inserted into a spin Hamiltonian, constitute the Holstein-Primakoff transformation. If S_ℓ^- is applied repeatedly until the state $n_\ell = 2S$ is reached, f_ℓ becomes zero and further spin lowering has no effect. Therefore, although strictly speaking the Bose operators a_ℓ^+ are defined by the above equations in a space of infinite dimensions (n_ℓ allowed to run from 0 to ∞), the presence of f_ℓ in a spin Hamiltonian operator will ensure that n_ℓ stops at 2S as it must in a real ferromagnet. Another way of deriving the Holstein-Primakoff transformation is to assume from the start the form (2.4-9). The requirement that the spin operators obey their usual commutation rules then yields the commutation relations (2.4-8) for the a_ℓ indicating that a correct transformation to creation and annihilation operators of Bosons has been achieved.

The presence of the square root operator f_ℓ in this Hamiltonian leads to many of the mathematical difficulties of spin wave theory. It is claimed by Holstein and Primakoff that at low temperatures

(i) $f_\ell = [1-(\langle N_\ell\rangle/2S)]^{\frac{1}{2}} \cong 1$ ... (2.4-11)

where $\langle N_\ell\rangle$ is the average over a statistical distribution of the ferromagnetic eigenstates ψ_E, of the expectation value of n_ℓ in these states.

A further approximation made by Holstein and Primakoff is the neglect of terms of the form.

(ii) $a_\ell^+ a_\ell a_m^+ a_m = N_\ell N_m$ ... (2.4-12)

(iii) $a_\ell^+ a_\ell a_m^+ = N_\ell a_m^+$ ... (2.4-13)

These terms are smaller than the retained terms in the expression for the Hamiltonian operator.

Spin waves are introduced by the following Fourier expansions in terms of wave vectors k within a Brillouin zone of the reciprocal lattice

$$a_\ell = N^{-\frac{1}{2}} \sum_k \exp(\mp ik.r_\ell)a_k, \quad a_k^+ a_k = n_k \, ; \quad a_\ell \equiv a_\ell^- \qquad \ldots (2.4\text{-}14)$$

where the permissible values of k are determined by periodic boundary conditions.

With use of the commutation relations (2.4-8), it is easy to verify that

$$\begin{aligned} [a_k , a_k^+] &= \delta_{k,k'} \\ [a_{k'}, a_k] &= 0 \end{aligned} \qquad \ldots (2.4\text{-}15)$$

and hence the spin wave creation and annihilation operators $a_k^\pm$ are also Bose operators and the transformation (2.4-14) is canonical. The eigenvalues of operators n_k will be the numbers of spin waves $\bar{n}_k$.

This Holstein-Primakoff formalism forms the basis of our further investigation reported in the next chapter.

CHAPTER III

INTERACTIONS I

By using a special expansion formalism we shall show here that spin waves, when quantized are ideal Bosons with an effective chemical potential effected by wave-wave interactions.

3.1 Spin wave - Spin wave Interactions and Expansion Formalism

The nearest neighbour exchange interaction model of a ferromagnet is described by the following Hamiltonian

$$H = -2J \sum_{j,\ell} S_j \cdot S_\ell + B_o g\mu_B \sum_{j=1}^{N} S_j^z \qquad \ldots (3.1\text{-}1)$$

Here S_j is the spin operator at the j^{th} atom, N is the total number of atoms, g the Lande-g factor, μ_B the Bohr magneton, the summation is taken over all nearest-neighbour pairs, and the external magnetic field B_o is directed along the z-axis.

The spin variables in quantum mechanics are operators which obey the following commutation relations

$$[S^2, S_z] = 0,\ [S_z, S_+] = \hbar S_+,\ [S_z, S_-] = -\hbar S_-,\ [S_+, S_-] = 2\hbar S_z \qquad \ldots (3.1\text{-}1$$

where $S_\pm = S_x \pm iS_y$, $S^2 = S_x^2 + S_y^2 + S_z^2$

We take the simultaneous set of normalized eigenvectors of the operators S^2 and S_z which mutually commute as the basic representation. We denote the corresponding eigenvalues with S and M whereas their common eigenvector we denote with $|SM\rangle$. Clearly, there are 2S+1 different values for M,

$$-S \leqslant M \leqslant S$$

and with $\Delta M = \pm 1$. Also we have for $\hbar = 1$

$$\begin{aligned} S^2|SM\rangle &= S(S+1)|SM\rangle, \\ S_z|SM\rangle &= M|SM\rangle \end{aligned} \qquad \ldots (3.1\text{-}2)$$

For a given value of S the eigenvectors $|SM\rangle$ span a (2S+1) dimensional space. These eigenvectors form a set of orthogonal unit vectors,

$$\langle SM|S'M'\rangle = \Delta(S-S')\Delta(M-M') \qquad \ldots (3.1\text{-}3)$$

It is the task of quantum mechanics to evaluate the non-vanishing matrix elements of the operators S_+ and S_-. Here we quote the final result:

$$\begin{aligned} S_+|SM\rangle &= [(S-M)(S+M+1)]^{\frac{1}{2}}|SM+1\rangle \\ S_-|SM\rangle &= [(S+M)(S-M+1)]^{\frac{1}{2}}|SM-1\rangle \end{aligned} \qquad \ldots (3.1\text{-}4)$$

Instead of dealing with the quantum number M, we may introduce a quantum number n such that

$$n = S-M, \ \Delta n = -\Delta m \qquad \ldots (3.1\text{-}5)$$

The quantum number n gives a departure of the z component S_z from the fixed values $S_z = S$. Using (3.1-5) the matrix elements for the Spin components in units $\hbar = 1$ becomes

$$S_+|S,n\rangle = [(2S+1-n)n]^{\frac{1}{2}}|S,n-1\rangle$$
$$S_-|S,n\rangle = [(2S-n)(n+1)]^{\frac{1}{2}}|S,n+1\rangle \qquad \ldots (3.1\text{-}6)$$
$$S_z|S,n\rangle = (S-n)|S,n\rangle$$

The quantum number n may further be replaced by a set of creation and annihilation operators as follows:

$$n = a^+a$$
$$a^+|S,n\rangle = (n+1)^{\frac{1}{2}}|S,n+1\rangle \qquad \ldots (3.1\text{-}7)$$
$$a|S,n\rangle = \sqrt{n}|S,n-1\rangle$$

where the operator a^+ creates a departure of the z component S_z from the fixed value $-S$ whereas the operator a annihilates a departure of this component from the fixed value $-S$. The minimum and maximum values for n determine the limiting eigenvectors $|S,n=0\rangle$ and $|S,n=2S\rangle$. These eigenvectors are characterized by

$$a|S,n=0\rangle = a^+|S,n=2S\rangle = 0 \qquad \ldots (3.1\text{-}8)$$

We shall call the state corresponding to the eigenvector $|S,n=0\rangle$ the vacuum or ground state.

Using the introduced operators we may rewrite the matrix elements (3.1-6) in the form,

$$S_+|S,n> = (2S)^{\frac{1}{2}}(1-\varepsilon_+)^{\frac{1}{2}}a|S,n>$$
$$S_-|S,n> = (2S)^{\frac{1}{2}}a^+(1-\varepsilon_-)^{\frac{1}{2}}|S,n> \qquad \ldots (3.1\text{-}9)$$
$$S_z|S,n> = (S-a^+a)|S,n>$$

where

$$\varepsilon_+ = \frac{n-1}{2S}, \quad \varepsilon_- = \frac{n}{2S} \qquad \ldots (3.1\text{-}10)$$

We may present the matrix elements (3.1-6) in an alternative operational form. We have

$$S_+|S,n> = (2S)^{\frac{1}{2}}(1-a^+a|2S)^{\frac{1}{2}}a|s,n>$$
$$S_-|S,n> = (2S)^{\frac{1}{2}}a^+(1-a^+a/2S)^{\frac{1}{2}}|s,n> \qquad \ldots (3.1\text{-}11)$$
$$S_z|S,n> = (S-a^+a)|s,n>$$

Going back to our Hamiltonian (3.1-1), we express the Spin operators in the forms,

$$S_j^+ = S_j^x + iS_j^y = (2S)^{\frac{1}{2}}f_j(s)a_j,$$
$$S_j^- = S_j^x - iS_j^y = (2S)^{\frac{1}{2}}a_j^+ f_j(s), \qquad \ldots (3.1\text{-}12)$$
$$S_j^z = S-a_j^+a_j,$$

where

$$f_j(s) = \left(1 - \frac{a_j^+ a_j}{2S}\right)^{\frac{1}{2}} \qquad \ldots (3.1\text{-}13)$$

and the operator $a_j^+a_j = N_j$ is called the number operator and a_j^+ and a_j are to be regarded as the creation and annihilation operator of the Spin deviation, and they satisfy the commutation rule

$$a_j a_\ell^+ - a_j^+ a_\ell = \delta_{j\ell} \qquad \ldots (3.1\text{-}14)$$

as demonstrated in Appendix A.

Using these operators, the Hamiltonian (3.1-1) can be written as follows,

$$H = -2J \sum_{j,\ell} \tfrac{1}{2}[\, S_j^- S_\ell^+ + S_j^+ S_\ell^-] + S_j^z S_\ell^z - B_o g\mu_B \sum_{j=1}^{N} S_j^z \qquad \ldots (3.1\text{-}15)$$

or

$$H = -2J \sum_{j,\ell} \tfrac{1}{2}[2Sa_j^+ f_j(s) f_\ell(s) a_\ell - 2Sa_j^+ a_j + a_j^+ a_j a_\ell^+ a_\ell] - B_o g\mu_B \sum_j a_j^+ a_j \qquad \ldots (3,1.\text{-}16)$$

B_o is the imposed magnetic field which we set equal to zero $J>0$ is the binary bond, and we assume that there are N spins in volume V_o, each with z nearest neighbours.

<u>Expansion Formalism</u>:

Several authors have used the above stated Hamiltonian and expanded $f_j(s)$ up to some order, and thereby obtained spin waves as quasi particles which obey Bose-Einstein distribution with zero chemical potential.

NOVAKOVIC (1975) expanded

$$f_j(s) = \frac{1 - a_j^+ a_j}{4S} \qquad \ldots (3.1\text{-}17)$$

whilst OGUCHI (1959) went a step further. He expanded

$$f_j(s) = 1 - \frac{a_j^+ a_j}{4S} - \frac{a_j^+ a_j a_j^+ a_j}{32S^2} \qquad \ldots (3.1\text{-}18)$$

These expansions are good enough for large values of S. But for small values of S, we have discovered that in order to take into account the complete wave-wave interaction, Oguchi's expansion is not sufficient. Within the wave wave interaction approximation, neglecting wave-wave-wave and wave-wave-wave-wave interactions, etc, $f_j(s)$ must be expanded to all orders, and the two- product terms $(a_j^+ a_j)$ in $f_j(s)f_\ell(s)$ collected. Surprisingly the infinite series, in the two product terms, has a compact form.

Noting that,

$$(1-x)^{\frac{1}{2}} = 1-x/2 - x^2/8 - x^3/16 - 5x^4/128 - 7x^5/256 + \ldots$$

$$\equiv 1-R(x) \qquad \ldots (3.1\text{-}19)$$

and putting $a_j = a$, $a_\ell = b$, for convenience, we obtain

$$f_j(s)-1 = \frac{-a^+ a}{2(2S)} - \frac{a^+ a a^+ a}{8(2S)^2} - \frac{a^+ a a^+ a a^+ a}{16(2S)^3} \qquad \ldots (3.1\text{-}20)$$

We notice that every term in (3.1-20) contains a two product term a^+a. Take for instance, $a^+aa^+aa^+aa^+a$, and use the commutation relation

$$[a,a^+] = 1, \qquad \ldots (3.1\text{-}21)$$

to see that

$$a^+aa^+aa^+aa^+a = a^+(1+a^+a)(1+a^+a)(1+a^+a)a = a^+a+\ldots \qquad \ldots (3.1\text{-}22)$$

We take only these two product terms in equation (3.1-20), because in equation (3.1-16) $a_j^+f_jf_\ell a_\ell$ makes such terms become 4-product terms, which are the only ones necessary in a wave-wave interaction approximation.

With equation (3.1-22) and others like it, $f_j(s)$ becomes

$$1-\left(\frac{1}{2(2S)}+\frac{1}{8(2S)^2}+\frac{1}{16(2S)^3}+\ldots\right)a^+a \qquad \ldots (3.1\text{-}23)$$

$$= 1-R\left(\frac{1}{2S}\right)a^+a$$

where

$$R\left(\frac{1}{2S}\right) = \left(1-\frac{1}{2S}\right)^{\frac{1}{2}}-1 = -\lambda<0 \qquad \ldots (3.1\text{-}24)$$

Thus, the operator f_j is approximated by $1+\lambda a^+a$, and

$$f_jf_\ell = (1+\lambda a^+a)(1+\lambda b^+b) = 1+\lambda a^+a + \lambda b^+b \qquad \ldots (3.1\text{-}25)$$

up to the two-product terms. Consequently,

$$H = -J \sum_{j=\ell} [\,2Sa_j^+(1+\lambda a_j^+a_j+\lambda a_\ell^+a_\ell)a_\ell - 2Sa_j^+a_j+a_j^+a_ja_\ell^+a_\ell\,] \quad \ldots (3.1\text{-}26)$$

Using the Fourier transformations

$$a_k = N^{-\frac{1}{2}}\sum_k \exp(-ik\ )a_k; \quad a_j^+ = N^{-\frac{1}{2}}\sum_k \exp(ik_{j})a_k^+ \quad \ldots (3.1\text{-}27)$$

where k denotes a reciprocal lattice vector and N is the total number of ferromagnetic spins, in the Fourier-transformed Hamiltonian, we have expressions like

$$J(k) = \sum J(j-\ell)\exp[\,ik(j-\ell)\,] = J(k)^* = J(-k) \quad \ldots (3.1\text{-}28)$$

Such expressions are calculated in Appendix B for crystal lattices having a cubic symmetry and Hexagonal symmetry. As k → o the expansion is given by

$$J(k) = J\{1-(ka)^2/z + A(\phi,\theta)(ka)^4 - B(\phi,\theta)(ka)^6, \ldots\} \quad \ldots (3.1\text{-}29)$$

for the crystal lattice having a cubic symmetry; ...

z denotes the number of nearest neighbours, a is the lattice constant, and J denotes an effective exchange integral.

We can now transform every term appearing in the above Hamiltonian with the help of the fourier transform (3.1-27)

$$\sum J(j-\ell) = zNJ \quad \ldots (3.1\text{-}30)$$

$$\begin{aligned} 2S\sum J(j-\ell)a_j^+a_\ell &= 2SN^{-1}\sum J(j-\ell)a_k^+a_{k'}\exp i(k.j-k'.\ell) \\ &= 2SN^{-1}\sum zJ(k)a_k^+a_{k+p}\exp(-ip.\ell) \\ &= 2s\sum zJ(k)a_k^+a_k \quad \ldots (3.1,\text{-}31) \end{aligned}$$

where we have used the substitution $k' = k+p$ and

$$\sum_{\ell} \exp(-ip.\ell) = N\Delta(p) = \begin{cases} N & \text{if } p = 0 \\ 0 & \text{if } p \neq 0 \end{cases} \qquad \ldots (3.1\text{-}32)$$

This follows from the translational property for the reciprocal lattice vectors. Also the following relationship holds

$$\begin{aligned} \Sigma J(j-\ell) a_j^+ a_j &= N^{-1} \Sigma J(j-\ell) a_k^+ a_{k'} \exp[\, i(k-k').R] \\ &= \Sigma z J a_k^+ a_k \end{aligned} \qquad \ldots (3.1\text{-}33)$$

We also transform the remaining three terms in (3.1.26) which depend on four operators. The first of such terms is equal to

$$\sum_{\text{all } j,\ell} J(j-\ell) a_j^+ a_j a_\ell^+ a_\ell = N^{-2} \sum_{\text{all } j,\, \text{all } k} J(j-\ell) a_k^+ a_{k'} a_{k''}^+ a_{k'''} (\exp i(k.j-k'.j \; k''.\ell-k'''.\ell))$$

Here we introduce the substitution

$$k'' = k'+p', \quad k''' = k+p,$$

which leads the above exponential factor to

$$\exp[\, i(k-k')(j-\ell)] \times \exp[\, i(p-p').\ell]$$

and the above term becomes

$$= N^{-2} \sum_{k,k',p,p'} J(k-k') a_k^+ a_{k'} a_{k'+p'}^+ a_{k+p} \times \exp[\, i(p-p').\ell]$$

The sum over ℓ may be performed giving the factor

$$N\Delta(p-p'),$$

therefore the above term becomes

$$= N^{-1} \sum_{k,k',p} zJ(k-k')a_k^+ a_{k'} a_{k'+p}^+ a_{k+p}$$

There are two important contributions coming from the above term one with p = 0, the other with k = k'. The former contribution is equal to

$$= N^{-1} \sum_{k,k'} zJ(k-k')a_k^+ a_{k'}^+ a_k a_{k'} + N^{-1} \sum_{k,k'} zJ(k-k')a_k^+ a_k \qquad \ldots (3.1\text{-}34)$$

The latter contribution is equal to

$$= N^{-1} \sum_{k,p} zJa_k^+ a_{k+p}^+ a_k a_{k+p} + N^{-1} \sum_{k,p} zJa_k^+ a_{k+p}\Delta(p) \qquad \ldots (3.1\text{-}35)$$

By neglecting the second sum in equations (3.1-34) and (3.1-35) we finally obtain

$$\sum_{j,\ell} J(j-\ell)a_j^+ a_j a_\ell^+ a_\ell = N^{-1} \sum_{k,k'} z[J+J(k-k')] a_k^+ a_{k'}^+ a_k a_{k'} \qquad \ldots (3.1\text{-}36)$$

Using a similar set of transformations we arrive at the result

$$\sum_{j,\ell} J(j-\ell)a_j^+ a_\ell^+ a_\ell a_\ell = \sum_{j,\ell} J(j-\ell)a_j^+ a_\ell^+ a_j a_\ell$$

$$= N^{-1} \sum_{k,k'} z[J(k)+J(k')] a_k^+ a_{k'}^+ a_k a_{k'} \qquad \ldots (3.1\text{-}37)$$

Now we can write the Hamiltonian in the transformed form as follows

$$H = E_o + 2sz\sum_k (J - J(k)) a_k^+ a_k$$

$$+ N^{-1} \sum_{k,k'} z[J(k)+J(k')-1-J(k-k')] + z(\alpha-1)[J(k)+J(k')] a_k^+ a_{k'}^+ a_k a_{k'} \quad \ldots (3.1\text{-}38)$$

Here E_o stands for the energy of the ground state

$$E_o = -zNS^2J$$

If we put $k' = q$ and we write the above Hamiltonian as

$$H - E_o = \sum_k A_k n_k + N^{-1} \sum_{k,q} V_{kq} n_k n_q + N^{-1} \sum_{k,q} W_{kq} n_k n_q \quad \ldots (3.1.\text{-}39$$

$$= A + B + C$$

where

$$A_k = 2SJz[1-\gamma(k)]$$

$$V_{kq} = zJ[\gamma(k)+\gamma(q)-1-\gamma(k-q)]$$

$$W_{kq} = z(\alpha-1)J[\gamma(k)+\gamma(q)]$$

and

$$\alpha = \alpha(s) = 4s\lambda = 4s(1-(1-\frac{1}{2S})^{\frac{1}{2}}),$$

$$\gamma(k) = \sum_a \exp(ik.a)/z, \quad a = |\underline{a}|, \quad a^3 = V_o/N$$

we have $n_k = a_k^+ a_k$.

The first term A_k gives the energy of the elementary excitations at zero temperature exactly, so $\hbar\omega \equiv A_k$ is a dispersion law. These elementary excitations are called agnons, and the energy of a single magnon is just A_k .

In the limiting cases where $k \to o$, the dispersion law for Magnons is

$$A(k) = 2SJa^2k^2 = \hbar\omega \equiv Fk^2 \qquad \ldots (3.1\text{-}40)$$

The second and third terms of expression (3.1-39), B and C, respectively describe an interaction which is often called the magnon-magnon interaction or Spin wave - Spin wave interaction.

With the expansion $\gamma(k) = 1 - \frac{k^2a^2}{z} + \ldots$ to order k^2a^2, in equation (3.1-39), the second term $\langle V_{kq} \rangle$ is zero on averaging over an angle(and this is why we shall need to expand $\gamma(k)$ up to k^4a^4), for the cubic lattice.

Writing out the third term of expression (3.1-39) we have

$$C = N^{-1}J \sum_{kq} (\alpha-1)[2z-k^2a^2-q^2a^2]n_kn_q \qquad \ldots (3.1\text{-}41)$$

To this order of expansion of $\gamma(k)$ the effect of the wave-wave interaction is included in C as encapsuled by $\alpha(s)$. Rewriting our Hamiltonian, we obtain

$$H = \sum_k\{[2JSa^2+(\alpha-1)\frac{Ja^2}{N}\langle n_q\rangle[k^2+\frac{(\alpha-1)J}{N}\langle[2z-q^2a^2]n_q\rangle\}n_k \qquad \ldots (3.1\text{-}42)$$

Or,

$$H = \sum_k (F_o k^2 - \mu) n_k \qquad \ldots (3.1\text{-}43)$$

where

$$F_o = 2JSa^2 + (\alpha-1)Ja^2 \frac{\langle n_q \rangle}{N} = 2JSa^2 + F_1 \qquad \ldots (3.1\text{-}44)$$

$$\approx 2JSa^2 \equiv F$$

$$\mu = -\frac{(\alpha-1)}{N} J \langle [2z - q^2 a^2] n_q \rangle$$

In each case averaging in q space is done over the Bose Einstein distribution

$$f(q) \equiv \frac{1}{\exp(\beta F q^2 - \beta\mu) - 1} \qquad \ldots (3.1\text{-}45)$$

3.2 Chemical Potential in Spin wave Interaction Theory

Expression (3.1-43) which follows from (3.1-42) shows that there exists an effective chemical potential μ.

For a weakly interacting system, in the second quantization formalism, the Hamiltonian

$$H = \sum_k A_k n_k + \sum_{k,q} W_{kq} n_k n_q \qquad \ldots (3.2\text{-}1)$$

Note that the part of $\langle W_{kq} n_q \rangle$ that is independent of k, we have called the quantity μ, so that

$$H = \sum_k (\lambda_k - \mu) n_k \; , \quad \lambda_k \equiv A_k + F_1 k^2 \qquad \ldots (3.2\text{-}2)$$

And the grand partition function is

$$Z = \prod_k \sum_{n_k} e^{-\beta(\lambda_k-\mu)n_k} = \prod_k \frac{1}{1-\exp(-\beta(\lambda_k-\mu))} \qquad \ldots (3.2\text{-}3)$$

which gives the Bose-Einstein distribution

$$<n_k> = \frac{1}{\exp\beta(\lambda_k-\mu)-1}$$

Thus the system behaves like an ideal Bose gas of chemical potential μ. For this system we proceed to find out the nature of μ (analytically and numerically).

Rewriting μ explicitly we have,

$$\mu = (1-\alpha)\frac{J}{N} <[2z-q^2a^2]n_q> \qquad \ldots (3.2\text{-}5)$$

According to BOGOLIUBOV and SHIRKOV (1959), we make a transition from a discrete momentum representation to the continuous momentum representation by using the prescription

$$\sum_q \frac{<n_q>}{N} = \frac{V}{(2\pi)^3N}\int_0^\infty 4\pi<n_q>q^2dq$$

$$= \frac{V}{2N\pi^2}\int_0^\infty <n_q>q^2dq \qquad \ldots (3.2\text{-}6)$$

Therefore

$$\mu = (1-\alpha)J[\frac{2ZV}{2\pi^2N}\int_0^\infty \frac{q^2dq}{\exp\beta(Fq^2-\mu)-1} - \frac{a^2V}{2\pi^2N}\int_0^\infty \frac{q^4dq}{\exp\beta(Fq^2-\mu)-1} \qquad \ldots (3.2\text{-}7)$$

$$\frac{V}{2\pi^2 N}\int_0^\infty \frac{q^2 dq}{\exp\beta(Fq^2-\mu)-1} = \int_0^\infty q^2 \exp(-\beta(Fq^2-\mu))[1-\exp(-\beta(Fq^2-\mu))]^{-1} dq\,\frac{V}{2\pi^2 N}$$

$$= \frac{V}{2\pi^2 N}\int_0^\infty q^2 \sum_{m=1}^{\infty} e^{-m\beta(Fq^2-\mu)} dq$$

$$= \sum_{m=1}^{\infty} \frac{e^{m\beta\mu}}{(m\beta F)^{3/2}}\,\frac{V}{4\pi^2 N}\left(\frac{\pi}{4}\right)^{\frac{1}{2}} \qquad \ldots (3.2\text{-}8)$$

and putting

$$r = \left(\frac{\pi}{4}\right)\frac{1}{4\pi^2} = 0,022, \quad \tau = \frac{k_B T}{2JS}, \quad F = 2JSa^2,$$

we have,

$$\sum_q \frac{\langle n_q \rangle}{N} = \frac{V}{2\pi^2 N}\int_0^\infty \frac{q^2 dq}{\exp\beta(Fq^2-\mu)-1} = \tau^{3/2} r \sum_{m=1}^{\infty} \frac{e^{m\beta\mu}}{m^{3/2}} \qquad \ldots (3.2\text{-}9)$$

Equation (3.2-7) becomes

$$\mu = (1-\alpha)J[2zr\tau^{3/2}\sum_{m=1}^{\infty}\frac{e^{m\beta\mu}}{m^{3/2}} - r\tau^{5/2}\sum_{m=1}^{\infty}\frac{e^{m\beta\mu}}{m^{5/2}}] \qquad \ldots (3.2\text{-}10)$$

$$\mu \approx 2(1-\alpha)rzJ\tau^{3/2}\sum_{m=1}^{\infty}\exp(\beta\mu m)/m^{3/2} \qquad \ldots (3.2\text{-}11)$$

Obviously $\mu<0$, as expected of Bosons. With $|\mu| = u$, and for very large β, we may approximate $\exp(-m\beta\mu)$ for some large L, by

$$u = (\alpha-1)2zr\,J\,\tau^{3/2}\,\frac{(k_B T)^L}{u^L}\sum_{m=1}^{\infty}\frac{1}{m^{L+3/2}}$$

$$u = [\frac{(\alpha-1)rz}{S}]^{\frac{1}{2}}\ 2JS\tau \ \equiv\ G(\alpha)k_B T$$

That is,

$$\mu = -G(\alpha)k_B T \qquad \ldots (3.2\text{-}12)$$

Equation (3.2-12) gives the approximate solution to equation (3.2-10). μ as we can see is the EFFECTIVE ELECTROCHEMICAL POTENTIAL in the Bose Einstein distribution that governs the corresponding quasi-particles, with the dispersion relation $\hbar\omega = Fk^2 = 2JSa^2k^2$.

Thus far, we have been able to show that in a consistent expansion of $f_j(s) = (1 - \frac{a_j^+ a_j}{2S})^{\frac{1}{2}}$ up to wave wave interaction only, for Heisenberg ferromagnet of N spins in a physical volume V_o, each of spin S, with z nearest neighbours, bond J>0, the spin waves called magnons at temperature T are Bosons with effective chemical potential μ.

Instead of the above approximation, using a computer, we have solved numerically equation (3.2-10).

Writing

$$w = \frac{|\mu|}{J}$$

we have

$$w = 2(\alpha-1)rz\tau^{3/2} \sum_{m=1}^{\infty} \exp(-mw/2S\tau)/m^{3/2} \qquad \ldots (3.2\text{-}13)$$

neglecting smaller terms,

Using iterative technique, w has been solved for the values of τ between 0 and 0,50 and graphs of w against τ is plotted and shown in Figs. (3,2-1 - 3.2-4).

By the method of least-square-error curve fitting, we obtain the following expressions of w, in terms of τ for cubic lattices, for example, the simple cubic, body centred cubic and face centred cubic.

(i) Body-centred cubic (e.g. Fe) with $s = \frac{1}{2}$, $z = 7{,}5$

$$w = -1{,}889\times10^{-3}+0{,}160\tau+0{,}23\tau^{2} = 0.16\tau+0{,}23\tau^{2} \qquad \ldots (3.2\text{-}14)$$

(ii) Body-centred cubic (e.g. Fe) with $s = \frac{1}{2}$, $z = 8$

$$w = -1{,}974\times10^{-3}+0{,}168\tau+0{,}24\tau^{2} = 0.17\tau+0.24\tau^{2} \qquad \ldots (3.2\text{-}15)$$

(iii) Face-centred cubic (e.g. Ni) with $s = \frac{1}{2}$, $z = 12$

$$w = -2{,}567\times10^{-3}+0{,}228\tau+0{,}30\tau^{2} = 0.23\tau+0{,}30\tau^{2} \qquad \ldots (3.2\text{-}16)$$

(iv) Simple cubic, with $s = .6$, $z = 6$

$$w = -8.701\times10^{-4}+6.80\times10^{-2}\tau+0.12\tau^{2} = 0{,}068\tau+0.12\tau^{2} \qquad \ldots (3{,}2\text{-}17)$$

(v) Simple cubic, with $s = .8$, $z = 6$

$$w = -5{,}674\times10^{-4}+4{,}28\times10^{-2}\tau+0.086\tau^{2} = 0{,}043\tau+0{,}086\tau^{2} \qquad \ldots (3{,}2\text{-}18)$$

(vi) Simple cubic, with $s = .9$, $z = 6$

$$w = -4{,}894\times10^{-4}+3{,}64\times10^{-2}\tau+7{,}64\times10^{-2}\tau^{2} = 0{,}036\tau+0{,}076\tau^{2} \qquad \ldots (3.2\text{-}19)$$

(vii) Simple cubic, with $s = 1{,}5$, $z = 6$

$$w = -2.708\times10^{-4}+1.95\times10^{-2}\tau+4.59\times10^{-2}\tau^{2} = 0.019\tau+0.046\tau^{2} \qquad \ldots (3.2\text{-}20)$$

Fig. 3.2.1: Graph of Chemical Potential/Exchange integral W against reduced temperature.

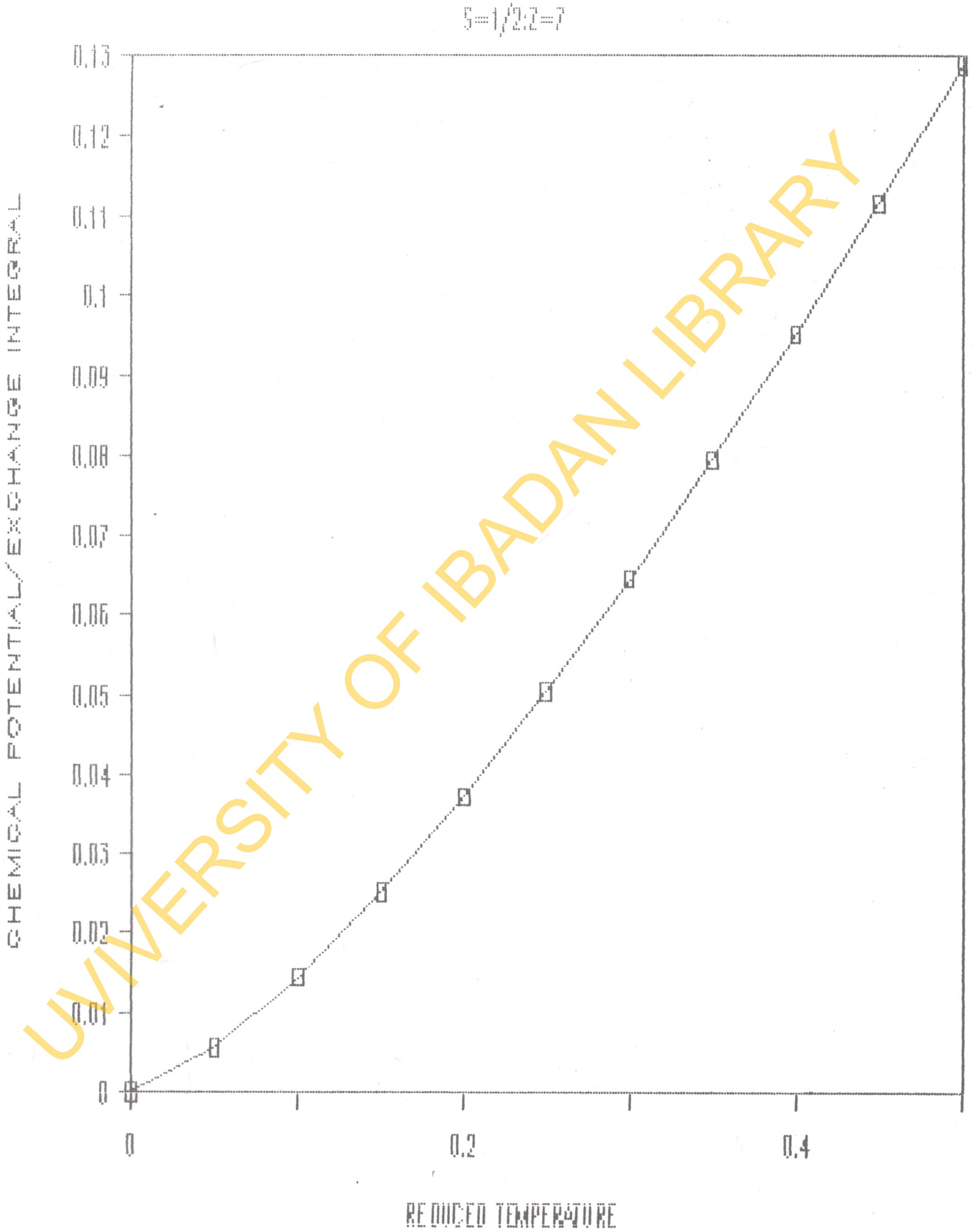


Fig. 3.2.2: Graph of Chemical Potential/Exchange integral W against reduced temperature

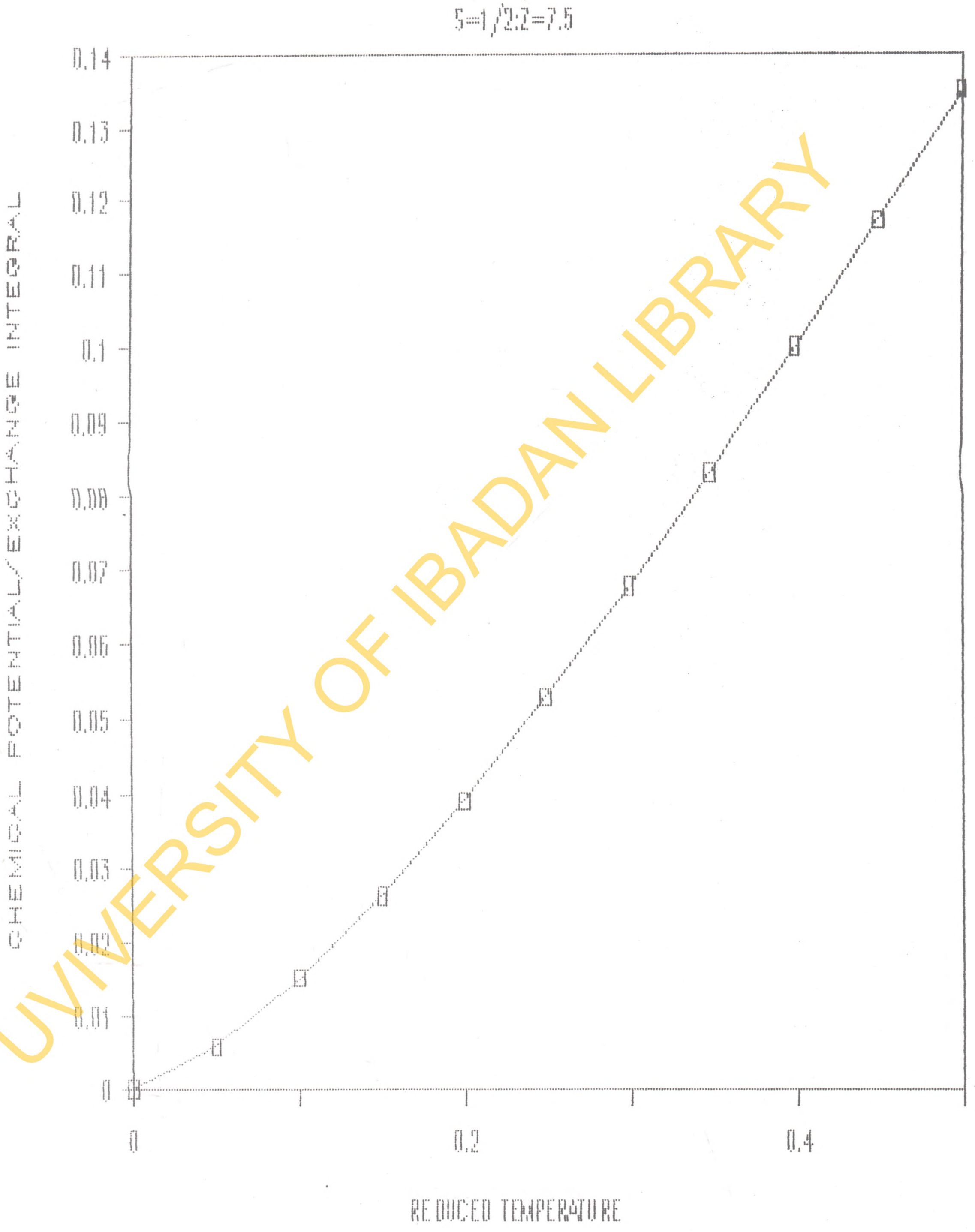


Fig. 3.2.3: Graph of Chemical Potential/Exchange integral W against reduced temperature.

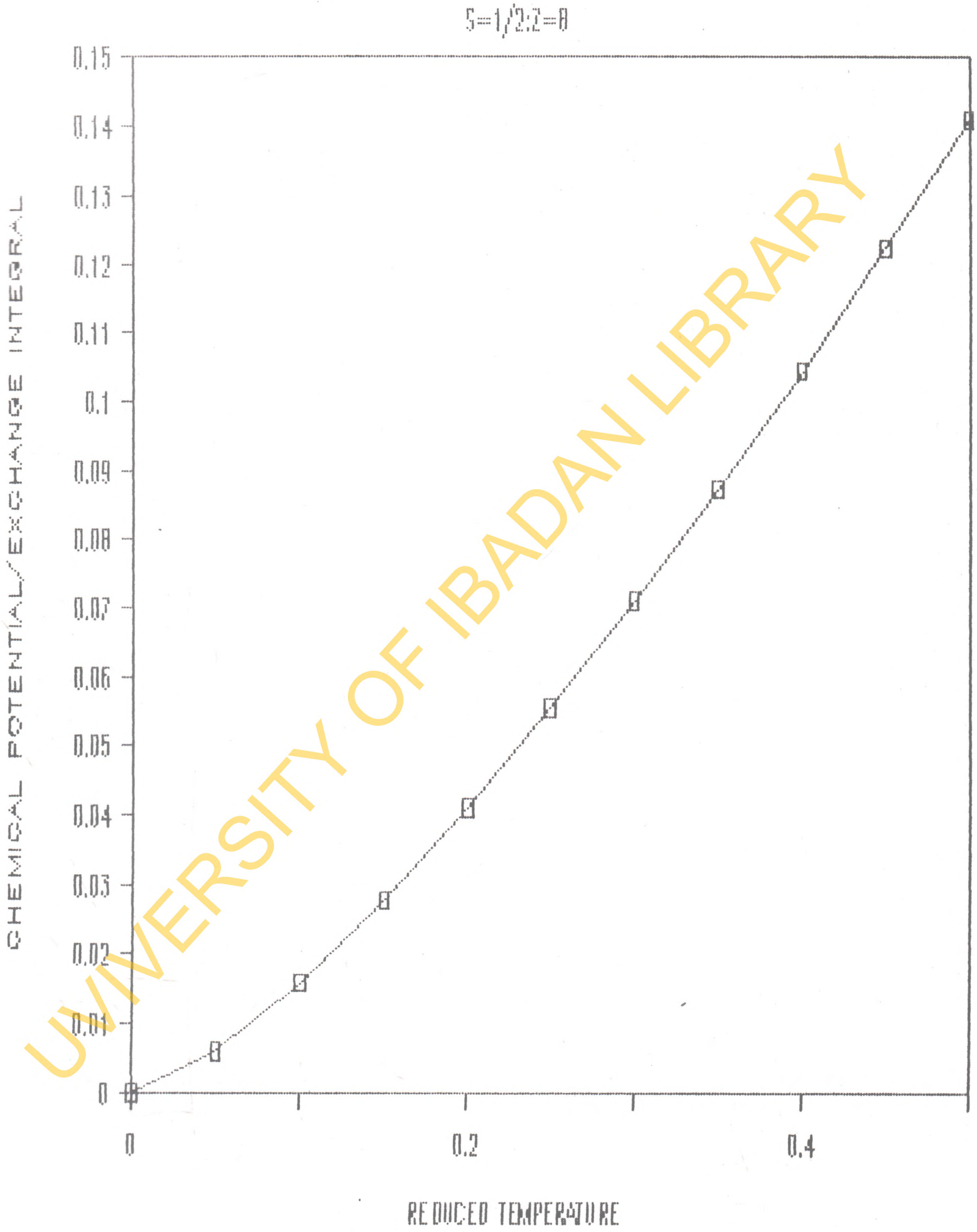


Fig. 3.2.4: Graph of Chemical Potential/Exchange integral W against reduced temperature.

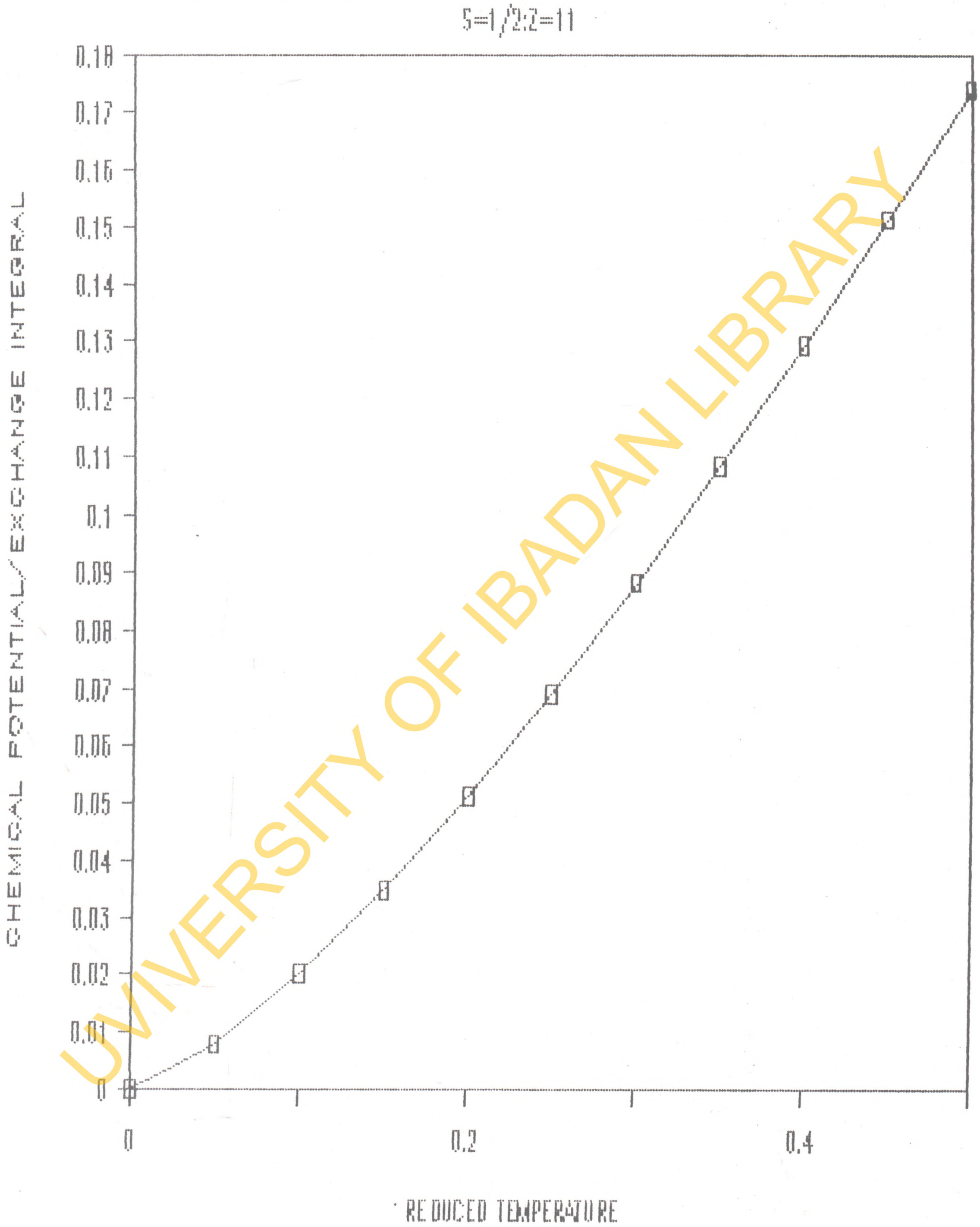
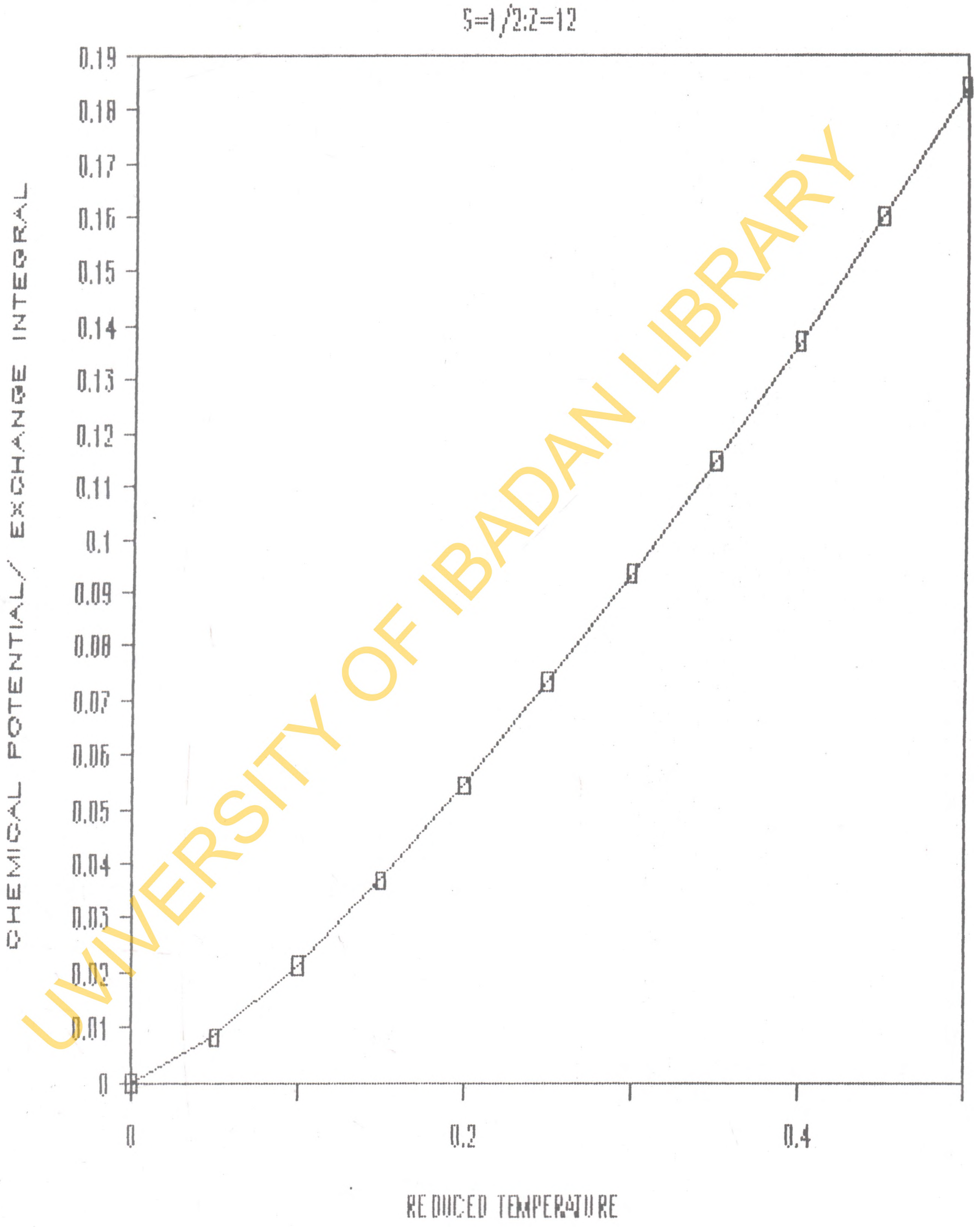


Fig. 3,2,5: Graph of Chemical Potential/Exchange integral W against reduced temperature.



(viii) Simple cubic, with s = 1,2, z = 6

$$w = -3.489\text{x}10^{-4}+2.54\text{x}10^{-2}\tau+5.72\text{x}10^{-2}\tau = 0.025\tau+0.057\tau^2 \qquad \ldots(3.2\text{-}21)$$

We see that in each case, w may be written as

$$w = w_1\tau + w_2\tau^2$$

so that G(α) from equation (3.2-12) becomes

$$G(\alpha) = \beta|\mu| = w_1/2S.$$

3.3 The Spontaneous Magnetization and Specific Heat

Having found the nature of the effective electro-chemical potential μ, we are interested in finding out the effect of μ on the coefficients of τ^ν in the expression for the spontaneous magnetization as well as on specific heat at low temperatures.

The spontaneous magnetization is defined by a thermal average of the z component of the magnetic moment and summed over a unit volume of the crystal.

$$M(T) = M(o)[1 - \frac{\langle n_k\rangle}{NS}] \qquad \ldots(3.3\text{-}1)$$

$$M(T) - M(o) \equiv \delta M(T) \qquad \ldots$$

$$\sum_k \frac{\langle n_k\rangle}{NS} = \frac{V}{(2\pi)^3 NS}\int \frac{k^2}{\exp\beta(Fk^2-\mu)-1}\,dk \qquad \ldots(3.3\text{-}2)$$

The third order approximation of F leads to

$$F = 2SJ[(ka)^2 - zA(\phi,\theta)(ka)^4 + zB(\phi,\theta)(ka)^6 + \ldots] \qquad \ldots (3.3\text{-}3)$$

$A(\phi,\theta)$ and $B(\phi,\theta)$ are evaluated in the Appendix C putting equation (3.3-3) in (3.3-2), we obtain

$$\sum_k \frac{\langle n_k \rangle}{NS} = \frac{V}{(2\pi)^2 NS} \int d\Omega \int_0^\infty \frac{k^2 dk}{\exp[\frac{k^2a^2}{\tau} - zA(\phi,\theta)\frac{(ka)^4}{\tau} + zB(\phi,\theta)\frac{(ka)^6}{\tau} - y] - 1} \qquad \ldots (3.3\text{-}4)$$

where $y = \mu/kT$

$$\sum_k \frac{n_k}{NS} = \frac{V}{(2\pi)^3 NS} \int d\Omega \sum_{m=1}^{\infty} e^{m\beta\mu} \int_0^\infty \frac{k^2 dk}{\exp[\frac{k^2a^2}{\tau} - zA(\phi,\theta)\frac{(ka)^4}{\tau} + zB(\phi,\theta)\frac{(ka)^6}{\tau}] - 1} \qquad \ldots (3.3\text{-}5)$$

Expression (3.3-5) is a very difficult integration, so we apply the technique of NOVAKOVIC (1975) by introducing the following substitutions.

$$S = C[1 - Dk^2 + Ek^4]k^2,$$

$$C = \frac{a^2}{\tau}$$

$$D = zA(\phi,\theta)a^2 \qquad \ldots (3.3\text{-}6)$$

$$E = zB(\phi,\theta)a^4$$

According to NOVAKOVIC (1975), we obtain

$$Ck^2 = S[1+D(\frac{S}{C} + \frac{DS^2}{C^2})-E(\frac{S^2}{C^2} + \frac{2DS^2}{C^3} + \frac{D^2S^2}{C^4})+D^2(\frac{S^2}{C^2} + \frac{2DS^2}{C^3} + \frac{D^2S^2}{C^4})] \quad \ldots (3.3\text{-}7)$$

$$k^2 = \frac{1}{C}[S^2+zA(\phi,\theta)\ S^2+(2z^2A^2(\phi,\theta)-zB(\phi,\theta)\ {}^2S^3+\ldots] \quad \ldots (3.3\text{-}8)$$

$$k^2dk = \frac{S^{\frac{1}{2}}}{2C^{3/2}}[1+\frac{S}{2}zA(\phi,\theta)\tau S+(8\ {}^2A^2(\phi,\theta)-\frac{7}{2}zB(\phi,\theta))(\tau S)^2+\ldots]dS \quad \ldots (3.3\text{-}9)$$

Equation (3.3-5) becomes

$$\sum_k \frac{\langle n_k\rangle}{NS} = \frac{V}{(2\pi)^3NS}\int_0^\infty dk \int_0^{2\pi} d\phi \int_0^\pi \frac{\sin\theta\, d\theta\, k^2}{\exp(S)-1}\sum_{m=1}^\infty e^{m\beta\mu} \quad \ldots (3.3\text{-}10)$$

Substituting (3.3-9) in (3.2-10) and writing

$$L_1 = \int_0^{2\pi} d\phi \int_0^\pi A(\phi,\theta)\sin\theta\ d\theta$$

$$L_2 = \int_0^{2\pi} d\phi \int_0^\pi A^2(\phi,\theta)\sin\theta\ d\theta \quad \ldots (3.3\text{-}11)$$

$$L_3 = \int_0^{2\pi} d\phi \int_0^\pi B(\phi,\theta)\sin\theta\ d\theta$$

we obtain

$$\sum_k \frac{\langle n_k\rangle}{NS} = \frac{V}{(2\pi)^3NS}C^{-3/2}\Sigma[\frac{e^{-my}}{m^{3/2}}\ 2\pi\ \Gamma(\frac{3}{2}) + \frac{5}{4}zL_1\Gamma(\frac{5}{2})\ \frac{e^{-my}}{m^{5/2}}\ \tau$$

$$+ (4z^2L_2 - \frac{7}{4}zL_3)\Gamma(\frac{7}{2})\frac{e^{-my}}{m^{7/2}}\ \tau^2+\ldots] \quad \ldots (3.3\text{-}12)$$

where Γ is the gamma function.

The first three terms of expression (3.3-12) gives the coefficients of $T^{3/2}$, $T^{5/2}$ and $T^{7/2}$ in the expression of

$$-\frac{\delta M(\tau)}{M(o)} \equiv C_1T^{3/2} + C_2T^{5/2} + C_3T^{7/2} + C_4T^4$$

In evaluating (3.3-12), we make use of $y = G(\alpha) = w_1/2S$ which has been evaluated in section (3.2).

The values of J are also needed for the various cubic structures. J is obtained from RUSHBROOKE and WOOD (1958) who arrived at the expression,

$$\theta_c = \frac{k_BT_c}{J} = \frac{5}{96}(z-1)(11S(S+1)-1) \qquad \ldots (3.3\text{-}13)$$

where k_B is the Boltzman's constant, T_c is the transition temperature, z is the number of the nearest neighbours, s is the spin values and J is the exchange integral. Writing

$$\tau = \frac{k_BT}{2JS} = \frac{\theta_c}{2ST_c} \cdot T \qquad \ldots (3.3\text{-}14)$$

With the substitution of (3.3-14) in (3.3-12), the various coefficients of T are obtained, and the effect of the electrochemical potential included. These have been done, and the results are tabulated in table 4.2. Note here that the coefficients so computed are the lower bounds, because of the presence of spin fluctuations discussed in chapter two.

We know that,

$$S_j(t) = S_j^o + T_j(t)$$

where

$$T_j(t) = \sum_k a_k e^{i(k_j - \omega t)}$$

$$\therefore \quad S = S_j = \langle S_j \rangle \geqslant \frac{1}{2} ,$$

we have made use of $s = \frac{1}{2}$. The average distance is $|\underline{a}| = a$ The average bound is J, the average number of nearest neighbours is z.

The specific heat is given by

$$C_v(T) = \frac{\partial}{\partial T}\langle H \rangle \qquad \ldots (3.3\text{-}15)$$

where

$$\langle H \rangle = N^{-1}\sum_k E(T,k)\langle n_k \rangle ; \quad E(T,k) = (Fk^2 - \mu)$$

and the internal energy $U(\mu)$ is given by

$$U \equiv \langle H \rangle = \frac{V}{2\pi^2 N}\int \frac{(Fk^2-\mu)}{\exp\beta(Fk^2-\mu)-1}\, k^2 \, dk \qquad \ldots (3.3\text{-}15a)$$

$$= \frac{V}{2\pi^2 N}\int \frac{Fk^2 \, dk}{\exp\beta(Fk^2-\mu)-1} - \frac{V}{2\pi^2 N}\int \frac{\mu k^2 dk}{\exp\beta(Fk^2-\mu)-1}$$

$$= \frac{V}{N}F\frac{3}{2}r(\beta F)^{-5/2}\sum \frac{e^{m\beta\mu}}{m^{5/2}} - \frac{V}{N}\mu r(\beta F)^{-3/2}\sum \frac{e^{m\beta\mu}}{m^{3/2}}$$

$$= \frac{2JS}{Q}\,\frac{3r}{2}(2JS)^{-5/2}(kT)^{5/2}\,\Sigma\,\frac{e^{+m\beta\mu}}{m^{5/2}} - \frac{\mu r}{Q}(2JS)^{-3/2}(kT)^{3/2}\,\Sigma\,\frac{e^{+m\beta\mu}}{m^{3/2}}$$

... (3.3-16)

$$C_v(T) = \frac{15}{4}\,\frac{2JS}{Q}(2JS)^{-5/2}k^{5/2}\,T^{3/2}\,\Sigma\frac{e^{+m\beta\mu}}{m^{5/2}} - \frac{yr}{2Q}\,3(2JS)^{3/2}k^{5/2}T^{3/2}\,\Sigma\,\frac{e^{+m\beta\mu}}{m^{3/2}}$$

$$= (2JS)^{-3/2}k^{5/2}T^{3/2}[\frac{15}{4Q}\,\Sigma\frac{e^{+m\beta\mu}}{m^{5/2}} + \frac{3\mu r\beta}{2Q}\,\Sigma\frac{e^{+m\beta\mu}}{m^{3/2}}$$

... (3.3-17)

where

$$r = \frac{1}{4\pi^2}\sqrt{\frac{\pi}{4}} = 0.022, \quad \beta\mu = Y, \quad \mu = YkT, \quad \frac{V}{N} = \frac{a^3}{Q}$$

and here k is Boltzmann constant. The second term of expression (3.3-17) is very small and may be neglected.

Calculations of the coefficients of $T^{3/2}$ for the specific heat has been made for Iron and Nickel with cubic lattice structures, and the effect of μ is significant on this coefficient (see table 4.2). We note that in eqn. (3.3-16)

$$U(\mu = 0) = \frac{2JS}{Q}\;\frac{3r}{2}(2JS)^{-5/2}(kT)^{5/2}\;\Sigma\frac{1}{m^{5/2}}$$

We now demonstrate that U increases with μ.

<u>On U(μ = 0) > U(μ<0)</u>

The internal energy per spin is

$$\frac{U}{N} = \frac{V}{2\pi^2 N}\int_0^\infty \frac{(Fk^2-\mu)k^2dk}{C-1} \quad \text{—}$$

... (3.3-17)

The number of magnons is

$$n = \frac{V}{2\pi^2 N}\int_0^{\infty} \frac{k^2 dk}{C-1} \qquad \ldots (3.3\text{-}18)$$

where $C = \exp(\beta(Fk^2-\mu))$

and

$$\frac{\partial C}{\partial \mu} = -\beta C; \quad \frac{dC}{\partial \beta} = (Fk^2-\mu)C$$

$$\frac{\partial n}{\partial \beta} = \frac{-V}{2\pi^2 N}\int_0^{\infty} \frac{(Fk^2-\mu)Ck^2 dk}{(C-1)^2} < 0 \qquad \ldots (3.3\text{-}19)$$

$$\frac{\partial (U/N)}{\partial \mu} = \frac{-V}{2\pi^2 N}\int_0^{\infty} \frac{k^2 dk}{C-1} + \frac{V}{2\pi^2}\frac{\beta}{N}\int_0^{\infty} \frac{(Fk^2-\mu)Ck^2 dk}{(C-1)^2}$$

$$= -n-\beta\frac{\partial n}{\partial \beta} \qquad \ldots (3.3\text{-}20)$$

Let

$$\beta\frac{\partial n}{\partial \beta} + n = \alpha(\beta) \quad \text{or}$$

$$\frac{\partial n}{\partial \beta} + \frac{1}{\beta}n = \frac{\alpha(\beta)}{\beta} \; ; \quad n(\infty) = 0 \qquad \ldots (3.3\text{-}21)$$

which has solution

$$n(\beta)-n(\infty) = \frac{1}{\beta}\int_{\infty}^{\beta} \alpha(\beta')d\beta' \qquad \ldots (3.3.22$$

For large β, but finite,

$$n(\beta)-n(\beta-\delta) = \frac{1}{\beta}\int_{\beta-\delta}^{\beta} \alpha(\beta')\delta\beta' \qquad \ldots (3.3\text{-}23)$$

with $o<\delta<<\beta$,

By (3.3.19), we have

$$0 > n(\beta)-n(\beta-\delta) \Rightarrow \alpha(\beta) < 0$$

That is

$$\partial\frac{(U/N)}{\partial\mu} = -n-\beta\frac{\partial n}{\partial\beta} = -\alpha(\beta) > 0$$

Therefore,

$$U(\mu = 0) > U(\mu < 0).$$

This implies that the existence of wave-wave interaction and hence of non-zero μ, gives rise to a lowering of the internal energy. In other words, the spin waves mutually interact in such a way that on the average they form bound states called spin complexes.

CHAPTER IV

THE HEXAGONAL CLOSE PACKED FERROMAGNETS

In this chapter, we apply the formalism used in Chapter III to the hexagonal ferromagnets.

4.1 The Hexagonal close packed ferromagnets

The ferromagnetic elements that have been discovered so far apart from the alloys includes Iron, Nickel, Cobalt, Dysprosium and Gadolinium. The first two have body centred and face centred cubic lattice structures respectively while the remaining three have Hexagonal close packed lattice structures.

In this section, we want to find the dependence of the coefficients of τ^{ν} on the electrochemical potential (μ) in the expression of spontaneous magnetization and specific heat for ferromagnets with Hexagonal close packed structures. This of course involves finding the correct expansion for the terms encapsuled in the dispersion relation.

For the cubic crystals, the Hamiltonian is written as

$$H = \sum_{k}(Fk^2-\mu)n_k \qquad \ldots (4.1\text{-}1)$$

where

$$F = 2zS[J-J(k)]/k^2 \qquad \ldots (4.1\text{-}2)$$

$$J(k) = \frac{1}{z}\sum_{\ell=1}^{z} J_{j\ell}\exp[ik.(R_j - R_\ell)]$$

$$= \frac{1}{z}\sum_{\ell=1}^{12} J_{j\ell}\text{Cos}[k.(R_j - R_\ell)] \qquad \ldots (4.1\text{-}3)$$

Let us put $R_j = (0,0,0)$ and $R_\ell = (x_\ell, y_\ell, z_\ell)$

The Reciprocal lattice vector is defined by

$k = \{k_x, k_y, k_z\}$

$k_x = k\text{Cos}\phi\text{Sin}\theta$

$k_y = k\text{Sin}\phi\text{Sin}\theta$

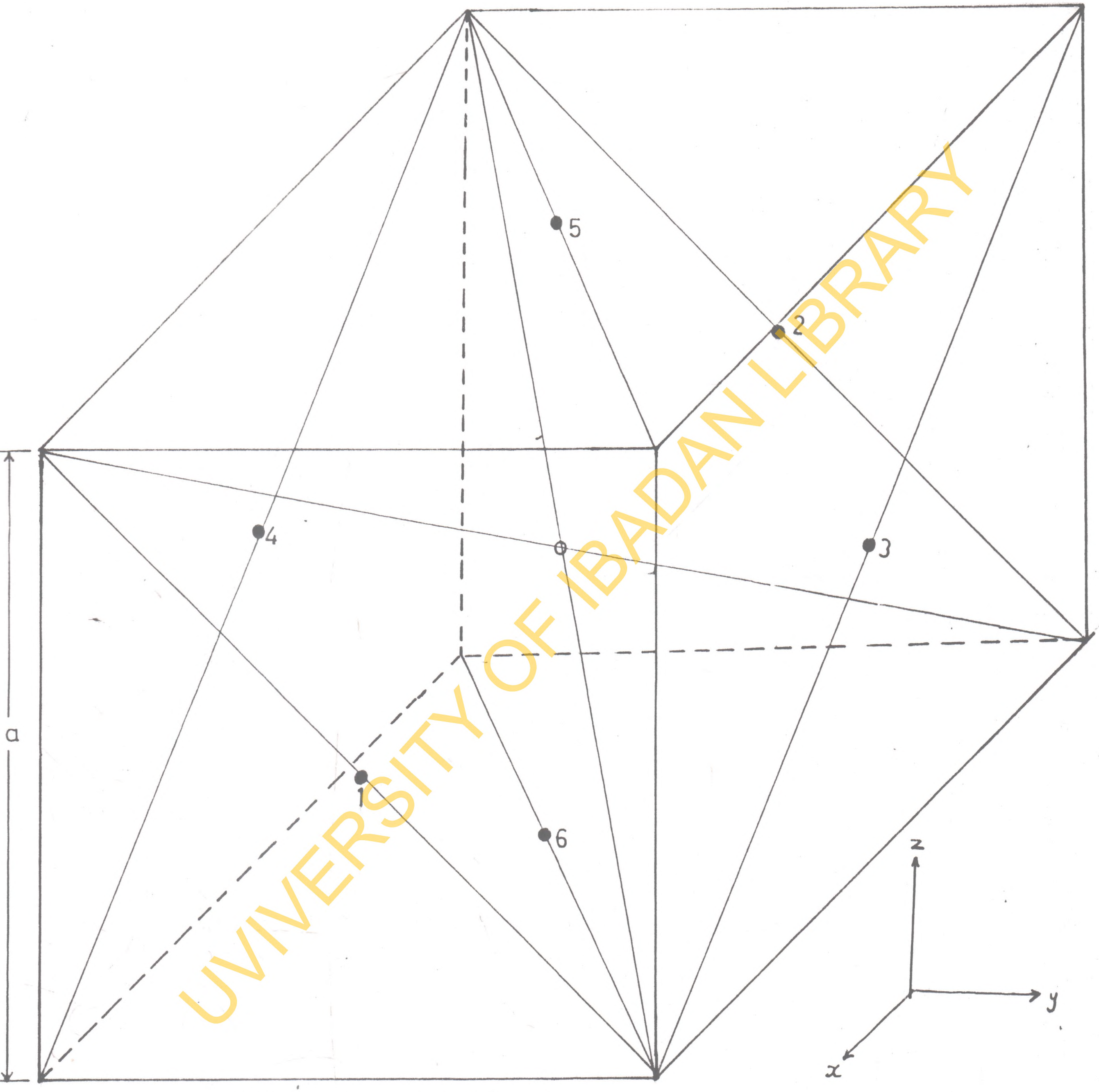
$k_z = k\text{Cos}\theta$

The nearest neighbour distances are given in Tables (4.1)i to (4.1)iii.

Table (4.1)i - Nearest neighbour Distances on a Simple cubic lattice in units a

ℓ	1	2	3	4	5	6	
x	1	-1	0	0	0	0	
y	0	0	1	-1	0	0	See Fig.(4.1)i
z	0	0	0	0	1	-1	

Fig. 4.1i - A given atom with six nearest neighbours on the simple cubic lattice



o ≡ given atom at (0,0,0)
● ≡ nearest neighbours.

Table (4,1ii) - Nearest neighbour Distances on body centered cubic lattice in units a/2

ℓ	1	2	3	4	5	6	7	8
x	1	1	-1	-1	1	1	-1	-1
y	-1	1	1	-1	-1	1	1	-1
z	1	1	1	+1	-1	-1	-1	-1

See Fig. (4,1ii)

Table (4,1iii) - Nearest neighbour Distances on a Face centered cubic lattice in units a/2

ℓ	1	2	3	4	5	6	7	8	9	10	1	12
x	1	1	-1	-1	0	0	0	0	1	1	-1	-1
y	1	-1	1	-1	1	1	-1	-1	0	0	0	0
z	0	0	0	0	1	-1	1	-1	1	-1	1	-1

(See Fig. (4,1iii)

Our estimates of the nearest-neighbour distances on a hexagonal close packed lattice in units of a, is shown in the following table 4.1(iv).

Table (4.1iv) - Nearest neighbour Distances on an Hexagonal close packed lattice in units of a.

ℓ	1	2	3	4	5	6	7	8	9	10	11	12
x	0	-0,5,	0.5,	0,	-0.5,	0.5,	1,	1,	-0.5,	0.5,	-1,	-1
y	-0,577,	0.289,	0.289,	-0.577,	0,289,	0.289,	0,00,	0.722,	-1.154,	-1.154	0,	0.722
z	$\frac{-1.632}{2}$,	$\frac{-1.632}{2}$,	$\frac{-1.632}{2}$,	$\frac{1.632}{2}$,	$\frac{1.632}{2}$,	$\frac{1.632}{2}$,	0,	0,	0,	0,	0,	0.

See our Fig. (4.1iv)

For a simple cubic lattice,

the Fourier transform $J(k) = \frac{1}{6}\sum_{\ell=1}^{z} J_{j\ell}\,\mathrm{Cos}[\,k.(R_j - R_\ell)]$

writing $kx = k_x$, $ky = k_y$, and $kz = k_z$

$$= \frac{J}{6}[\mathrm{Cos}\ kxa + \mathrm{Cos}(-kxa) + \mathrm{Cos}(kya) + \mathrm{Cos}(-kya) + \mathrm{Cos}(kza) + \mathrm{Cos}(-kza)]$$

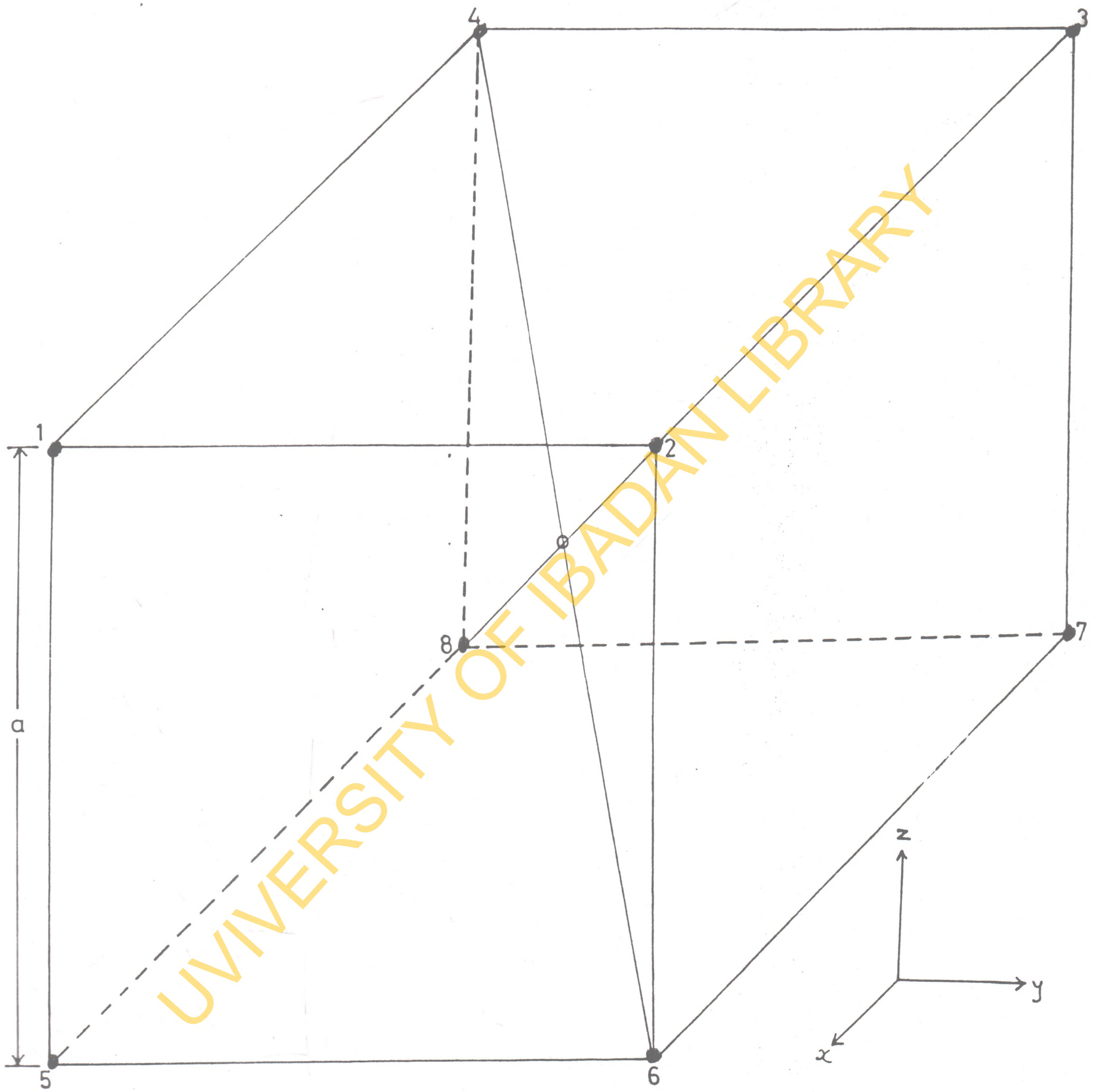
$$= \frac{J}{3}[\,\mathrm{Cos}(kxa) + \mathrm{Cos}(kya) + \mathrm{Cos}(kza)]\,.$$

For a body centred cubic lattice,

the Fourier transform

$$J(k) = \frac{J}{8}[\mathrm{Cos}(kxa - kya + kza)/2 + \mathrm{Cos}(kxa + kya + kza)/2 + \mathrm{Cos}(-kxa+kya+kza)/2 + \mathrm{Cos}(-kxa-kya+kza)/2 + \mathrm{Cos}(kxa-kya-kza)/2 + \mathrm{Cos}(kxa+kya-kza)/2 + \mathrm{Cos}(-kxa+kya-kza)/2 + \mathrm{Cos}(-kxa-kya-kza)/2]$$

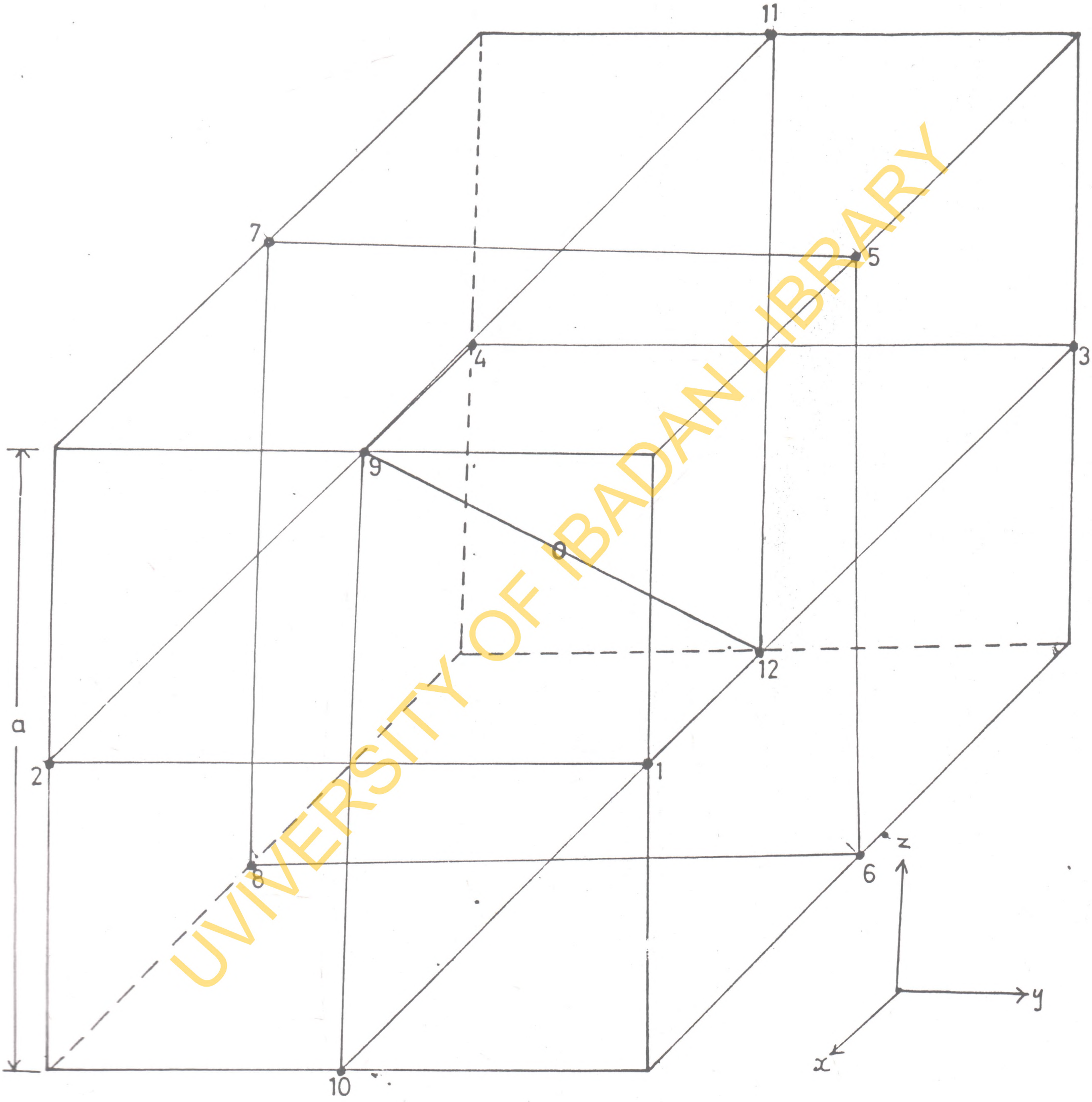
Fig. 4.1ii - A given atom with eight neighbours on the body-centered cubic lattice.



o ≡ given atom at (0,0,0)

● ≡ nearest neighbours

Fig.4.1iii - A given atom with twelve neighbours on the face centred cubic lattice



○ ≡ given atom at (0,0,0)

● ≡ nearest neighbours

Fig. 4.1iv - A given atom with twelve nearest neigbours on the Hexagonal close packed lattice.

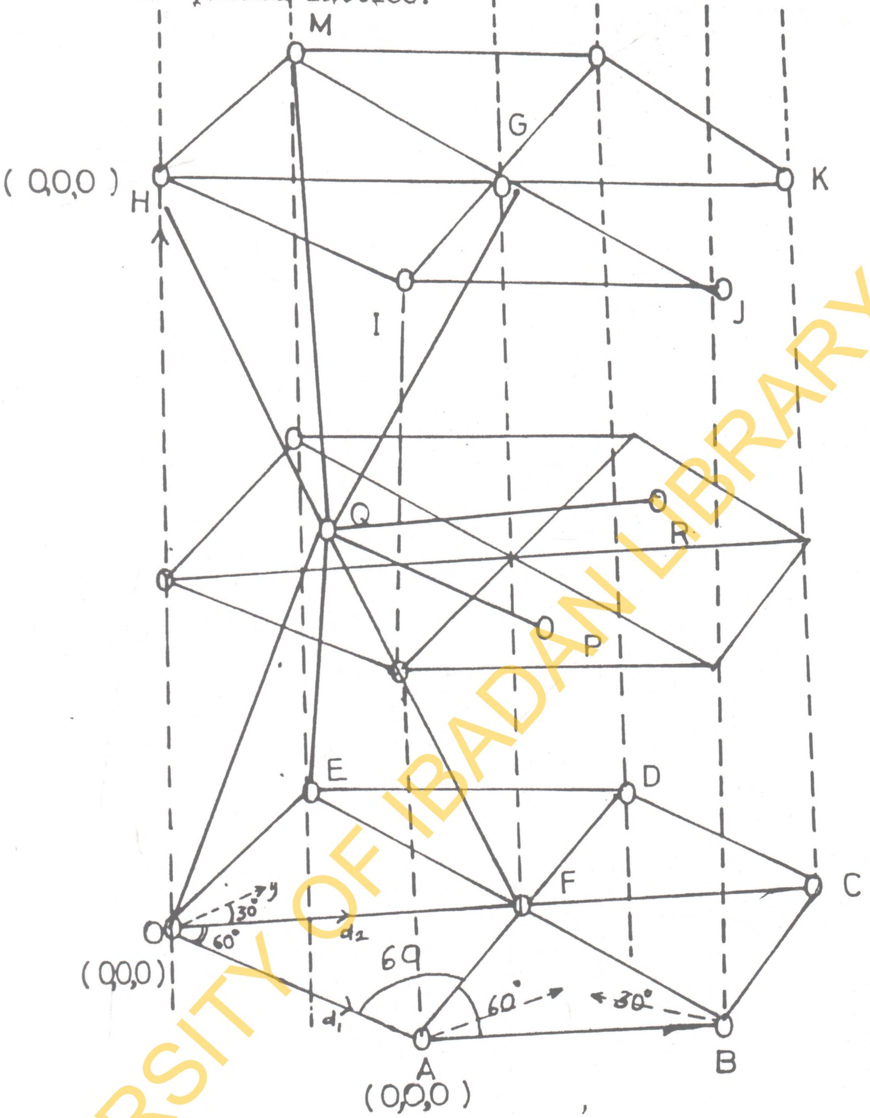
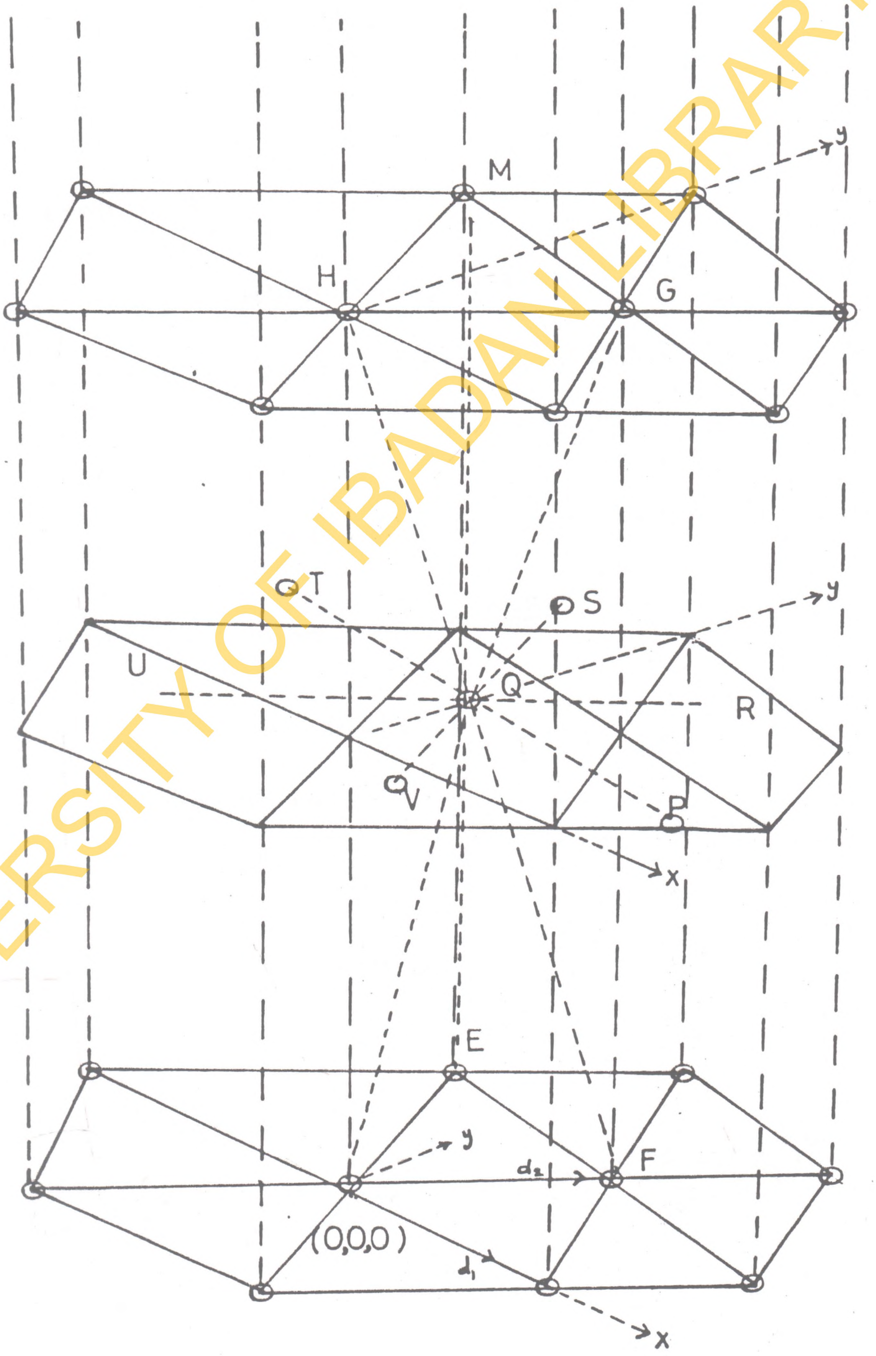


Fig. 4.1v - A given atom with twelve nearest neighbours on the Hexagonal close packed lattice.



$$= \frac{J}{8}[\ 2\mathrm{Cos}(kxa+kza)/2\mathrm{Cos}\ kya+2\mathrm{Cos}(-kya+kza)/2\mathrm{Cos}kya$$

$$+2\mathrm{Cos}(kxa-kza)\mathrm{Cos}\ kya+2\mathrm{Cos}(-kxa-kza)/2\mathrm{Cos}\ kya$$

$$= J[\ \mathrm{Cos}\ \frac{kxa}{2}\ \ \mathrm{Cos}\ \frac{kya}{2}\ \mathrm{Cos}\ \frac{kza}{2}]$$

For a face centred cubic,

the Fourier transform $J(k)$

$$J(k) = \frac{J}{12}[\ \mathrm{Cos}(kxa+kya)+\mathrm{Cos}(kxa-kya)+\mathrm{Cos}(-kxa+kya)$$

$$+\ \mathrm{Cos}(-kxa-kya)+\mathrm{Cos}(kya+kza)+\mathrm{Cos}(kya-kza)$$

$$+\ \mathrm{Cos}(-kya+kza)+\mathrm{Cos}(-kya-kza)+\mathrm{Cos}(kxa+kza)$$

$$+\ \mathrm{Cos}(kxa-kza)+\mathrm{Cos}(-kxa+kza)+\mathrm{Cos}(-kxa-kza)]$$

$$= \frac{J}{3}[\ \mathrm{Cos}\ \frac{kxa}{\sqrt{2}} + \mathrm{Cos}\ \frac{kya}{\sqrt{2}} + \mathrm{Cos}\ \frac{kza}{\sqrt{2}}]$$

We proceed to obtain the fourier transform J(k) for a hexagonal close packed lattice.

For a Hexagonal close-packed lattice, we have

$$J(k) = J_\gamma(k) = \frac{J}{z}\sum_{\ell=1}^{12} \mathrm{Cos}\ k.R = \frac{J}{z}\sum_{\ell=1}^{12}\mathrm{Cos}(k_x x_\ell+k_y y_\ell+k_z z_\ell) \qquad \ldots\ (4.1\text{-}4)$$

$\mathrm{Cos}(k_x x_\ell+k_y y_\ell+k_z z_\ell)$

$$= 1 - \frac{(k_x x_\ell+k_y y_\ell+k_z z_\ell)^2}{2!} + \frac{(k_x x_\ell+k_y y_\ell+k_z z_\ell)^4}{2!} + \ldots$$

$$- \frac{(k_x x_\ell + k_y y_\ell + k_z z_\ell)^6}{6!} + \ldots \qquad \ldots (4.1\text{-}5)$$

To obtain J(k), we substitute the values on the table (4.1iv) into the expression obtained after putting (4.1-5) into (4.1-4). Taking each term separately, we have the following

$$\frac{1}{12} \sum_{\ell=1}^{12} \frac{(k_x x_\ell + k_y y_\ell + k_z z_\ell)^2}{2!} = \frac{1}{24}[D''(\phi,\theta)(ka)^2] \qquad \ldots (4.1\text{-}6)$$

where

$$D''(\phi,\theta)(ka)^2 = \sum_{\ell=1}^{12} (k_x^2 x_\ell^2 + k_y^2 y_\ell^2 + k_z^2 z_\ell^2 + 2k_y k_x x_\ell y_\ell + 2k_x k_z x_\ell z_\ell + 2k_y k_z y_\ell z_\ell) \qquad \ldots (4.1\text{-}7)$$

$$\frac{1}{12} \sum_{\ell=1}^{12} \frac{(k_x x_\ell + k_y y_\ell + k_z z_\ell)^4}{4!} = \frac{1}{12}(\frac{1}{24}) A''(\phi,\theta)(ka)^4 \qquad \ldots (4.1\text{-}8)$$

where

$$A''(\phi,\theta)(ka)^4 = \sum_{\ell=1}^{12} (k_x^4 x_\ell^4 + k_y^4 y_\ell^4 + k_z^4 z_\ell^4 + 6k_x^2 k_y^2 x_\ell^2 y_\ell^2 + 6k_y^2 k_z^2 y_\ell^2 z_\ell^2 + 6k_x^2 k_z^2 x_\ell^2 z_\ell^2 + 4k_x^3 k_y x_\ell^3 y_\ell + 4k_x^3 k_z x_\ell^3 z_\ell + 4k_y^3 k_x x_\ell y_\ell^3 + 4k_y^3 k_z y_\ell^3 z_\ell + 4k_z^3 k_x x_\ell z_\ell^3 + 4k_z^3 k_y y_\ell z_\ell^3) \qquad \ldots (4.1\text{-}9)$$

$$\frac{1}{12}\sum_{\ell=1}^{12}\frac{(k_x x_\ell + k_y y_\ell + k_z z_\ell)^6}{6!} = \frac{1}{12}\left(\frac{1}{720}\right)[B''(\phi,\theta)(ka)^6]$$

Writing $B''(\phi,\theta)(ka)^6 = a+b$

$$a = \sum_{\ell=1}^{12}(k_x^6 x_\ell^6 + k_y^6 y_\ell^6 + k_z^6 z_\ell^6 + 7k_z^4 k_y^2 z_\ell^4 y_\ell^2 + 7k_x^4 k_y^2 x_\ell^4 y_\ell^2 + 7k_y^4 k_x^2 y_\ell^4 x_\ell^2$$

$$+ 7k_x^2 k_z^4 x_\ell^2 z_\ell^4 + 7k_x^4 k_z^2 x_\ell^4 z_\ell^2 + 7k_y^4 k_z^2 y_\ell^4 z_\ell^2 + 4k_x^5 k_y x_\ell^5 y_\ell + 4k_x^5 k_z x_\ell^5 z_\ell$$

$$+ 4k_y^5 k_x x_\ell y_\ell^5 + 4k_y^5 k_z y_\ell^5 z_\ell + 4k_z^5 k_x x_\ell z_\ell^2 + 4k_z^5 k_y z_\ell^5 y_\ell$$

$$+ 8k_y^3 k_x^3 x_\ell^3 y_\ell^3 + 8k_z^3 k_y^3 z_\ell^3 y_\ell^3 + 8k_z^3 k_x^3 x_\ell^3 z_\ell^3 + 16k_y^3 k_x^2 k_z y_\ell^3 z_\ell x_\ell^2$$

$$+ 16k_z^3 k_y k_x^2 y_\ell z_\ell^3 x_\ell^2 + 16k_x^3 k_y k_z^2 x_\ell^3 y_\ell z_\ell^2 + 16k_y^2 k_x^3 k_z y_\ell^2 x_\ell^3 z_\ell$$

$$+ 16k_z^3 k_x k_y^2 z_\ell^3 x_\ell y_\ell^2 + 16k_y^3 k_x k_z^2 y_\ell^3 z_\ell^2 x_\ell + 18k_y^2 k_z^2 k_x^2 x_\ell^2 y_\ell^2 z_\ell^2$$

$$+ 12k_x^4 k_y k_z x_\ell^4 y_\ell z_\ell + 12k_y^4 k_x k_z y_\ell^4 x_\ell z_\ell + 12k_x k_y k_z^4 x_\ell y_\ell z_\ell^4$$

and

$$b = \sum_{\ell=1}^{12}(2k_x^5 k_y x_\ell^5 y_\ell + 2k_y^5 k_x x_\ell y_\ell^5 + 2k_x^5 k_z x_\ell^5 z_\ell + 2k_z^5 k_x x_\ell z_\ell^5 + 2k_y^5 k_z y_\ell^5 z_\ell$$

$$+ 2k_z^5 k_y z_\ell^5 y_\ell + 8k_x^4 k_y^2 x_\ell^4 y_\ell^2 + 8k_y^4 k_x^2 x_\ell^2 y_\ell^4 + 8k_x^4 k_z^2 x_\ell^4 z_\ell^2$$

$$+ 8k_z^4 k_x^2 x_\ell^2 z_\ell^4 + 8k_y^4 k_z^2 y_\ell^4 z_\ell^2 + 8k_z^4 k_y^2 y_\ell^2 z_\ell^4 + 18k_z^4 k_x k_y x_\ell y_\ell z_\ell^4$$

$$+ 18k_y^4k_xk_zx_\ell z_\ell y_\ell^4 + 18k_x^4k_yk_zx_\ell^4y_\ell z_\ell + 12k_x^3k_y^3x_\ell^3y_\ell^3 + 12k_y^3k_z^3y_\ell^3z_\ell^3$$

$$+ 12k_x^3k_z^3x_\ell^3z_\ell^3 + 72k_x^2k_y^2k_z^2x_\ell^2y_\ell^2z_\ell^2 + 44k_z^3k_x^2k_yx_\ell^2z_\ell^3y_\ell$$

$$+ 44k_z^3k_y^2k_xy_\ell^2z_\ell^3x_\ell + 44k_y^3k_z^2k_xy_\ell^3z_\ell^2x_\ell + 44k_x^3k_yx_\ell^3z_\ell^2y_\ell$$

$$+ 44k_y^3k_x^2k_zy_\ell^3z_\ell x_\ell^2 + 44k_x^3k_y^2k_zx_\ell^3y_\ell^2z_\ell) \qquad \ldots (4.1\text{-}10)$$

The fourier transform J(k) for an Hexagonal close packed lattice is markedly different from that of the cubic lattice.

Replacing F with F', for a Hexagonal close packed lattice, the transformed Hamiltonian is written as

$$H = \sum_k (F'k^2 - \mu)n_k \qquad \ldots (4.1\text{-}11)$$

where

$$F' = 2SzJ[D''(\phi,\theta)a^2k^2 - A''(\phi,\theta)(ka)^4 + B''(\phi,\theta)(ka)^6 + \ldots] \qquad \ldots (4.1\text{-}12)$$

The quantities $D''(\phi,\theta)$, $A''(\phi,\theta)$ and $B''(\phi,\theta)$ have been outlined and evaluated in the appendix D.

We proceed to find the effect of the electrochemical potential μ on the coefficients of τ^ν in the expression of spontaneous magnetization and specific heat. As in eqn. (3.3-2)

$$\sum_k \frac{\langle n_k \rangle}{NS} = \frac{V}{(2\pi)^3 NS} \int \frac{k^2 \, dk}{\exp(F'k^2 - \mu) - 1} \qquad \ldots (4.1\text{-}13)$$

This integration is of course not a trival one. We extend our previous technique of doing it by writing

$$S_o = [D''(\phi,\theta)a^2k^2 - A''(\phi,\theta)(ka)^4 + B''(\phi,\theta)(ka)^6]\frac{1}{\tau}$$

and $\qquad \ldots (4.1\text{-}14)$

putting $P = D''(\phi,\theta)$, $C = \frac{a^2}{\tau}$, $G = zA''(\phi,\theta)a^2$, $F'k^2 = 2SzJS_o$, $H = B''(\phi,\theta)a^4z$. Equation (4.1-14) becomes

$$S_o = C[P - Gk^2 + Hk^4]k^2 \qquad \ldots (4.1\text{-}15)$$

$$Ck^2 = \frac{S_o}{P}[1 + \frac{GS_o}{CP^2}2(1 + \frac{GS_o}{CP^2})] - \frac{H}{P}[\frac{S_o^2}{C^2P^2}(1 + \frac{2GS_o}{CP^2} + \frac{G^2S_o^2}{C^2P^4})]$$

$$+ \frac{G^2}{P^2}[\frac{S_o^2}{C^2P^2}(1 + \frac{2GS_o}{CP^2} + \frac{G^2S_o^2}{C^2P^4})] \qquad \ldots (4.1\text{-}16)$$

$$= \frac{S_o}{P}[1 + \frac{GS_o}{CP^2} + (\frac{2G^2}{C^2P^4} - \frac{H}{P^3C^2})S_o^2]$$

$$k^2dk = \frac{S_o^{\frac{1}{2}}}{2C^{3/2}P^{3/2}}[1 + \frac{5GS_o}{2CP^2} + \frac{8G^2S_o^2}{C^2P^4} - \frac{7}{2}\frac{H}{P^3}\frac{S_o^2}{C^2}] \qquad \ldots (4.1.17)$$

$$k^2dk = \frac{S_o^{\frac{1}{2}}}{2C^{3/2}P^{3/2}}[1 + \frac{5}{2}\frac{zA''(\phi,\theta)}{D''^2(\phi,\theta)}S_o\tau + \frac{8z^2A''^2(\phi,\theta)S_o^2\tau^2}{D''^4(\phi,\theta)}$$

$$- \frac{7}{2} \cdot \frac{B''(\phi,\theta)z\tau^2S_o^2}{D''^3(\phi,\theta)} + \ldots]\,dS_o \qquad \ldots (4.1\text{-}18)$$

Substituting (4.1-18) into (4.1-13) and by the techniques of numerical methods, we have been able to compute the first three coefficients of $-\delta m(\tau)/m(o)$.

The first term of $-\delta m(\tau)/m(o)$ is

$$= \frac{V}{(2\pi)^2 NS} \int_0^\infty dS_o \int_0^{2\pi} d\phi \int_0^\pi \frac{\text{Sin}\,\theta\; S_o^{\frac{1}{2}}}{2C^{3/2}P^{3/2}} e^{-m\beta\mu}$$

$$= \frac{V}{(2\pi)^3 NS} \tau^{3/2}\Gamma(\tfrac{3}{2}) \sum_{m=1}^{\infty} \frac{e^{+m\beta\mu}}{m^{3/2}} \int_0^{2\pi} \int_0^{\pi} [D''(\phi,\theta)]^{-3/2} \text{Sin}\theta\, d\theta\, d\phi$$

$$D''(\phi,\theta) = (\text{Cos}\phi\text{Sin}\theta)^2 \sum_{\ell=1}^{12} x_\ell + (\text{Sin}\phi\text{Sin}\theta)^2 \sum_{\ell=1}^{12} y_\ell + (\text{Cos}\theta)^2 \sum_{\ell=1}^{12} z_\ell / 24 \qquad \ldots (4.1\text{-}19)$$

The second term of $-\delta m(\tau)/m(o)$ is

$$= \frac{V}{(2\pi)^3 NS} \tau^{3/2}\Gamma(\tfrac{5}{2}) \sum_{m=1}^{\infty} \frac{e^{-my}}{m^{5/2}} \frac{5}{4}z \int_0^{2\pi} \int_0^{\pi} \frac{A''(\phi,\theta)\text{Sin}\theta}{[D''(\phi,\theta)]^{3/2}} d\theta\, d\phi$$

where

$$A''(\phi,\theta) = \frac{1}{24}(\text{Cos}\phi\text{Sin}\theta)^4 \sum_{\ell=1}^{12} X_\ell^4 + (\text{Sin}\phi\text{Sin}\theta)^4 \sum_{\ell=1}^{12} y_\ell^4 + (\text{Cos}\theta)^4 \sum_{\ell=1}^{12} z_\ell^4$$

$$+ (\text{Cos}\phi\text{Sin}\theta)^3\text{Sin}\phi\text{Sin}\theta \sum_{\ell=1}^{12} x_\ell y_\ell^3 + 4(\text{Sin}\phi\text{Sin}\theta)^3\text{Cos}\theta \sum_{\ell=1}^{12} y_\ell^3 z_\ell +$$

$$+ 6(\text{Cos}\phi\text{Sin}\theta)^2(\text{Sin}\phi\text{Sin}\theta)^2 \sum_{\ell=1}^{12} x_\ell^2 z_\ell^2 + 6(\text{Sin}\phi\text{Sin}\theta)^2(\text{Cos}\theta)^2 \sum_{\ell=1}^{12} y_\ell^2 z_\ell^2$$

$$+ 6(\mathrm{Cos}\phi\mathrm{Sin}\theta)^2(\mathrm{Cos}\theta)^2 \sum_{\ell=1}^{12} x_\ell^2 z_\ell^2 + 12(\mathrm{Cos}\theta)^2(\mathrm{Sin}\phi\mathrm{Sin}\theta)(\mathrm{Cos}\phi\mathrm{Sin}\theta) \sum_{\ell=1}^{12} x_\ell y_\ell z_\ell^2$$

$$+ 12(\mathrm{Cos}\phi\mathrm{Sin}\theta)^2(\mathrm{Sin}\phi\mathrm{Sin}\theta)\mathrm{Cos}\theta \sum_{\ell=1}^{12} x_\ell^2 y_\ell z_\ell + 12(\mathrm{Sin}\phi\mathrm{Sin}\theta)^2$$

$$\mathrm{Cos}\phi\mathrm{Sin}\theta\mathrm{Cos}\theta \sum_{\ell=1}^{12} y_\ell^2 x_\ell z_\ell \qquad \ldots (4.1\text{-}20)$$

The third term of $-\delta(m(\tau))/m(o)$ is

$$= \frac{V}{(2\pi)^3 NS} \tau^{3/2} \Gamma(\tfrac{7}{2}) \Sigma \frac{e^{-my}}{m^{3/2}} \left[4z^2 \iint \frac{A''(\phi,\theta)\mathrm{Sin}\theta d\theta d\phi}{[D''(\phi,\theta)]^4} - \frac{7z}{4} \iint \frac{B''(\phi,\theta)\mathrm{Sin}\theta d\theta d\phi}{[D''(\phi,\theta)]^3} \right]$$

$$\ldots (4.1\text{-}21)$$

where

$$B''(\phi,\theta) = (\mathrm{Cos}\phi\mathrm{Sin}\theta)^6 \sum_{\ell=1}^{12} x_\ell^6 + (\mathrm{Sin}\phi\mathrm{Sin}\theta)^6 \sum_{\ell=1}^{12} y_\ell^6 + (\mathrm{Cos}\theta)^6 \sum_{\ell=1}^{12} z_\ell^6$$

$$+ 6\mathrm{Cos}^3\phi\mathrm{Sin}^6\theta\mathrm{Sin}\phi \sum_{\ell=1}^{12} x_\ell^5 y_\ell + 6\mathrm{Sin}^6\theta\mathrm{Sin}^5\phi\mathrm{Cos}\phi \sum_{\ell=1}^{12} x_\ell y_\ell^2 + 6\mathrm{Cos}^5\phi\mathrm{Sin}^5\theta\mathrm{Cos}\theta \sum_{\ell=1}^{12} z_\ell x_\ell^5$$

$$+ 6\mathrm{Cos}^5\theta\mathrm{Cos}\phi\mathrm{Sin}\theta \sum_{\ell=1}^{12} x_\ell z_\ell^2 + 6\mathrm{Sin}^5\phi\mathrm{Sin}^5\theta\mathrm{Cos}\theta \sum_{\ell=1}^{12} z_\ell y_\ell^2 + 6\mathrm{Cos}^5\theta\mathrm{Sin}\phi\mathrm{Sin}\theta \sum_{\ell=1}^{12} y_\ell z_\ell^5$$

$$+ 15\mathrm{Sin}^6\theta\mathrm{Cos}^4\phi\mathrm{Sin}^2\theta \sum_{\ell=1}^{12} x_\ell^4 y_\ell^2 + 15\mathrm{Sin}^6\theta\mathrm{Sin}^4\phi\mathrm{Cos}^2\phi \sum_{\ell=1}^{12} x_\ell^2 y_\ell^4$$

$$+ 15\mathrm{Cos}^4\phi\mathrm{Sin}^4\theta\mathrm{Cos}^2\theta \sum_{\ell=1}^{12} x_\ell^4 z_\ell^2 + 15\mathrm{Cos}^4\theta\mathrm{Cos}^2\phi\mathrm{Sin}^2\theta \sum_{\ell=1}^{12} x_\ell^2 z_\ell$$

$$+ 15\mathrm{Sin}^4\phi\mathrm{Sin}^4\theta\mathrm{Cos}^2\theta \sum_{\ell=1}^{12} y_\ell^2 z_\ell^2 + 15\mathrm{Cos}^4\theta\mathrm{Sin}^2\phi\mathrm{Sin}^2\theta \sum_{\ell=1}^{12} y_\ell^2 z_\ell^4$$

$$+ 30\mathrm{Cos}^4\theta\,\mathrm{Sin}^2\theta\,\mathrm{Cos}\phi\,\mathrm{Sin}\phi \sum_{\ell=1}^{12} x_\ell y_\ell z_\ell^4 + 30\mathrm{Sin}^5\theta\,\mathrm{Sin}^4\phi\,\mathrm{Cos}\phi\,\mathrm{Cos}\theta \sum_{\ell=1}^{12} x_\ell y_\ell^4 z_\ell$$

$$+ 30\mathrm{Sin}^5\theta\,\mathrm{Cos}^4\phi\,\mathrm{Sin}\phi\,\mathrm{Cos}\theta \sum_{\ell=1}^{12} y_\ell z_\ell x_\ell^4 + 20\mathrm{Sin}^6\theta\,\mathrm{Cos}\phi\,\mathrm{Sin}^3\theta \sum_{\ell=1}^{12} x_\ell^3 y_\ell^3$$

$$+ 20\mathrm{Sin}^3\phi\,\mathrm{Sin}^3\theta\,\mathrm{Cos}^3\theta \sum_{\ell=1}^{12} y_\ell^3 z_\ell^3 + 20\mathrm{Cos}^3\phi\,\mathrm{Sin}^3\theta\,\mathrm{Cos}^3\theta \sum_{\ell=1}^{12} x_\ell^3 z_\ell^3$$

$$+ 90\mathrm{Sin}^4\theta\,\mathrm{Cos}^2\phi\,\mathrm{Sin}^2\phi\,\mathrm{Cos}^2\theta \sum_{\ell=1}^{12} x_\ell^2 y_\ell^2 z_\ell^2 + 60\mathrm{Cos}^3\theta\,\mathrm{Sin}^3\theta\,\mathrm{Cos}^2\phi\,\mathrm{Sin}\phi \sum_{\ell=1}^{12} x_\ell^2 y_\ell z_\ell^3$$

$$+ 60\mathrm{Cos}^3\theta\,\mathrm{Sin}^3\theta\,\mathrm{Sin}^2\phi\,\mathrm{Cos}\phi \sum_{\ell=1}^{12} y_\ell^2 z_\ell^3 x_\ell + 60\mathrm{Sin}^4\theta\,\mathrm{Sin}^3\phi\,\mathrm{Cos}\phi\,\mathrm{Cos}^2\theta \sum_{\ell=1}^{12} y_\ell^3 z_\ell^2 x_\ell$$

$$+ 60\mathrm{Sin}^5\theta\,\mathrm{Sin}^3\phi\,\mathrm{Cos}^2\phi\,\mathrm{Cos}\theta \sum_{\ell=1}^{12} x_\ell^3 z_\ell^2 y_\ell + 60\mathrm{Sin}^5\theta\,\mathrm{Cos}^3\phi\,\mathrm{Sin}^2\phi\,\mathrm{Cos}\theta \sum_{\ell=1}^{12} y_\ell^3 x_\ell^2 z_\ell$$

$$+ 60\mathrm{Sin}^4\theta\,\mathrm{Cos}^3\phi\,\mathrm{Sin}\phi\,\mathrm{Cos}^2\theta \sum_{\ell=1}^{12} x_\ell^3 y_\ell^2 z_\ell \,]/720$$

In evaluating our terms (4.1-19), (4.1-20) and (4.1-21), after integration, we require the value of J, the exchange integral for ferromagnets with hexagonal close packed lattice structure.

4.2 Evaluation of the Exchange Integral

RUSHBROOKE and WOOD (1958) have in their work calculated the first six coefficients in the expansion of the susceptibility X, and its inverse X^{-1} in ascending powers of the reciprocal temperature for the Heisenberg model of a ferromagnet with cubic symmetry. From these coefficients of X, estimates have been made of the reduced curie temperature $\theta_c = \frac{k_B T_c}{J}$ for the simple, body centred and face centred cubic lattices.

It was found that formula

$$\theta_c = \frac{5}{96}(z-1)(11x-1), \qquad \ldots (4.2\text{-}1)$$

where $X = S(S+1)$ and z, the lattice coordination number reproduces the estimated curie temperatures fairly accurately.

In evaluating J for the cubic lattices, we have made use of the above formula by writing

$$\tau = \frac{k_B T}{2JS} = \frac{\theta_c}{2ST_c} T \qquad \ldots (4.2\text{-}2)$$

Since (4.2-1) does not apply to crystals with close packed Hexagonal lattice structure, following RUSHBROOKE and WOOD (1958) and DOMB and SYKES (1957) we have a technique of calculating the reduced curie temperature (θ_c) from which J the exchange integral is obtained.

In what follows we write the reduced susceptibility $\bar{X}$ as $\frac{JX}{Ng^2\mu\beta^2}$ where N is the number of lattice sites, $\mu\beta$ denotes the Bohr magneton and g the gyromagnetic ratio. It has been shown by Rushbrooke and Wood that

$$\bar{X}\theta = \frac{1}{3}S(S+1)\sum_{n=o}^{\infty}\frac{a_n}{\theta^n}, \qquad \ldots (4.2\text{-}3)$$

and

$$\frac{1}{\bar{X}\theta} = \frac{3}{S(S+1)}\sum_{n=o}^{\infty}\frac{b_n}{\theta^n} \qquad \ldots (4.2\text{-}4)$$

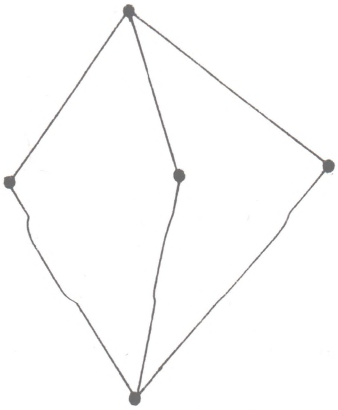
where $\theta = \frac{kT}{J}$ is the reduced temperature.

According to Rushbrooke and Wood, the general expression for the coefficients b_1, b_2, b_3, b_4, b_5 and b_6 are given below in terms of the following parameters p_n, q, r, t whose meaning are given as follows.

1. $\frac{1}{2(n+2)}zNP_n$ = number of (unlabelled) close, non-crossing circuits of n+2 points on the lattice

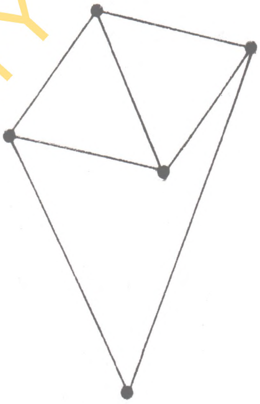
   for example, $\frac{1}{6}N_2P_1$ = number of triangles the sides of which join neighbouring lattice sites.

2. $\frac{1}{12}zNq$ = number of (unlabelled) diagrams of the type which can be found on the lattice.



3. $\frac{1}{24}zNr$ = number of (unlabelled) tetrahedra which can be found on the lattice

4. $\frac{1}{4}zNt$ = number of (unlabelled) diagram of the



type which can be found on the lattice.

Their values for the various lattices are tabulated below:

Lattice	z	p_1	p_2	p_3	p_4	p_5	q	r	t
Simple cubic	6	0	4	0	44	0	0	0	0
Body centred cubic	8	0	12	0	222	0	18	0	0
Face centred cubic	12	4	22	140	970	7196	36	4	16
Hexagonal close pack	12	4	22	140	970	7196	37	4	16

DOMB and SYKE (1957) observed that the lattice parameter which we have called q in the table above has, the value 37 for the hexagonal close-packed lattice in contrast to 36 for the face centred cubic lattice. Consequently, the value a_6 and b_6 are slightly different for the hexagonal close packed and face-centred cubic lattice. The general coefficients $b_1, \ldots, b_6$ are given as follows

$$b_1 = -\frac{2}{3} zX$$

$$b_2 = \frac{1}{9} zX[4x+3]$$

$$b_3 = \frac{4}{135} z\ x\ [-4x^2-9x-6+10p_1x^2+5p_1x]$$

$$b_4 = \frac{1}{405} z\ x\ [(80P_2-96P_1-16)x^3 + 40P_2-159P_1+64-40z)x^2 + (-54P_1 + 96 - 45z)x + 45]$$

$$b_5 = \frac{2}{42525}Z \; x[(2800P_3-3360P_2-3360P_1^2-1456P_1+800)x^4$$

$$+ (1400P_3-6160P_2-3360P_1^2-4200zP_1+12936P_1+80+1120z)x^3$$

$$+(2898P_1-4752-3780z)x-1728]$$

$$b_6 = \frac{Z}{127575} x[-4480q-26880P_1P_2+11200P_4-13440P_3-25984P_2+5824P_1^2$$

$$+24960P_1-128)x^5+(-4480q-26880P_1P_2+5600P_4$$

$$-27440P_3 + 42784_2 - 22400zP_2 + 112896P_1^2 - 11200zP_1^2$$

$$-62800P_1 + 24640zP_1 - 12960 + 3064z)x^4$$

$$+(-840r - 1260q-5040P_1P_2 - 12600P_3 + 66612P_2 - 15860zP_2$$

$$+81648P_1^2 - 6440zP_1^2 - 164760P_1 + 61320zP_1 - 204$$

$$-11844z + 58802^2)x^3 + (-210r + 26082P_2 + 7623P_1^2$$

$$-108900P_1 + 35490zP_1 + 27978 - 38052z + 9660)x^2$$

$$+ -19440P_1 + 29116 - 29862z)x + 8694. \qquad \ldots (4.2\text{-}5)$$

where

$$X = S(S+1),$$

These coefficients have been computed with the aid of a computer for cobalt Co, Dysprosium Dy and Gd, Gadolinium. We have also extended it to cover, both Iron and Nickel, so as to make a comparison with the values of θ_c calculated using Rushbrooke and Wood formula (3.4-1).

The method originally used by OPECHOWSKI (1938) and ZEHLER (1950) for estimating the curie temperature from a knowledge of the first few a or b coefficients was to find the smallest positive real root of the equation

$$1+b_1x + b_2x^2 + \ldots, = 0 \qquad \ldots (4.2\text{-}6)$$

Denoting this by X^*, $X^{-1} = 0$ when $\theta = \frac{1}{X^A}$ so that $\frac{1}{X^A}$ is the estimate of the curie temperature.

We have in this work, taken all the six coefficients into consideration and by the use of Pade approximants (see Appendix B) expressed susceptibility as rational functions, with a reduced number of terms

$$X = \frac{1}{\sum\limits_{\ell=o}^{6} b_\ell x^\ell} = \frac{\Sigma d_j x^j}{\Sigma n_p x^p} \qquad \ldots (4.2\text{-}7)$$

Equation (4.2-7) after a cross multiplication gives for Nickel (N_i)

$$(1-6x+6x^2+6x^3+0.75x^4-3.55x^5-28.389x^6)(d_o+d_1x+d_2x^2) = 1+n_1x \qquad \ldots (4.2\text{-}8)$$

Equating coefficients of like terms, we obtain with

$$d_o = 1 = n_o$$

$$d_1 = n_1+6$$

$$-6d_1+d_2 = -6$$

$$6d_1-6d_2+d_3 = -6$$

$$6d_1+6d_2-6d_3+d_4 = -0,75$$

$$0,75d_1+6d_2+6d_3-6d_4+d_5 = 3,55$$

$$-3,55d_1+0,75d_2+6d_3+6d_4-6d_5 = 28.389 \qquad \ldots (4.2\text{-}9)$$

Solving the equations above, we have

$d_1 = 1,6807$, $d_2 = 4,0842$, $d_3 = 8.421$, $d_4 = 15.186$,

$d_5 = 4,8105$ and $n_1 = -4,3193$,

Therefore,

$$X = \frac{1}{\Sigma b_\ell x^\ell} = \sum_{j=o}^{2} \frac{d_j x^j}{(1-4,319X)} \qquad \ldots (4.2\text{-}10)$$

$$X_c = \frac{1}{4,3193}$$

$$\theta_c = 4.3193$$

The critical point exponent

$$\gamma = 1 + \frac{1.6807}{4.3193} + \frac{4.0847}{(4.3193)^2} = 1.61.$$

θ_c has been obtained using this technique for, Iron, Nickel, Cobalt, Dysprosium and Gadolinium and the results compared with the results from Rushbrooke and Wood formula. This technique has enabled us to calculate the critical point exponents and all these have been tabulated and shown in the following table 4.1.

These values of θ_c calculated now enable us to calculate the exchange integral J from equation (4.2-2).

These values of J when substituted into equations (4.1-19), (4.1-20) and (4.1-21) give the coefficients $T^{3/2}$, $T^{5/2}$, and $T^{7/2}$ of spontaneous magnetization respectively and the effect of the electrochemical potential is examined. The coefficient of the specific heat is also computed by the method outlined in chapter III and the results tabulated, for the various ferromagnetic elements.

All these coefficients are shown in the table 4.2.

4.3 Spin wave - Spin wave - Spin wave Interaction

We have extended our formalism and technique to take into account the wave-wave-wave interactions and the effect thereof.

As usual, by the method of second quantization and using Holstein and Primakoff transformation, the Hamiltonian

Table 4.1 – Reduced curie temperature (θ_c) and the critical point exponent for some ferrometals.

Ferromagnetic Elements	Lattice Structure	Rushbrooke and Wood θ_c	Pade' Approximinants θ_c	Spin (s)	Critical point exponent
IRON (FE)	Body Centred Cubic (BCC)	7.656	8.057	1	1.45
COBALT (Co)	Hexagonal Close Packed (HCP)	12.030	12.659	1	1.40
NICKEL (Ni)	Face-Centred Cubic (FCC)	4.153	4.319	$\frac{1}{2}$	1.61
DYSPROSIUM (Dy)	Hexagonal Close Packed (HCP)	188.489	201.110	5	1.30
GADOLINIUM (Gd)	Hexagonal Close Packed (HCP)	98.680	105.120	$\frac{7}{2}$	1.31

Table 4.2 - Coefficients of $T^{3/2}$, $T^{5/2}$, $T^{7/2}$ and T^4 of spontaneous magnetization and the coefficient of $T^{3/2}$ of specific heat for some ferrometals

ELEMENTS	LATTICE STRUCTURE	SPIN (s)/ NEAREST NEIGHBOURS(z)	CHEMICAL POTENTIAL (μ)	TRANSITION TEMP. $(T_c)^oK$	REDUCED TEMP(θ_c)	$C_1T^{3/2}$	$C_2T^{5/2}$	$C_3T^{7/2}$	C_4T^4	SPECIFIC HEAT $\tau^{3/2}10^{-23}$
-	SC	$s = \frac{1}{2}, z = 6$	0.123	1043	1.88	5.203×10^{-6}	1.345×10^{-9}	5.525×10^{-13}	3.590×10^{-15}	4.54
IRON (Fe)	BCC	$s = \frac{1}{2}, z = 7$	0.152	1043	2.34	2.292×10^{-6}	0.828×10^{-9}	3.167×10^{-13}	2.669×10^{-15}	2.94
		$s = \frac{1}{2}, z=7.5$	0.161		2.45	3.647×10^{-6}	0.894×10^{-9}	3.420×10^{-13}	4.607×10^{-15}	2.73
		$s = \frac{1}{2}, z=8$	0.169		2.64	4.000×10^{-6}	1.065×10^{-9}	4.008×10^{-13}	5.726×10^{-15}	2.70
COBALT (Co)	HCP	$s = \frac{1}{2}, z=11$	0.214	1400	3.77	2.008×10^{-6}	0.357×10^{-9}	1.355×10^{-13}	1.351×10^{-15}	1.27
		$s = \frac{1}{2}, z=12$	0.228		4.15	2.259×10^{-6}	0.496×10^{-9}	2.271×10^{-13}	2.070×10^{-15}	1.25
NICKEL (Ni)	FCC	$s = \frac{1}{2}, z=12$	0.228	672	4.15	7.395×10^{-6}	0.360×10^{-8}	3.787×10^{-12}	5.146×10^{-14}	1.25
GADOLINIUM (Gd)	HCP	$s = \frac{7}{2}, z=12$	0.00215	292	105.19	2.279×10^{-6}	7.70×10^{-7}	9.275×10^{-8}	4.95×10^{-10}	1.728
DYSPROSIUM (Dy)	HCP	$s = 5, z=12$	0.00103	85	201.11	1.671×10^{-4}	2.497×10^{-5}	6.929×10^{-6}	2.235×10^{-7}	1.731

of a Heisenberg ferromagnet is written as,

$$H = -2J \sum_{j,\ell} [\, 2Sa_j^{+} f_j(s) f_\ell(s) a_\ell - 2Sa_j^{+} a_j + a_j^{+} a_j a_\ell^{+} a_\ell \,] - g\mu_B H_o \sum_j a_j^{+} a_j \qquad \ldots(4.3\text{-}1)$$

In equation (4,3-1), $f_j(s) = (1-a_j^{+}a_j/2S)^{\frac{1}{2}}$ and the expansion of $f_j(s)$ takes into consideration all the two-product and four product terms in order to account for the wave-wave-wave interaction. Hence,

$$(1 - \frac{a^{+}a}{2S})^{\frac{1}{2}} = 1 - \frac{1}{2}(\frac{a^{+}a}{2S}) - \frac{1}{8}(\frac{a^{+}a}{2S})^2 - \frac{1}{16}(\frac{a^{+}a}{2S})^3 - \frac{5}{128}(\frac{a^{+}a}{2S})^4 - \frac{7}{256}(\frac{a^{+}a}{2S})^5 - \ldots \qquad \ldots (4.3\text{-}2)$$

where

$$(a^{+}a)^2 = (a^{+}aa^{+}a) = a^{+}(1+a^{+}a)a = a^{+}a+a^{+}a^{+}aa,$$

$$(a^{+}a)^3 = (a^{+}aa^{+}aa^{+}a) = a^{+}(1+a^{+}a)(a+a^{+}a)a = a^{+}(1+2a^{+}a+a^{+}a+a^{+}a^{+}aa)a$$

$$= a^{+}a+3a^{+}a^{+}aa+a^{+}a^{+}a^{+}aaa$$

$$= a^{+}a+3a^{+}a^{+}aa,$$

$$(a^{+}a)^4 = (a^{+}aa^{+}aa^{+}aa^{+}a) = a^{+}(1+a^{+}a)(1+a^{+}a)(1+a^{+}a)a$$

$$= a^{+}[\,(1+a^{+}a+a^{+}a^{+}aa)(1+a^{+}a)\,]a$$

$$= a^{+}a+7a^{+}a^{+}aa+6a^{+}a^{+}a^{+}aaa+a^{+}a^{+}a^{+}a^{+}aaaa$$

$$= a^{+}a+7a^{+}a^{+}aa,$$

$$(a^{+}a)^{5} = (a^{+}aa^{+}aa^{+}aa^{+}aa^{+}a) = a^{+}(1+a^{+}a)(1+a^{+}a)(1+a^{+}a)(1+a^{+}a)a$$

$$= a^{+}[(1+7a^{+}a+6a^{+}a^{+}aa+a^{+}a^{+}a^{+}aaa)(1+a^{+}a)]a$$

$$= a^{+}a+15a^{+}a^{+}aa+25a^{+}a^{+}a^{+}aaa+9a^{+}a^{+}a^{+}a^{+}aaaa$$

$$+ 2a+a^{+}a^{+}a^{+}a^{+}aaaaa$$

$$= a^{+}a+15a^{+}a^{+}aaa,$$

$$(a^{+}a)^{6} = (a^{+}aa^{+}aa^{+}aa^{+}aa^{+}aa^{+}a) =$$

$$a+[1+15a^{+}a+25a^{+}aaa+10a^{+}a^{+}a^{+}aaa+a^{+}a^{+}a^{+}a^{+}aaaa+a^{+}a+15a^{+}a+15a^{+}a^{+}aa$$

$$+50a^{+}a^{+}aa+25a^{+}a^{+}a^{+}aaa+30a^{+}a^{+}a^{+}aaa+10a^{+}a^{+}a^{+}a^{+}aaaa+4a^{+}a^{+}a^{+}a^{+}aaaa$$

$$+a^{+}a^{+}a^{+}a^{+}a^{+}aaaaa]a,$$

$$= a^{+}(1+31a^{+}a+90a^{+}a^{+}aa+65a^{+}a^{+}a^{+}aaa+15a^{+}a^{+}a^{+}a^{+}aaaa+a^{+}a^{+}a^{+}a^{+}a^{+}aaaaa)a$$

$$= a^{+}a+31a^{+}a^{+}aa,$$

Equation (4,3-2) becomes

$$(1 - \frac{a^{+}a}{2S})^{\frac{1}{2}} = 1-[\frac{1}{2}(\frac{1}{2S}) + \frac{1}{8}(\frac{1}{2S})^{2} + \frac{1}{16}(\frac{1}{2S})^{3} + \frac{5}{128}(\frac{1}{2S})^{4} + \ldots]a^{+}a$$

$$-[\frac{1}{8}(\frac{1}{2S})^{2} + \frac{3}{16}(\frac{1}{2S})^{3} + \frac{7.5}{128}(\frac{1}{2S})^{4} + \frac{7.15}{256}(\frac{1}{2S})^{5} + \ldots]a^{+}a^{+}aa \qquad \ldots (4,3\text{-}3)$$

$$(1 - \frac{a^{+}a}{2S})^{\frac{1}{2}} = 1 + \lambda a^{+}a + \gamma a^{+}aa^{+}a$$

where

$$\lambda = (1-(1 - \frac{1}{2S})^{\frac{1}{2}})$$

$$\gamma = \frac{1}{8}(\frac{1}{2S})^2 + \frac{3}{16}(\frac{1}{2S})^3 + \frac{7.5}{128}(\frac{1}{2S})^4 + \frac{7.15}{256}(\frac{1}{2S})^5+\ldots \qquad \ldots (4.3\text{-}4)$$

Equation (4.3-1) can be written with the above modification and $H_o = 0$ to give

$$H = \Sigma-2J[\,2Sa^+(1+\lambda a^+a+\gamma a^+a^+aa)(1+\lambda b^+b+\gamma b^+b^+bb)b+(S-a^+a)(S-b^+b)] \qquad \ldots (4.3\text{-}5)$$

Putting $a_j = a$, $a_\ell = b$

$$H = \Sigma-2J[\,2Sa^+(1+\lambda(a^+a+b^+b)+\gamma(a^+a^+aa+b^+b^+bb)+\lambda^2a^+ab^+b)b$$

$$- (S^2-S(a^+a+b^+b)+a^+ab^+b)]$$

$$= \Sigma-2J[2S(a^+b+\lambda(a^+a^+ab+a^+b^+bb)+\gamma(a^+a^+a^+aab+a^+b^+b^+bbb)$$

$$+ \lambda^2(a^+a^+ab^+bb) + (S^2-S(a^+a+b^+b)+a^+ab^+b] \qquad \ldots (4,3\text{-}6)$$

$$= \Sigma-2J[2S(a^+b-a^+a)+2S\lambda(a^+a^+ab+a^+b^+bb)+a^+ab^+b$$

$$+ 2S\beta(a^+a^+a^+aab + a^+b^+b^+bbb)+\lambda^2(a^+a^+ab^+bb)] \qquad \ldots (4.3\text{-}7)$$

Using the transformation

$$a_k = N^{-\frac{1}{2}}\sum_j \exp(-ik_j)a_j, \quad a_k^+ = N^{-\frac{1}{2}}\sum_j \exp(ik_j)a_j^+ \qquad \ldots (4,3-8)$$

where k denotes a reciprocal lattice vector and N is the total number of ferromagnetic spins.

We can now transform every term which has not been transformed appearing in the above Hamiltonian with the help of the fourier transform (4,3-8)

$$\sum_{\text{all } j} Ja^+a^+ab^+bb^+ = \sum N^{-3}Ja_k^+ a_{k^i}^+ a_{k^{ii}} a_{k^{iii}}^+ a_{k^{iv}} a_{k^v}^+ \exp i(k.j+k^i.j-k^{ii}.j+k^{iii}.\ell - k^{iv}.\ell-k^v.\ell)$$

where

$$k^{iii} = k^{ii}+p^{ii}, \quad k^{iv} = k^i+p^i, \quad k^v = k+p$$

on substitution, we have

$$\sum_{\text{all } j} Ja^+a^+ab^+bb = N^{-3}\sum Ja_k^+ a_{a^i}^+ a_{k^{ii}} a^+_{k^{ii}+p^{ii}} a_{k^i+p^i} a_{k+p} \exp i(k.j+k^i.j-k^{ii}.j+k^{ii}.\ell - p.\ell+p^{ii}.\ell-k^i.\ell-p^i.\ell-k.\ell)$$

$$= N^{-3}\sum Ja_k^+ a_{k^i}^+ a_{k^{ii}} a_{k^{ii}+p^{ii}} a_{k^i+p^i} a_{k+p} \exp i(k+k^i-k^{ii})(j-\ell) \exp i(p^{ii}-p^i-p).\ell \qquad \ldots (4.3-9)$$

There are three important contributions coming from the above term one with $p_1 = p = 0$, $k = k^i$, and $k = k^{ii}$.

The first contribution gives

$$= N^{-2}\Sigma J(k+k^{i}-k^{ii})z\, a^{+}_{k}a^{+}_{k^{i}}a^{+}_{k^{ii}}a_{k^{ii}}a_{k^{i}}a_{k}$$

The second contribution gives

$$N^{-2}\Sigma J(2k-k^{ii})z\, a^{+}_{k}a^{+}_{k^{i}}a_{k^{ii}}a^{+}_{k^{ii}+p^{i}+p}a_{k+p^{i}}a_{k+p}$$

The third contribution gives

$$N^{-2}\Sigma J(k^{i})z\, a^{+}_{k^{ii}}a^{+}_{k^{i}}a_{k^{ii}}a^{+}_{k^{ii}}a^{+}_{k^{ii}+p^{i}+p}a_{k^{i}+p^{i}}a_{k^{ii}+p}$$

Adding all contributions, we obtain,

$$\sum_{\text{all } j} Ja^{+}a^{+}ab^{+}bb = N^{-2}z\Sigma[J(k+k^{i}-k^{ii})+J(2k^{i}-k^{ii})+J(k^{i})]\, a^{+}_{k}a^{+}_{k^{i}}a^{+}_{k^{ii}}a_{k}a_{k^{i}}a_{k^{ii}} \qquad \ldots\ (4.3\text{-}10)$$

Similarly,

$$\sum_{\text{all } j} J(a^{+}b^{+}b^{+}bbb) = N^{-3}\Sigma Ja^{+}_{k}a^{+}_{k^{i}}a^{+}_{k^{ii}}a_{k^{iii}}a_{k^{iv}}a_{k^{v}} \exp i(k.j+k^{i}.\ell+k^{ii}.\ell-k^{iii}.\ell -k^{iv}.\ell-k^{v}.\ell)$$

with

$$k^{iii} = k^{ii}+p^{ii},\quad k^{iv} = k^{i}+p^{i},\quad k^{v} = k+p.$$

On substitution we have

$$\Sigma J(a^{+}b^{+}b^{+}bbb) = N^{-3}\Sigma J a^{+}_{k} a^{+}_{k^{i}} a^{+}_{k^{ii}} a_{k^{ii}+p^{ii}} a_{k^{i}+p^{i}} a_{k+p}\ \exp i(k.j+k^{i}.\ell+k^{ii}.\ell-$$

$$k^{ii}.\ell-p^{ii}.\ell-k^{i}.\ell-p^{i}.\ell-k.\ell-p.\ell)$$

$$= N^{-3}\Sigma J a^{+}_{k} a^{+}_{k^{i}} a^{+}_{k^{ii}} a_{k^{ii}+p^{ii}} a_{k^{i}+p^{i}} a_{k+p} \exp i(k(j-\ell)\exp -i(p^{ii}+p^{i}+p).\ell \qquad \ldots (4.3\text{-}11)$$

With contributions $p = p^{i} = p^{ii} = 0$, $k = k'$ and $k = k^{ii}$

$\Sigma J a^{+}b^{+}b^{+}bbb$

$$= N^{-2}\Sigma zJ(k)+J(k^{i})+J(k^{ii}) a^{+}_{k} a^{+}_{k^{i}} a^{+}_{k^{ii}} a_{k^{ii}} a_{k^{i}} a_{k} \qquad \ldots (4.3\text{-}12)$$

Now, we can write the Hamiltonian in the transformed form as follows

$$H = E_{o} + \sum_{k} A(k) a^{+}_{k} a_{k} + N^{-1} \sum_{k,k^{i}} V(k,k^{i}) a^{+}_{k} a^{+}_{k^{i}} a_{k} a_{k^{i}} + N^{-2} \sum_{k,k^{i},k^{ii}} V(k,k^{i},k^{ii})$$

$$a^{+}_{k} a^{+}_{k^{i}} a^{+}_{k^{ii}} a_{k} a_{k^{i}} a_{k^{ii}} \qquad \ldots (4,3\text{-}13)$$

where

$A(k) = 2zSJ(1-\gamma(k))$

$V(k,k^{i}) = 4S\ zJ[\gamma(k)+\gamma(k^{i})] - zJ[1+\gamma(k-k^{i})]$

$V(k,k^{i},k^{ii}) = -4S\gamma zJ[\gamma(k)+\gamma(k^{i})+\gamma(k^{ii})] - \lambda^{2} zJ[\gamma(k+k^{i}-k^{ii})+\gamma(2k^{i}-k^{ii})\gamma(k^{i})]$

and

$$E_o = -zNS^2J, \quad \gamma(k) = \sum_a \exp(ik.a)/z; \quad |a|^3 = V_o/N$$

Writing $V(k,k^i,k^{ii})$ fully we have

$$\Sigma V(k,k^i,k^{ii}) = N^{-2}\Sigma 4s\gamma zJ(1-\frac{(ka)^2}{z}+1-\frac{(k^ia)^2}{z}+1-\frac{(k^{ii}a)^2}{z})$$

$$+\frac{\lambda^2 zJ}{z}\Sigma(1-\frac{(k+k^i-k^{ii})^2}{z}a^2+1-\frac{(2k^i-k^{ii})^2}{z}a^2+1-\frac{(k^ia)^2}{z}) \qquad \ldots (4.3\text{-}14)$$

Averaging over k^{ii} space we have

$$= \frac{4s\gamma J}{N^2}\Sigma<(3z-k^2a^2-{k^i}^2a^2-{k^{ii}}^2a^2)><n_{k^{ii}}> + \frac{\lambda^2 J}{N}\Sigma<3z-k^2a^2-6{k^i}^2a^2-2{k^{ii}}^2a^2n_{k^{ii}}) \qquad \ldots (4,3\text{-}15)$$

$$= \frac{4s\gamma J}{N^2}\Sigma(3z-k^2a^2-{k^i}^2a^2)r\,\tau^{3/2}\sum_{m=1}^{\infty}\frac{e^{m\beta\mu}}{m^{3/2}} + \frac{\lambda^2 J}{N}\Sigma<3z-k^2a^2-6{k^i}^2a^2)r\tau^{3/2}\sum_{m=1}^{\infty}\frac{e^{m\beta\mu}}{m^{3/2}} \qquad \ldots (4.3\text{-}16)$$

averaging over k', we have

$$= 4s\gamma J[(3z-k^2a^2)r^2\tau^3(\sum_{m=1}^{\infty}\frac{e^{m\beta\mu}}{m^{3/2}})^2 + \lambda^2 J(3z-k^2a^2)r^2\tau^3(\Sigma\frac{e^{m\beta\mu}}{m^{3/2}})^2 \qquad \ldots (4.3\text{-}17)$$

Rewriting our transformed Hamiltonian, we obtain

$$H = \sum_k(A(k)-\mu+A^1-B^1k^2a^2)n_k$$

$$= \sum_k A(k)-(\mu-A^1)-B^1k^2a^2)n_k \qquad \ldots (4.3\text{-}18)$$

where

$$A^1 = 3z\tau^3 r^2 J(4s\gamma+\lambda^2)\left(\sum_{m=1}^{\infty}\frac{e^{m\beta\mu}}{m^{3/2}}\right)^2$$

$$B^1 = (4s\gamma+\lambda^2)Jr^2\tau^3\left(\sum_{m=1}^{\infty}\frac{e^{m\beta\mu}}{m^{3/2}}\right)^2 \quad \ldots (4.3\text{-}19)$$

Equation (4,3-19) clearly shows the effect of the wave-wave-wave interaction on the dispersion relation of the magnons. The energy of a magnon is altered slightly by the additional term $-B^1$, while, the electrochemical potential of a magnon is altered by the additional term $-A^1$.

Our interest here is to find out the effect of $-A^1$ on μ. Writing $w = |\mu|/J$. We have

$$w = (\alpha-1)\,2rZ\tau^{3/2}\sum_{m=1}^{\infty}\frac{e^{-mw/2S\tau}}{m^{3/2}} + (4s\gamma+\lambda^2)r\tau^3 2z\left[\sum_{m=1}^{\infty}\frac{\frac{e^{-mw}}{2S\tau}}{m^{3/2}}\right]^2 \quad \ldots (4.3\text{-}20)$$

with the aid of the computer, we solve numerically the above equation and by the method of least square error fitting, we obtain the following expression for w, for Iron, Cobalt, Nickel, Dysprosium and Gadolinium.

(i) Iron Fe, ($s = \frac{1}{2}$, $z = 7.5$)

$$w = -1.699\times10^{-3}+0.154\tau+0.28\tau^2 = 0.15\tau+0.28\tau^2 \quad \ldots (4.3\text{-}21a)$$

(ii) Iron Fe, ($s = \frac{1}{2}$, $z = 8$)

$$w = -1.846\times10^{-3}+0.164\tau+0.27\tau^2 = 0.16\tau+0.27\tau^2 \quad \ldots (4.3\text{-}21b)$$

(iii) Cobalt Co, $(s = \frac{1}{2},\ z = 11)$

$$w = -2.304\times10^{-3}+0.209\tau+0.32\tau^{2} = 0.21\tau+0.32\tau^{2} \qquad \ldots (4.3\text{-}21c)$$

(iv) Cobalt Co. $(s = \frac{1}{2},\ z = 12)$

$$w = -2.441\times10^{-3}+0.223\tau+0.33\tau^{2} = 0.22\tau+0.33\tau^{2} \qquad \ldots (4.3\text{-}21d)$$

(v) Nickel Ni, $(s = \frac{1}{2},\ z = 12)$

$$w = -2.441\times10^{-3}+0.233\tau+0.33\tau^{2} = 0.22\tau+0.33\tau^{2} \qquad \ldots (4.3\text{-}21e)$$

(vi) Gadolinium Gd. $(s = \frac{1}{2},\ z = 12)$

$$w = -1.919\times10^{-4}+1.444\times10^{-2}\tau+4.172\times10^{-2}\tau^{2} = 1.44\times10^{-2}\tau+4.17\times10^{-2}\tau^{2} \qquad \ldots (4.3,21f)$$

(vii) Dysprosium Dy $(s = 5,\ z = 12)$

$$w = -1.319\times10^{-4}+0.990\times10^{-2}\tau+2.921\times10^{-2}\tau^{2} = 0.99\times10^{-2}\tau+2.92\times10^{-2}\tau^{2} \qquad \ldots (4.3\text{-}21g)$$

$G(\alpha)$ from equation (4.3-7) becomes

$$G(\alpha) = \beta|\mu| = w_1/2S$$

We proceed to find the effect of this new μ on the coefficient of $T^{3/2}$ in the expression of the spontaneous magnetization. This has been done and the table below compares this new 'μ' with the μ of chapter III. We see that the two μ's hardly differ in each case. That is, wave-wave-wave interactions is negligible in comparison with wave-wave interaction. The following figures shows the graphs of w against I.

Table 4.3 - Coefficients of $T^{3/2}$ with chemical potential in wave-wave-wave interactions and wave wave wave interactions.

ELEMENTS	CHEMICAL POTENTIAL IN WAVE-WAVE INTERACTION (μ_1)	CHEMICAL POTENTIAL IN WAVE-WAVE-WAVE INTERACTION (μ_2)	$C_1T^{3/2}$ (μ_1)	$C_1T^{3/2}$ (μ_2)	C_1 experimental
BCC $s = \frac{1}{2}$, $z=7.5$ e.g. Iron	0.16069	0.15369	$3.647\text{x}10^{-6}$	$3.701\text{x}10^{-6}$	$3.41\text{x}10^{-6}$ (Iron)
BCC $s = \frac{1}{2}$, $z=8$ e.g. Iron	0,16880	0.16417	$4.00\text{x}10^{-6}$	$4.039\text{x}10^{-6}$	$3.41\text{x}10^{-6}$ (Iron)
HCP $s = \frac{1}{2}$, $z = 11$ e.g. Cobalt	0.21400	0.20940	$2.008\text{x}10^{-6}$	$2.026\text{x}10^{-6}$	$1.7\text{x}10^{-6}$ (Cobalt)
HCP $s = \frac{1}{2}$, $z = 12$ e.g. Cobalt	0.2280	0.2233	$2,259\text{x}10^{-6}$	$2.279\text{x}10^{-6}$	$1.7\text{x}10^{-6}$ (Cobalt)
FCC $s = \frac{1}{2}, z = 12$	0,2280	0.2230	$7,395\text{x}10^{-6}$	$7.459\text{x}10^{-6}$	$7.4\text{x}10^{-6}$ (Nickel)
HCP $s = \frac{1}{2}, z = 12$	0.00215	0.00206	$2.79\text{x}10^{-6}$	$2.280\text{x}10^{-6}$	- (Gadolinium)
HCP $s = 5, z = 12$	0.00103	0.00099	$1.671\text{x}10^{-4}$	$1.6714\text{x}10^{-4}$	- (Dysprosium)

Fig. 4.3-1: Graph of Chemical Potential/Exchange integral W against reduced temperature T.

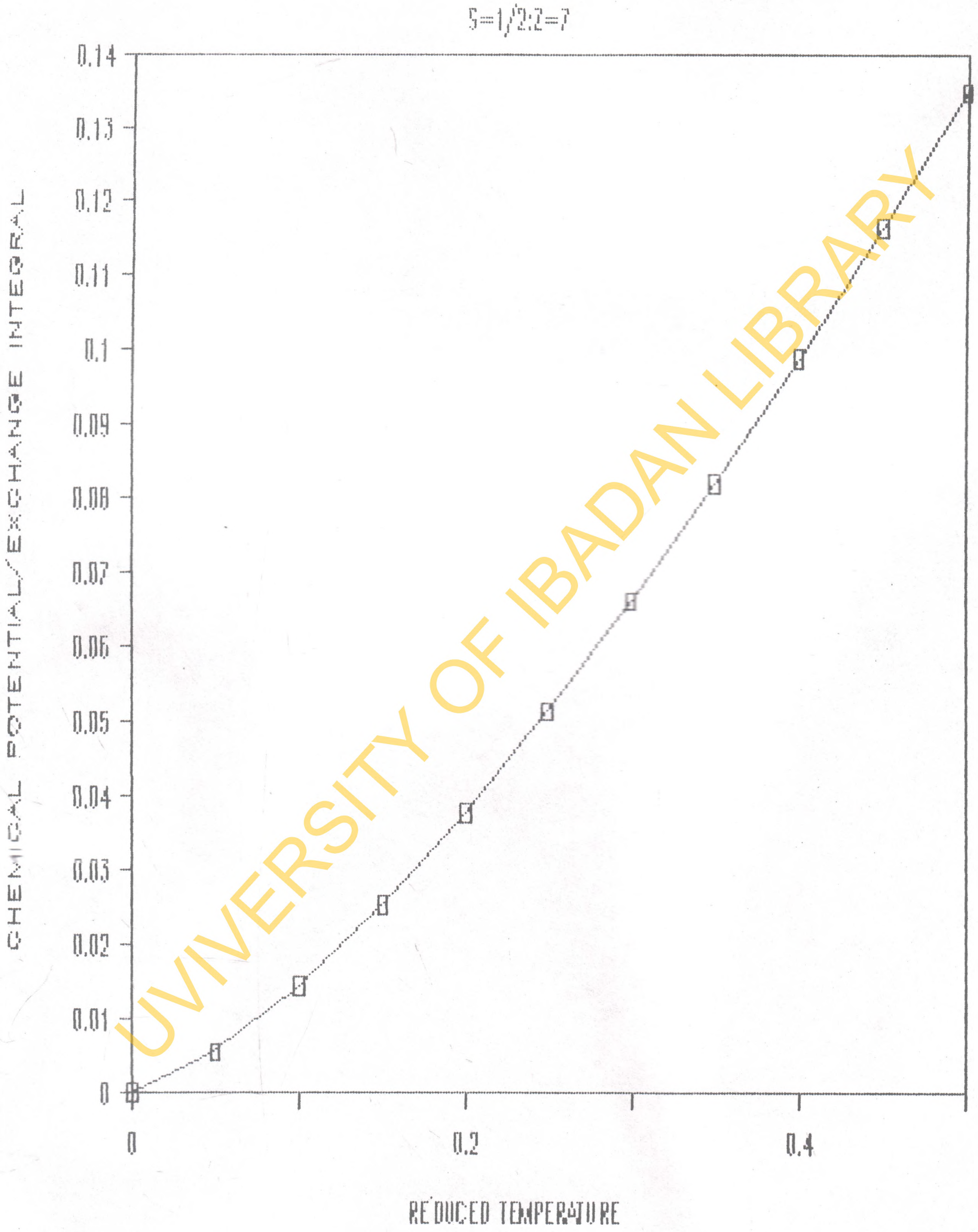


Fig. 4.3-2 Graph of Chemical Potential/Exchange integral W against reduced temperature T

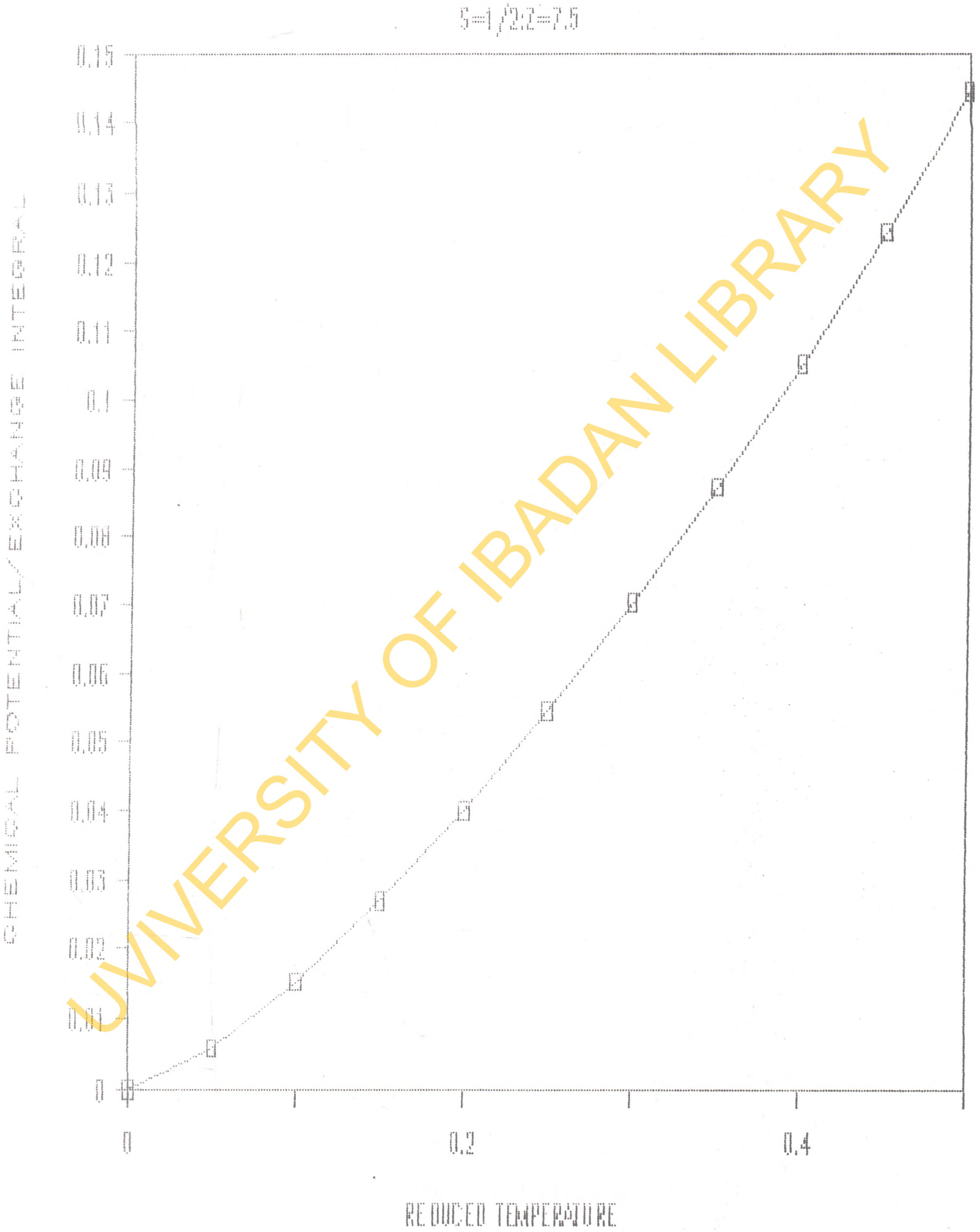
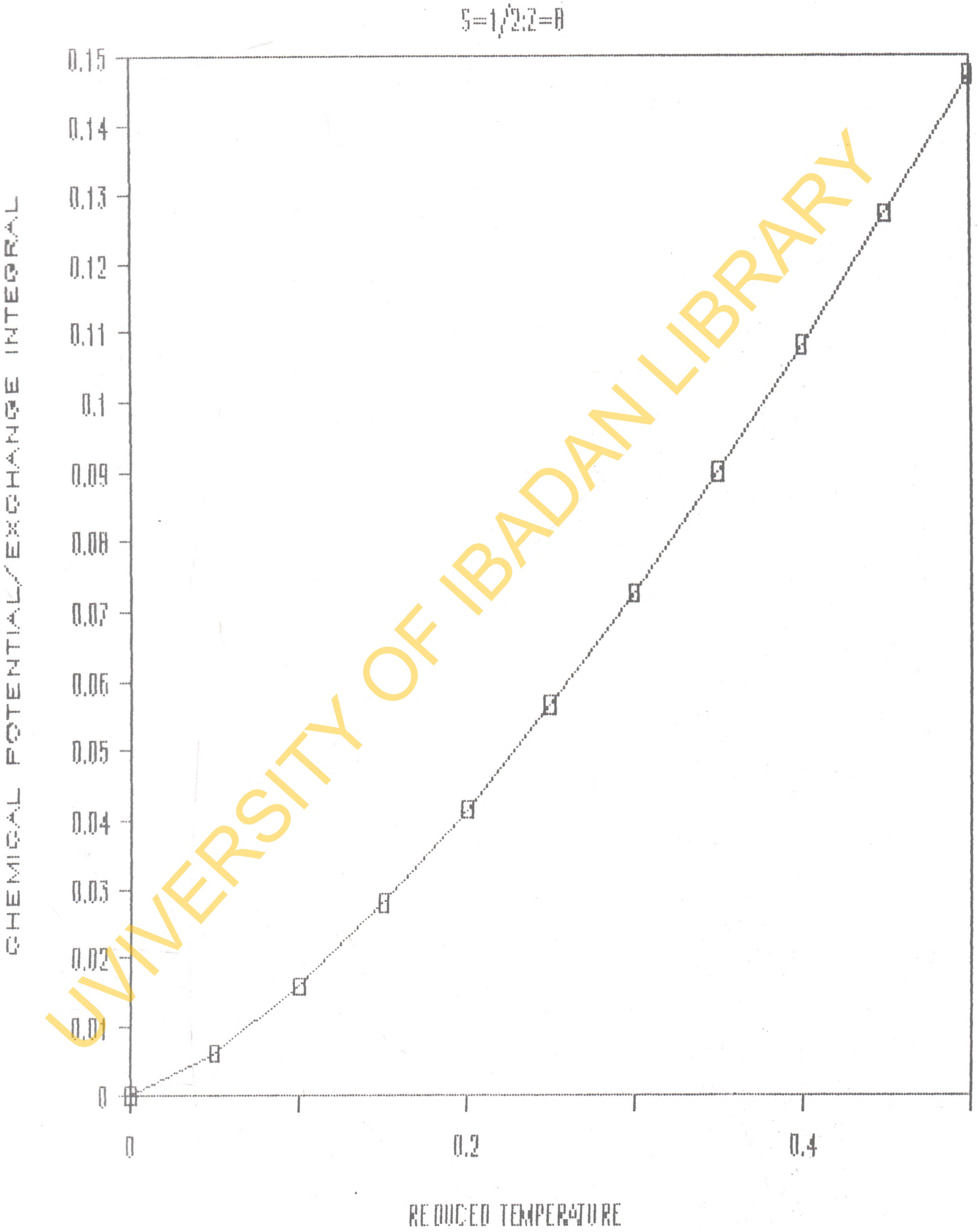


Fig. 4.3-3 Graph of Chemical Potential/Exchange integral W against reduced temperature T.



Fig, 4.3-4: Graph of Chemical Potential/Exchange integral W against reduced temperature T.

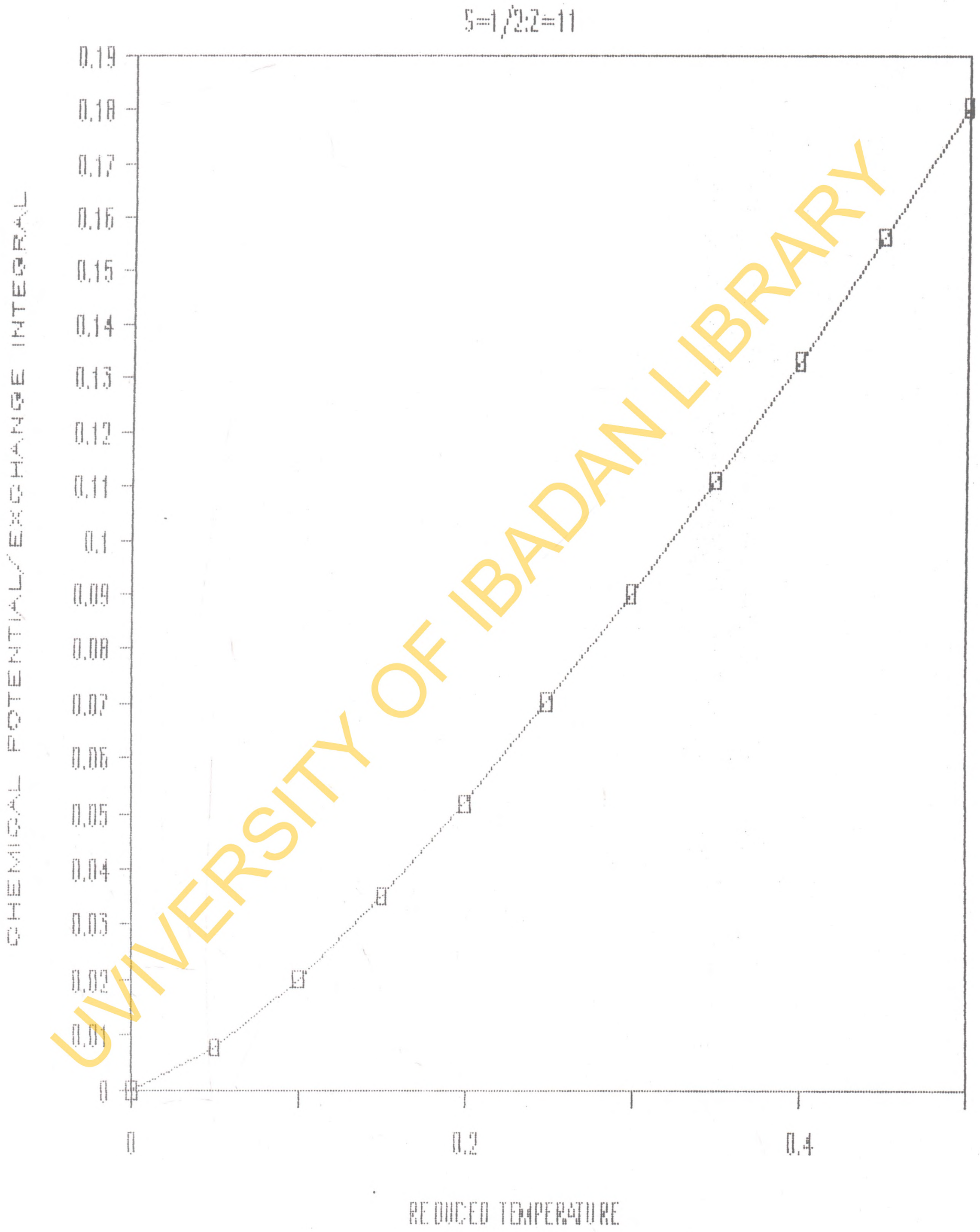
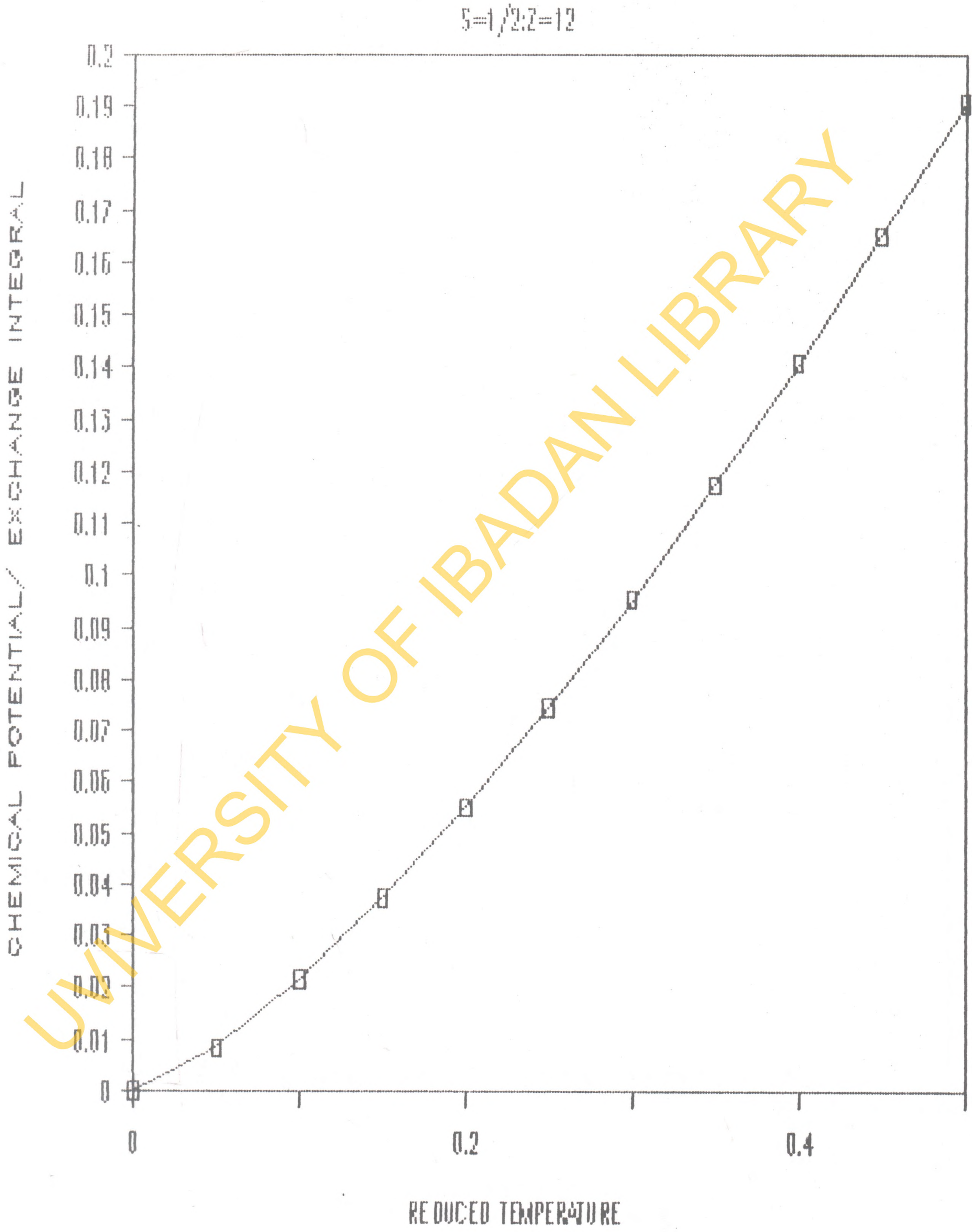


Fig. 4.3-5: Graph of Chemical Potential/Exchange integral W against reduced temperature T.



CHAPTER V

INTERACTIONS II

It has been suggested that magnons, by virtue of their motion do mutually interact, dynamically and secondly they are strictly speaking not Bosons. In this chapter, we examine these two suggestions.

5.1 The Dynamical Interaction

To the best of our knowledge and in agreement with several authors, the spontaneous magnetization at low temperatures contains terms of the form $T^{3/2}$, $T^{5/2}$ and $T^{7/2}$, which correspond to the terms k^2, k^4 and k^6 of the dispersion law respectively. In this section, we are interested in finding the next degree of T contributes to the magnetization. We shall also find the effect of the electrochemical potential on the coefficient of this degree of T.

Going back to our transformed Hamiltonian Expression (3.1-39) is

$$H-E_o = \sum_k A_k n_k + N^{-1}\sum_{k,q} V_{kq} n_k n_q + N^{-1}\sum_{k,q'} W_{kq} n_k n_q = A+B+C$$

where

$$V_{kk'} = zJ[\gamma(k)+\gamma(q)-1-\gamma(k-q)], \quad W_{kq} = z(\alpha-1)J[\gamma(k)+\gamma(q)]$$

$$A_k = 2sJz[1-\gamma(k)]$$

If we expand $\gamma(k)$ to order k^4a^4, we have that

$$\gamma(k) = 1 - \frac{k^2a^2}{z} + A(\phi,\theta)(ka)^4.$$

Note here that the term B on averaging over an angle is not zero and

$$V_{kk'} = zJ[1- \frac{(ka)^2}{z} + A(\phi,\theta)(ka)^4 + 1 - \frac{(k'a)^2}{z} + A(\phi',\theta')(k'a)^4 - 1 - 1 + \frac{(k-k')^2a^2}{z}$$

$$-A(\alpha,\beta)(k-k')^4a^4] \qquad \text{... (5,1-1)}$$

$$= zJ[-A(\alpha,\beta)(k^4+k'^4+4k^2k'^2)a^4+A(\phi,\theta)(ka)^4+A(\phi',\theta')(k'a)^4] \qquad \text{... (5,1-1)}$$

Averaging in k' space and neglecting small terms, we have

$$<V_{kq}\ n_q> = -zJ<[A(\alpha,\beta)4k^2a^4]n_q\ q^2> \qquad \text{... (5.1-2)}$$

Our fourier transformed Hamiltonian is written as

$$H = \sum_k (Fk^2-\mu)n_k \qquad \text{... (5.1-3)}$$

where

$$F = 2SJa^2 - N^{-1}zJ<A(\alpha,\beta)4q^2a^4n_q> \qquad \text{... (5.1-4)}$$

$$F = 2SJa^2[1-\eta] \qquad \text{... (5.1-5)}$$

where

$$\eta = N^{-1}zJ<A(\alpha,\beta)4q^2a^4n_q>/2SJa^2.$$

$$\eta = \frac{V}{2\pi^2 N} zJa^4 \int \frac{A(\alpha,\beta)4q^4 dq}{\exp(Fq^2-\mu)-1}$$

$$= \frac{3}{4}\,\frac{V}{N}\left(\frac{1}{4\pi}\right)^{5/2}\left(\frac{2JSa^2}{kT}\right)^{-5/2}\sum_{m=1}^{\infty}\frac{e^{+m\beta\mu}}{m^{5/2}}\,a^4 x 4\,\frac{\alpha zJ}{2SJa^2} L_1,$$

where

$$L_1 = \int_0^{2\pi} d\alpha \int_0^{\pi} A(\alpha,\beta)\sin\beta d\beta \qquad \ldots(5.1\text{-}6)$$

We should note here that the presence of η has caused a modification of the Dispersion law. There is a shift in the energy of the Spinwave, because of the presence of other Spin waves. This kind of interaction between Spin waves is called the Dynamical interaction (Dyson (1959)).

With the presence of the Dynamical interaction between Spin waves, we are interested in finding the effect of this interaction as well as the effect of the electrochemical potential on the coefficient of spontaneous magnetization,

$$\delta M = \sum_k \frac{\langle n_k \rangle}{NS} = \frac{1}{QS}\left(\frac{kT}{8\pi JS}\right)^{3/2}\sum_{m=1}^{\infty}\frac{e^{+m\beta\mu}}{m^{3/2}}(1-\eta)^{-3/2} \qquad \ldots (5.1\text{-}7)$$

where the number N of atoms per unit volume is Q/a^3.

Therefore for small η,

$$\sum_k \frac{\langle n_k \rangle}{NS} = \frac{1}{QS}\left(\frac{kT}{8\pi JS}\right)^{3/2} \sum_{m=1}^{\infty} \frac{e^{m\beta\mu}}{m^{3/2}} \left(1 + \frac{3}{2}\eta\right)$$

$$= \frac{1}{QS}\left(\frac{kT}{8\pi JS}\right)^{3/2} \sum_{m=1}^{\infty} \frac{e^{+m\beta\mu}}{m^{3/2}} + \frac{3}{Q^2} \frac{3\pi}{4S^2} zL, \left(\frac{kT}{8\pi JS}\right)^4 \sum \frac{e^{+m\beta\mu}}{m^{3/2}} \sum \frac{e^{m\beta\mu}}{m^{5/2}}$$

... (5.1-8)

The second term of expression (5.1-8) clearly gives the coefficient of T^4. This coefficient has been calculated for some ferromagnetic elements, and shown in Table 4.2. This T^4 dependence, due to Dynamical interaction, is experimentally negligible as compared with the other coefficients of T.

5.2 The Kinematical Interaction

According to DYSON (1956), the kinematical interaction arises because the Spin wave states which contain more than one Spin wave are not members of an orthogonal set. The non-orthogonality of these states produces an interaction between Spins which we call the kinematical interaction. The Physical cause of this interaction is the fact that more than (2S+1) units of reversed Spin cannot be attached to the same atom. There is therefore some form of exclusion at work, to limit any dense packing of many spin waves within a given volume.

The kinematical interaction is a purely statistical effect which reduces the statistical weight of states containing a high density of spin waves per unit volume. They appear in calculation of the statistical and thermodynamical properties of the spin wave system, but not in the dynamics of individual spin waves.

In this section, we show the effect of the kinematical interaction of Spin waves by recomputing the coefficients of T in the expression of the spontaneous magnetization, for Iron, Nickel, Cobalt, Dysprosium and Gadolinium. This time, all averaging in k space is done over intermediate statistics.

The intermediate statistics, is so-called because the largest number of particles p allowed in any state is intermediate between Fermi-Dirac Statistics with p = 1 and Bose-Einstein statistics with p = ∞. For this statistics, it is the case that the grand partition function is

$$Z = \sum_{n_k=o}^{p} a_k^{n_k} \qquad \ldots (5.2\text{-}1)$$

where

$$a_k = e^{-\beta(E_k-\mu)} = b_k z, \quad 1<p<\infty$$

$$z = e^{\beta\mu}, \quad b_k = e^{-\beta E_k}$$

$$Z = \frac{1-a_k^{p+1}}{1-a_k} = \frac{1-(b_k z)^{p+1}}{1-(b_k z)} \qquad \ldots (5.2\text{-}2)$$

The number distribution is defined as

$$n_k = z\frac{\partial}{\partial z}\ln Z \qquad \ldots (5.2\text{-}3)$$

Thus the distribution becomes

$$\langle n_k \rangle = \frac{1}{(b_k z)^{-1}-1} - \frac{(p+1)}{(b_k z)^{-(p+1)}-1}$$

$$= \frac{1}{\exp\beta(E_k-\mu)-1} - \frac{(p+1)}{\exp\beta(E_k-\mu)(p+1)-1} \qquad \ldots (5.2\text{-}4)$$

For Spin waves, $p = 2S+1$

$$\langle n_k \rangle = \frac{1}{\exp\beta(E_k-\mu)-1} - \frac{(2S+2)}{\exp\beta(E_k-\mu)(2S+2)-1} \qquad \ldots (5.2\text{-}5)$$

Averaging under this distribution, the chemical potential μ in (3.2-5) becomes

$$\mu = (1-\alpha)\,\frac{J}{N}\langle[\,2z-\alpha^2 a^2\,]\,n_\alpha\rangle \qquad \ldots (5.2\text{-}6)$$

$$\mu = (1-\alpha)J[2z-k^2a^2]\frac{V}{2\pi^2N}[\int_0^\infty \frac{k^2\,dk}{\exp\beta(Fk^2-x)-1} - \int_0^\infty \frac{(2S+2)k^2dk}{\exp\beta(Fk^2-x)(2S+2)-1}] \qquad \ldots (5.2\text{-}7)$$

neglecting smaller terms, we have

$$\mu = (1-\alpha)J\frac{2zV}{2\pi^2N}[\int_0^\infty \sum_{m=1}^\infty e^{-m\beta(Fk^2-x)}k^2dk - \int_0^\infty (2S+2)\sum_{m=1}^\infty e^{-m\beta(Fk^2-x)(2S+2)}k^2dk \qquad \ldots (5.2\text{-}8)$$

$$= (1-\alpha)2zJ[\sum_{m=1}^\infty - \frac{e^{m\beta x}}{(m\beta F)^{3/2}}\frac{V}{4\beta^2N}(\frac{\pi}{4})^{\frac{1}{2}} - (2S+2)\sum_{m=1}^\infty \frac{e^{m\beta x(2S+2)}}{[(m\beta F)(2S+2)]^{3/2}}\frac{V}{4\pi^2N}(\frac{\pi}{4})^{\frac{1}{2}}] \qquad \ldots (5.2\text{-}9)$$

Put

$$r = \frac{1}{4\pi^2}(\frac{\pi}{4})^{\frac{1}{2}}, \quad w = \frac{|\mu|}{J}, \quad \tau = \frac{k_BT}{2SJ}, \quad F = 2SJa^2,$$

$$w = (1-\alpha)2zr\tau^{3/2}[\sum_{m=1}^\infty \frac{e^{\frac{-mw}{2S\tau}}}{m^{3/2}} - 2S+2\sum_{m=1}^\infty \frac{e^{\frac{-mw}{2S\tau}(2S+2)}}{m^{3/2}}(2S+2)^{-3/2} \qquad \ldots (5.2\text{-}10)$$

$$= (1-\alpha)2zr\tau^{3/2}[\sum_{m=1}^\infty (\frac{e^{(\frac{-mw}{2S\tau})}}{m^{3/2}}) - \sum_{m=1}^\infty \frac{e^{\frac{-mw}{2S\tau}(2S+2)}}{m^{3/2}}(2S+2)^{-\frac{1}{2}} \qquad \ldots (5.2.11)$$

We proceed to solve μ numerically from equation (5.2-11), for the values of τ between 0 and 0.50.

By the method of least square error fitting, we obtain the following expressions of w, for Iron, Cobalt, Nickel, Dysprosium and Gadolinium.

(i) Body-centred cubic (e,g, Fe) with $s = \frac{1}{2}$, $z = 7,5$

$$w - 1,476\text{x}10^{-3} + 0.108\tau + 0,21\tau^2 = 0,11\tau + 0.21\tau^2 \qquad \ldots (5.2\text{-}12a)$$

(ii) Body-centred cubic (e,g, Fe) with $s = \frac{1}{2}$, $z = 8$

$$w = -1.564\text{x}10^{-3} + 0.115\tau + 0.22\tau^2 = 0.12\tau + 0.22\tau^2 \qquad \ldots (5.2\text{-}12b)$$

(iii) Hexagonal close packed (e.g. Co.) with $s = \frac{1}{2}$, $z = 11$

$$w = -2.058\text{x}10^{-3} + 0,154\tau + 0,28\tau^2 = 0,15\tau + 0,28\tau^2 \qquad \ldots (5.2\text{-}12c)$$

(iv) Hexagonal-close packed (e.g. Co) with $s = \frac{1}{2}$, $z = 12$

$$w = -2.659\text{x}10^{-3} + 0,172\tau + 0,29\tau^2 = 0.17\tau + 0.29\tau^2 \qquad \ldots (5.2\text{-}12d)$$

(v) Face centred cubic (e.g. Ni) with $s = \frac{1}{2}$, $z = 12$

$$= -2,659\text{x}10^{-3} + 0,172\tau + 0,29\tau^2 = 0.17\tau + 0,29\tau^2 \qquad \ldots (5.2\text{-}12e)$$

(vi) Hexagonal close packed (e.g. Gd) with $s = \frac{7}{2}$, $z = 12$

$$w = -1.466\text{x}10^{-4} + 1,027\text{x}10^{-2}\tau + 2,861\text{x}10^{-2}\tau^2 = 1,03\text{x}10^{-2}\tau + 2.86\text{x}10^{-2}\tau^2 \qquad \ldots (5.2\text{-}12f)$$

(vii) Hexagonal close packed (e.g. Dy) with $s = 5$, $z = 12$

$$w = -1,053\text{x}10^{-4} + 7,422\text{x}10^{-3}\tau + 2,060\text{x}10^{-2}\tau^2 = 7,42\text{x}10^{-3}\tau + 2,06\text{x}10^{-2}\tau^2 \qquad \ldots 5.2\text{-}12g)$$

As usual μ (the electrochemical potential) is computed for all the ferromagnetic elements. We proceed to find the effect of this new μ on the coefficients of T^{ν} in the expression for the spontaneous magnetization.

$$\sum_k \frac{n_k}{NS} = \frac{V}{(2\pi)^3 NS}\left[\int_0^\infty \frac{k^2 dk}{\exp\beta(Fk^2-\mu)-1} - 2S+2\int_0^\infty \frac{k^2 dk}{\exp\beta(Fk^2-\mu)(2S+2)-1}\right] \quad \ldots (5,2\text{-}13)$$

The third order approximation of F leads to

$$= 2sJ[(ka)^2 - zA(\phi,\theta)(ka)^4 + zB(\phi,\theta)(ka)^6 + \ldots] \quad \ldots (5.2\text{-}14)$$

Putting (5.2-14) into (5.2-13) and evaluating, we have

$$\sum_k \frac{\langle n_k \rangle}{NS} = \frac{V}{(2\pi)^3 N} C^{-3/2} \sum_{m=1}^{\infty}\left\{\frac{e^{-my}}{m^{3/2}} - \frac{e^{-my(2S+2)}}{m^{3/2}}(2+2S)^{-\frac{1}{2}}\right\} 2\pi\Gamma(\tfrac{3}{2})$$

$$+ \frac{5}{4}zL_1\Gamma(\tfrac{5}{2})\left\{\frac{e^{-my}}{m^{5/2}} - \frac{e^{-my(2S+2)}}{m^{5/2}}(2S+2)^{-\frac{1}{2}}\right\}\tau$$

$$(4z^2L_2 - \frac{7}{4}zL_3)\Gamma(\tfrac{7}{2})\left\{\frac{e^{-my}}{m^{7/2}} - \frac{e^{-my(2S+2)}}{m^{3/2}}(2S+2)^{-\frac{1}{2}}\right\}\tau^2 \quad \ldots (5.2\text{-}15)$$

where Γ is the gamma function $y = \frac{\mu}{kT}$, and all other terms retain their previous meanings and definitions.

Expression (5,2-15) gives the effect of the kinematical interaction, as well as the effect of the electrochemical potential on the coefficients of spontaneous magnetization.

The table 5.2 shows μ'' (the new effective chemical potential and the various coefficients of T^{ν}.

The coefficient of T^4 shows the effect of both Dynamical and kinematical interactions.

Table 5.2 - Coefficients of $T^{3/2}$, $T^{5/2}$, $T^{7/2}$ and T^{4} with Kinematical interactions.

FERROMAGNETIC ELEMENTS	CHEMICAL POTENTIAL (μ'')	$C''_1(T^{3/2})$	$C''_2(T^{5/2})$	$C''_3(T^{7/2})$	$C''_4(T^{4})$
SC $s=\frac{1}{2}$, $z=6$	0,113	$4{,}513\text{x}10^{-6}$	$0{,}672\text{x}10^{-7}$	$2{,}762\text{x}10^{-13}$	$1{,}795\text{x}10^{-15}$
BCC $s=\frac{1}{2}$, $z=7.5$	0,108	$2.546\text{x}10^{-6}$	$0.543\text{x}10^{-9}$	$1{,}984\text{x}10^{-13}$	$1.132\text{x}10^{-15}$
(Fe) $s=\frac{1}{2}$, $z=8$	0,115	$2{,}820\text{x}10^{-6}$	$0{,}655\text{x}10^{-9}$	$2.351\text{x}10^{-13}$	$2{,}504\text{x}10^{-15}$
HCP $s=\frac{1}{2}$, $z=11$	0.154	$1{,}489\text{x}10^{-6}$	$0{,}235\text{x}10^{-9}$	$0.853\text{x}10^{-13}$	$0.659\text{x}10^{-15}$
(Co) $s=\frac{1}{2}$, $z=12$	0,172	$1.689\text{x}10^{-6}$	$0{,}332\text{x}10^{-9}$	$1.460\text{x}10^{-13}$	$1.036\text{x}10^{-15}$
FCC $s=\frac{1}{2}$, $z=12$ (Ni)	0.172	$5.529\text{x}10^{-6}$	$0.241\text{x}10^{-8}$	$2.434\text{x}10^{-12}$	$2.403\text{x}10^{-14}$
HCP $s=\frac{1}{2}$, $z=12$ (Gd)	0.00147	$1.582\text{x}10^{-6}$	$5{,}191\text{x}10^{-7}$	$6.231\text{x}10^{-8}$	$2.298\text{x}10^{-10}$
HCP $s=5$, $z=12$ (Dy)	0.000742	$1.217\text{x}10^{-4}$	$1{,}787\text{x}10^{-5}$	$4.950\text{x}10^{-6}$	$1{,}165\text{x}10^{-7}$

The table 5.3 below gives the computed coefficients of $T^{3/2}$ for all the five ferromagnetic elements, with the inclusion of the effect of the presence of

(i) the electrochemical potential μ

(ii) the kinematical interaction,

(iii) both the electrochemical potential as well as the kinematical interaction, and

(iv) no interaction.

In table 5.3, we also give the available experimental values for some of the elements for comparative studies.

Table 5.3: The Coefficient of $T^{3/2}$

	IRON $(s=\frac{1}{2}, z=7.5)$	IRON $(s=\frac{1}{2}, z=8)$	COBALT $(s=\frac{1}{2}, z=11)$	COBALT $(s=\frac{1}{2}, z=12)$	NICKEL $(s=\frac{1}{2}, z=12)$	GADOLINIUM $(s=7/2, z=12)$	DYSPROSIUM $(s=5, z=12)$
With the electrochemical potential μ	$3.647x10^{-6}$	$4.000x10^{-6}$	$2.008x10^{-6}$	$2.259x10^{-6}$	$7.393x10^{-6}$	$2.279x10^{-6}$	$1.671x10^{-4}$
With the Kinematical interaction	$2.818x10^{-6}$	$3.239x10^{-6}$	$1.495x10^{-6}$	$1.479x10^{-6}$	$6.546x10^{-6}$	$2.635x10^{-6}$	$1.940x10^{-4}$
With both electrochemical potential (μ) and kinematical interaction	$2.546x10^{-6}$	$2.820x10^{-6}$	$1.489x10^{-6}$	$1.689x10^{-6}$	$5.529x10^{-6}$	$1.582x10^{-6}$	$1.217x10^{-4}$
With no interaction	$6.687x10^{-6}$	$6.479x10^{-6}$	$4.102x10^{-6}$	$4.726x10^{-6}$	$15.49x10^{-6}$	$4.27x10^{-6}$	$2.95x10^{-4}$
Experimental value	$3.41x10^{-6}$	$3.41x10^{-6}$	$1.7x10^{-6}$	$1.7x10^{-6}$	$7.4x10^{-6}$	-	-

CHAPTER VI

DISCUSSION

In this chapter, we give a detailed discussion of our results and extensions thereof to antiferromagnetism.

6.1 Results

The temperature T_o, below which magnons are well defined quasi-particles for cubic crystals as shown in chapter two is given by

$$T_o = 2x10^{-3}\left(\frac{T_c}{z-1}\right)^2 \qquad \ldots (6.1-1)$$

T_o, for crystals with Hexagonal close packed lattice structure is

$$T_o = 1.23x10^{-3}\, S^3\left(\frac{T_c}{\theta_c}\right)^2 \qquad \ldots (6.1-2)$$

where T_c is the transition temperature, θ_c is the reduced curie temperature k_B is the Boltzmann's constant, $\hbar$ is the planck's constant, z is the number of nearest neighbours, a is the interatomic distance and S is the Spin value.

Thus for b_{cc} Iron $T_o = 44k$, for fcc Nickel $T_o = 7k$ for fcc Cobalt $T_o = 28k$, for h_{cp} Gadolinium $T_o = 0.4k$ and for h_{cp} Dysprosium, $T_o = 0.02k$.

For temperatures $T > T_o$, the interaction among the Spin waves is important. The spin operators S^+ and S^- respectively contain the term $f_j(s)$, (see equation 3.1-12). Within the spin wave - spin wave interaction approximation,

$$f_j(s) = [1 - \frac{a_j^+ a_j}{2S}]^{\frac{1}{2}}$$

where a_j^+ and a_j are the creation and annihilation operators respectively and S, has been expanded to all orders.

The infinite series in the two product terms has the form

$$f_j(s) = 1 + \lambda a_j^+ a_j \qquad \ldots (6.1\text{-}3)$$

where

$$-\lambda = (1 - \frac{1}{2S})^{\frac{1}{2}} - 1$$

The Fourier transformed Hamiltonian of a ferromagnet as shown in chapter three is given by

$$H - E_o = \sum_k A_k n_k + N^{-1} \sum_{k,q} V_{kq} n_k n_q + N^{-1} \sum_{k,q} W_{kq} n_k n_q \qquad \ldots (6.1\text{-}4)$$

where $E_o = -zNS^2J$ is the energy of the ground state

$$A_k = 2SJz[1-\gamma(k)]$$

$$V_{kq} = zJ[\gamma(k) + \gamma(q) - 1 - \gamma(k-q)]$$

$$W_{kq} = z(\alpha-1)J[\gamma(k) + \gamma(q)] \qquad \ldots (6.1\text{-}5)$$

and $\alpha = \alpha(s) = 4s\lambda = 4s(1-(1-\frac{1}{2S})^{\frac{1}{2}})$

$$\gamma(k) = \sum_a \exp(ik.a)/z, \qquad n_k = a_k^+ a_k$$

With the expansion $\gamma(k) = 1 - \frac{k^2a^2}{z} + \ldots$, to order k^2a^2, V_{kq} on averaging over an angle gives a zero, hence the effect of the wave wave interation is included in the third term of expression (6.1-4) as encapsuled by $\alpha(s)$.

Rewriting the Hamiltonian, we obtain,

$$H = \sum_k (Fk^2 - \mu)n_k$$

where $F = 2JSa^2 + (\alpha-1)Ja^2 \frac{<n_q>}{J} \simeq 2JSa^2$ ... (6.1-6)

and $\mu = -\frac{(\alpha-1)}{N} J<[2z - q^2a^2]\, n_q>$

μ is the effective electrochemical potential.

OGUCHI (1959) in his attempts to find the correction to the spontaneous magnetization produced by spin-wave interactions has calculated the grand partition function of the system defined by

$$Z = \text{Trace} \exp(-\beta H), \quad \beta = \frac{1}{k_BT} \qquad \ldots (6.1\text{-}7)$$

With,

$$\beta H = \beta\sum_{k} A_k n_k + \beta\sum W_{kq} n_k n_q = A+\varepsilon B$$

Instead of Oguchi's Z of eqn. (6.1-7), we have used,

$$Z = \mathrm{Tr}e^{-A}(1-\varepsilon B)$$

$$Z = \mathrm{Tr}e^{-A} - \varepsilon \mathrm{Tr}\ Be^{-A} \qquad \ldots (6.1\text{-}8)$$

$$= \mathrm{Tr}\ e^{-A} - \varepsilon\left[\frac{\mathrm{Tr}\ Be^{-A}}{\mathrm{Tr}\ e^{-A}}\right]\mathrm{Tr}\ e^{-A}$$

$$Z = \mathrm{Tr}\ e^{-A}[1-\varepsilon\langle B\rangle] \qquad \ldots (6.1\text{-}9)$$

Since A and B commute, $[A, B] = 0$; then,

$$\mathrm{In}\ Z = \mathrm{In}\ Z_o - \varepsilon\langle B\rangle$$

where $\langle B\rangle = \frac{\beta}{E}\langle \sum W_{kq} n_k n_q\rangle$

$$\simeq \frac{\beta}{E} n_k \langle \sum W_{kq} n_q\rangle \equiv \mu n_k$$

Essentially,

$$Z = \mathrm{Tr}e^{-A'}$$

$$A' = \beta\sum_{k}(A_k-\mu)n_k \qquad \ldots (6.1\text{-}10)$$

The analytic expression of μ is given by

$$-\mu = 2J(\alpha-1)rZ\tau^{3/2}\sum_{m=1}^{\infty}\exp^{(m\beta\mu)}/m^{3/2} \qquad \ldots (6.1\text{-}11)$$

μ has been computed for some ferromagnets, (see Table 4.2). As we see, μ is appreciable for ferromagnets with small

S values, and can be neglected for those with large values of S. The effect of μ on the coefficients of $T^{3/2}$, $T^{5/2}$, $T^{7/2}$ and T^4 of spontaneous magnetization and the coefficient of $T^{3/2}$ of specific heat of some ferromagnets have been calculated and shown in Table 4.2. We see that in the two cases of Iron and Nickel for which experimental values are available from the work of ARGYLE, CHARAP and PUGH (1963), the computed values of the coefficients of $T^{3/2}(C_1)$ and $T^{5/2}(C_2)$ respectively are in impressive agreement with the experimental ones, as shown in table 6.1

Table 6.1 - Values of C in units of $(10^{-6}/k^{3/2})$

Metal	C_1	C_2	C_1 (experimental)	C_2 (experimental)
Iron	3.645	0.894×10^{-3}	3.4 ± 0.2	$1\pm1 \times 10^{-3}$
Nickel	7.395	0.360×10^{-2}	7.5 ± 0.2	$(1.5\pm0.2)\times10^{-2}$

In finding the effect of the electrochemical potential on the coefficients of T^{υ} in the expression of the spontaneous magnetization for ferromagnets with the Hexagonal close packed structures, we required the correct expansion for the terms encapsuled in the dispersion relation.

For the Hexagonal close packed crystals, the Hamiltonian is

$$H = \sum_k (Fk^2 - \mu)n_k$$

where

$$F = 2SzJ[D''(\phi,\theta)a^2k^2 - A''(\phi,\theta)(ka)^4 + B''(\phi,\theta)(ka)^6 + \ldots]/k^2$$

where $D''(\phi,\theta)$, $A''(\phi,\theta)$ and $B''(\phi,\theta)$ have been outlined and evaluated in Appendix D.

Following RUSHBROOKE and WOOD (1958) and DOMB and SYKES (1957) and by the use of Pade' Approximants, we have calculated the Reduced Curie temperature θ_c for some ferromagnets as well as their critical point exponent. Rushbrooke and Wood's formula for θ_c (eqn. 4.2-1) is for cubic crystals while our technique is adaptable for all types of crystals.

From Table 4.1, we see that for cubic crystals, the Reduced temperature (θ_c) calculated by our technique differs slightly from the Reduced temperature calculated using Rushbrooke and Wood's formula. There is a remarkable difference for crystals with the hexagonal close packed lattice structures. This implies that Rushbrooke and Wood's formula cannot be used for crystals with Hexagonal close packed lattice structures.

The internal energy U with $(\mu = 0)$ is given by

$$U(\mu = 0) = \frac{2JS}{Q}\frac{3r}{2}(2JS)^{-5/2}(kT)^{5/2}\sum_m \frac{1}{m^{5/2}} \qquad \ldots (6.1\text{-}12)$$

we have shown that $\partial U/\partial\mu > o$ and hence

$U(\mu = 0)$ is greater than $U(\mu<0)$,

$$U(\mu<o) = \frac{2JS}{Q}\frac{3r}{2}(2JS)^{-5/2}(kT)^{5/2}\sum \frac{e^{+m\beta\mu}}{m^{5/2}} - \frac{\mu r}{Q}(2JS)^{-3/2}(kT)^{3/2}\sum \frac{e^{+m\beta\mu}}{m^{3/2}} \qquad \ldots (6.1.13)$$

Similarly, the entropy $\hat{S}$ with $\mu = o$ is not less than the entropy $\hat{S}$ with $\mu<o$, because $o<T = \partial U/\partial\hat{S} = \frac{\partial U}{\partial\mu}/\frac{\partial\hat{S}}{\partial\mu}$.

This implies that the existence of the wave-wave interaction and hence of non-zero μ, gives rise to a lowering of the thermodynamic internal energy and entropy In other words, the spin waves on the average form bound states called spin complexes.

Within the spin wave - spin wave - spin wave interactions, the energy of a magnon is altered slightly by the additional term $-B'$, while the electrochemical potential of a magnon is altered by the additional term $-A'$, (see equation (4.3-18 - 4.3-19). The effect of the new μ is found on the coefficient of $T^{3/2}$ in the expression of the spontaneous magnetization and compared with the effect of the μ of chapter III, See table (4.3). We see that the two μ's hardly differ in each case, which implies that wave-wave-wave interactions is negligible in comparison with wave-wave interactions.

In agreement with several authors, the spontaneous magnetization at low temperature contains terms $T^{3/2}$, $T^{5/2}$ and $T^{7/2}$ which correspond to the terms k^2, k^4 and k^6 of the dispersion law respectively. With the expansion of $\gamma(k)$ of expressions (3.1-39) and (6.1-4) to order k^4a^4, we obtain an additional term $-\eta$ in the dispersion relation, which gives the coefficient of T^4 in the expression for spontaneous magnetization. The presence of η causes a shift in the energy of the spin wave. This is due to the presence of other spin waves. This kind of interaction between spin waves according to DYSON (1956) is called the dynamical interaction. The electrochemical potential μ affects this dynamical term; the coefficient of T^4 has been calculated for some ferromagnetic elements and shown in Table 4.2.

From our results, this T^4 dependence, which is due to the dynamical interaction is experimentally negligible as compared with the other coefficients of T^{ν}. The effect of the kinematical interaction of the spin waves is obtained by recomputing the various coefficients of T^{ν} in the expression of the spontaneous magnetization for some ferromagnets, and treating the magnons as quasi-particles obeying intermediate statistics.

Table 5.2 shows that the kinematical interaction can be neglected for ferromagnets with large exchange integral J values.

6.2 Antiferromagnetism

Our expansion formalism can be extended to spin complexes in antiferromagnetism. ANDERSON (1952) presented an approximate quantum theory of antiferromagnets on the basis of the semi-classical spin wave theory, first introduced by Kramers and Heller. The spin wave theory of antiferromagnets is far more complicated than that of ferromagnets. Following Anderson, Kubo (1952), in his spin wave theory of anti-ferromagnetics used the formulation devised by Holstein and Primakoff and using quantum statistics derived some thermodynamic quantities of antiferromagnets.

We report that in a consistent expansion of $(1 - \frac{a^+a}{2S})^{\frac{1}{2}}$ up to wave-wave interaction only for antiferromagnets, and using quantum statistics, there exists some modifications in the thermodynamic quantities that were derived quantum statistically by Kubo.

In the antiferromagnetic case, where the lattice is assumed to be divided into two interpenetrating sublattices we introduce two different definitions of the spin deviation operators, that is,

$$\begin{aligned} S_{xj} + iS_{yj} &= (2S)^{\frac{1}{2}}[1 - \frac{n_j}{2S}]^{\frac{1}{2}} a_j \\ S_{xj} - iS_{yj} &= (2S)^{\frac{1}{2}} a_j^*[1 - \frac{n_j}{2S}]^{\frac{1}{2}} \qquad \ldots (6.1\text{-}14) \\ S_{zj} &= S - n_j \end{aligned}$$

For a spin j on one of the sublattices, say the (+) lattice, and

$$\begin{aligned} S_{xk} + iS_{yk} &= (2S)^{\frac{1}{2}} b_k[1 - \frac{n_k}{2S}]^{\frac{1}{2}} \\ S_{xk} - iS_{yk} &= (2S)^{\frac{1}{2}}[1 - \frac{n_k}{2S}]^{\frac{1}{2}} b_k \qquad \ldots (6.1\text{-}15) \\ S_{zk} &= -S + n_k \end{aligned}$$

For a spin k on the other lattice, say the (-) lattice. the operators b and b^* are naturally defined in the same way as a and a^* and satisfy the equation

$$b_k^* b_k = n_k, \quad b_k b_k^* - b_k^* b_k = 1 \qquad \ldots (6.1\text{-}16)$$

The simplest form of the Hamiltonian of an antiferromagnet is usually assumed to be

$$H_{ex} = |J| \sum_{j,k} S_j \cdot S_k \qquad \ldots (6.1\text{-}17)$$

Inserting equations (6.1-14) and (6.1-15) into equation (6,1-17) we obtain

$$H_{ex} = -\frac{1}{2}Nz|J|S^2 + z|J|S(\sum_j n_j + \sum_k n_k)$$

$$+ |J|S \sum_{j,k} \{f_s(n_j) a_j f_s(n_k) b_k + a_j^* f_s(n_j) b_k^* f_s(n_k) \qquad \ldots (6.1.\text{-}18)$$

where

$$f_s(n_k) = (1 - \frac{n_k}{2S})^{\frac{1}{2}},$$

We have

$$H_{ex} = H^o + H^1 \qquad \ldots (6.1\text{-}19)$$

where $H^o = -\frac{1}{2}Nz|J|S^2 + z|J|S(\sum_j n_j + \sum_k n_k)$

$$+ |J|S \sum_{j,k} (a_j^+ b_k^+ + a_j b_k),$$

and

$$H^1 = \lambda |J| S \sum_{j,k} (n_j a_j b_k + a_j n_k b_k + a_j^* n_j b_k + a_j b_k^* n_k)$$

$$- |J| \sum_{j,k} (a_j^* a_j b_k^* b_k)$$

where $\lambda = (1 - \frac{1}{2S})^{\frac{1}{2}} - 1 \qquad \ldots (6.1\text{-}20)$

Note that λ contains all the coefficients of the two product terms as shown in the ferromagnetic case. The classical treatment of spins in the limit of $S \to \infty$ is called the zeroth approximation. The first approximation is the approach by the Spin wave theory on the basis of the simplified Hamiltonian H^o. By taking account of some of the higher terms omitted in the first approximation and applying the first order perturbation theory, we obtain the second approximation, and fortunately for us here, the results are convergent.

By the canonical transformation defined by

$$a_j = \frac{1}{2}(Q_j + iP_j), \quad a_j^* = \frac{1}{2}(Q_j - iP_j)$$

$$b_k = \frac{1}{2}(R_k + iS_k), \quad b_k^* = \frac{1}{2}(R_k - iS_k)$$

and using the following Fourier transforms, we have

$$P_\lambda = \left(\frac{2}{N}\right)^{\frac{1}{2}} \sum_j e^{i\lambda j} P_j, \qquad Q_\lambda = \left(\frac{2}{N}\right)^{\frac{1}{2}} \sum_j e^{-i\lambda j} Q_j$$

$$S_\lambda = \left(\frac{2}{N}\right)^{\frac{1}{2}} \sum_j e^{-i\lambda k} S_k, \qquad R_\lambda = \left(\frac{2}{N}\right)^{\frac{1}{2}} \sum_j e^{i\lambda k} R_k,$$

We introduce also the fourier components of the creation and annihilation operators by

$$a_\lambda = \left(\frac{2}{N}\right)^{\frac{1}{2}} \Sigma a_j e^{i\lambda j} = \frac{1}{2}(X_{1\lambda} + X_{2\lambda}),$$

$$a_\lambda^* = \left(\frac{2}{N}\right)^{\frac{1}{2}} \Sigma a_j^* e^{-i\lambda j} = \frac{1}{2}(X_{1\lambda}^* + X_{2\lambda}^*)$$

$$b_\lambda = \left(\frac{2}{N}\right)^{\frac{1}{2}} \Sigma b_k e^{-i\lambda k} = \frac{1}{2}(X_{1\lambda} - X_{2\lambda}) \qquad \ldots (6.1\text{-}22)$$

$$b_\lambda^* = \left(\frac{2}{N}\right)^{\frac{1}{2}} \sigma b_k^* e^{i\lambda k} = \frac{1}{2}(X_{1\lambda}^* - X_{2\lambda})$$

where $X_{1\lambda} = q_{1\lambda} + iP_{1\lambda}$, $X_{1\lambda}^* = q_{1\lambda} - iP_{1\lambda}$,

$$P_\lambda = (P_{1\lambda} + P_{2\lambda})/\sqrt{2}$$

$$Q_\lambda = (q_{1\lambda} + q_{2\lambda})/\sqrt{2}$$

$$S_\lambda = (P_{1\lambda} - P_{2\lambda})/\sqrt{2} \qquad \ldots (6.1\text{-}23)$$

$$R_\lambda = (q_{1\lambda} - q_{2\lambda})/\sqrt{2}$$

H^1 is written as,

$$H^1 = \lambda|J|SN \sum\sum\sum_{\lambda+k=\mu+\nu}\sum_{\rho} [a_\lambda^* a_\mu a_\nu b_k + a_\lambda b_\lambda^* b_\mu b_\nu + a_\mu^* a_\nu^* a_\lambda b_k$$

$$+ a_k^* b_\mu^* b_\nu^* b_\lambda] e^{ik\rho} - \frac{1}{N}|J| \sum\sum\sum_{\lambda+\nu=\mu+k}\sum_{\rho} a_\lambda^* a_\mu b_\nu b_k^* e^{i(k-\nu)\rho} \qquad (6.1\text{-}24)$$

Using the following averages,

$$\langle a_\lambda^* a_\lambda \rangle = \langle b_\lambda^* b_\lambda \rangle = \frac{1}{4}\langle q_{1\lambda}^2 + P_{1\lambda}^2 + q_{2\lambda}^2 + P_{2\lambda}^2 - 2\rangle$$

$$\langle a_\lambda^* b_\lambda \rangle = \langle a_\lambda^* b_\lambda^* \rangle = 0, \qquad \ldots (6.1\text{-}25)$$

$$\langle a_\lambda^2 \rangle = \langle b_\lambda^2 \rangle = \langle a_\lambda^{*2} \rangle = \langle b_\lambda^{*2} \rangle = 0$$

$$\langle a_\lambda b_\lambda \rangle = \langle a_\lambda^* b_\lambda^* \rangle = \frac{1}{4}\langle q_{1\lambda}^2 - P_{1\lambda}^2 - q_{2\lambda}^2 + P_{2\lambda}^2 \rangle$$

To the first order of H^1, the Partition Function can be written as

$$e^{-\frac{F}{kT}} = \mathrm{Trace}[\exp(-H^o/kT)(1-H^1/kT)]$$

$$=[\mathrm{Trace}(\exp(-H^o/kT))](1-\langle H^1\rangle/kT) \quad \ldots (6.1\text{-}26)$$

and the free energy as

$$\frac{-F}{kT} = \log[\mathrm{Trace}(\exp(-H^o/kT))] - \langle H^1\rangle/kT \quad \ldots (6.1\text{-}27)$$

The derivation of (6.1-27) from (6.1-26) is known to be unsatisfactory, from the mathematical point of view, but (6.1-27) is rigorous in the first order approximation of H^1. Noticing that all products of operators such as $a_\lambda a_\mu$, $a_\lambda b_\mu$, $b_\lambda b_\mu$, $a^*_\lambda a_\mu$ and so on have averages equal to zero, if the wave number λ and μ are different, we find that

$$\langle H^1\rangle = -\frac{1}{2}Nz|J|(A+C)^2 + N|J|(1+4\lambda S)AC \quad \ldots (6.1\text{-}28)$$

where

$$A = \frac{2}{N}\sum_\lambda \langle a^*_\lambda a_\lambda\rangle$$

$$= \frac{2}{N}\sum_\lambda \langle b^*_\lambda b_\lambda\rangle$$

and

$$C = \left(\frac{2}{N}\right)\sum_\lambda \langle a_\lambda b_\lambda\rangle$$

$$= \frac{2}{N}\sum_\lambda \langle a^*_\lambda b^*_\lambda\rangle$$

If we insert, the expressions of E_o and E_T given in table E_1 in appendix E, we obtain the energy in the second approximation

$$E = -\frac{1}{2}Nz|J|S(S+C_o-\lambda(C_o^2S^{-1})$$
$$+ Nz|J|S(1+2\lambda DC_oS^{-1})C_1\theta^{D+1}$$

where C_o, and C_1 are easily found in Appendix E, and D is the Dimentionality of the lattice.

The following tables shows the ground state energies of antiferromagnets calculated respectively by Kubo and by us using our method for $s = \frac{1}{2}$

TABLE 6.2 - Ground state energies of antiferromagnets (by Kubo)

Lattice	z	$-E_o/(Nz\|J\|S/2)$
Linear chain	2	$S+0.363 + 0.033S^{-1} = S+0.363 + 0.066$
Quadratic layers	4	$S+0.158 + 0.0062S^{-1} = S+0.158 + 0.012$
NaCl-type	6	$S+0.097 + 0.0024S^{-1} = S+0.097 + 0.005$
CsCl-type	8	$S+0.073 + 0.0013S^{-1} = S+0.073 + 0.003$

TABLE 6.3 - Ground state energies of antiferromagnets (by our technique)

Lattice	z	$-E_o/(Nz\|J\|S/2)$
Linear chain	2	S + 0.363 + 0.130
Quadratic layer	4	S + 0.158 + 0.024
NaCl-type	6	S + 0.097 + 0.009
CsCl-type	8	S + 0.073 + 0.005

Indeed our expansion formalism can be extended to antiferromagnetism. This is quite encouraging in view of the recent researches (Mackintosh 1988, Sogo, 1987) which indicate that Spin waves in antiferromagnetism are relevant to high temperature superconductivity. In other words, unlike low-temperature superconductors which are diamagnetic, the age-old spin-wave theory may be the starting point for the exciting new phenomenon of superconductivity in antiferromagnetics. We envisage that, since an antiferromagnet is essentially an interlace of two ferromagnets, our investigations reported here will be highly germane to the current effort to understand high temperature superconductivity and ferromagnetism itself.

6.3 Conclusion

The Developed Formalism of Holstein-Primakoff-Oguchi actually deals with a system consisting of some abstract quasi-particles whose statistical behaviour is to be determined. A point of view suggests that such a gas consists of quasi-particles whose field amplitudes obey a set of commutation relations. Therefore it looks as if the system is a system of Bosons. However such a boson system is not real owing to the fact that the occupation number operator $a_j^+ a_j$ is restricted to the eigenvalues $n_j = 0,1,...,2S$ whereas the real boson system would require also the eigenvalues for $n_j > 2S$. As we know, these latter values are unphysical. However, there are two limiting situations, where the boson picture represents a fair approximation to the real system. The first is the case where S is large enough to justify the use of commutation relations for bosons. The other case is that of the Dynamical behaviour of the system in the ground state or state very close to it.

In both cases, NOVAKOVIC (1975) and OGUCHI (1959) considered the operator $a_j^+ a_j / 2S$ when applied to the eigenvectors as a small quantity compared to unity.

Therefore expansions were made in powers of $a_j^+ a_j/2S$ to some order to investigate the thermodynamic properties of an exchange interaction acting between the ferromagnetic spins at low temperatures.

In our work, we have expanded $a_j^+ a_j/2S$ to all orders in S and we have shown that in a consistent expansion of

$$f_j(S) = (1 - \frac{a_j^+ a_j}{2S})^{\frac{1}{2}}$$

up to wave-wave interaction for Heisenberg Ferromagnet of N spins in a physical volume V_o each of spins S, with z nearest neighbours, bond $J>0$, the quantized spin waves called magnons at temperature T are Bosons with effective chemical potential μ.

The existence of wave-wave interaction and hence of non-zero μ gives rise to a lowering of the thermodynamic internal energy and entropy. The spin waves, on the average thus form spin complexes. The wave-wave-wave interactions is negligible in comparison with the wave-wave interactions.

The dynamical term which is depicted by the coefficient of T^4 is both numerically and experimentally negligible, as compared with the other coefficients of T^{ν}.

The kinematical term accounted for with intermediate statistics is negligible for ferromagnets with large exchange integral J values.

The phenomenon of magnetism still remains incompletely understood, even though it is one of the oldest observed in the annals of physics. In the quest to elucidate it, spin-wave theory remains an amenable theory at low temperatures. Within the theory, for both Ferro- and antiferro-magnetism, our expansion formalism simplifies the logic of spin wave- spin wave interaction by enabling one to treat the waves as ideal magnons with effective chemical potential and obeying Bose-Einstein or intermediate statistics.

6.4 Suggestions for Further Work

Our work is basically on the Ferromagnets. The following are some suggestions for further research work.

(i) A consistent expansion of $(1-a^{+}a/2S)^{\frac{1}{2}}$ up to wave-wave interactions can be done for the antiferromagnets as we have attempted and outlined in the discussion (section 6.1), the perpendicular susceptibility can be examined and its dependence on T obtained.

(ii) The fundamental question "Are the magnetic electrons localized or itinerant needs to be fully answered.

(iii) The intimate link between magnetism and superconductivity in the high temperature superconductors can be found since the progenitor of the high temperature superconductors, $LaCuO_4$ exhibits antiferromagnetism, even though band calculations indicate that the exchange interaction is far two small to induce magnetic ordering in a pure, perfect crystal.

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APPENDIX A

COMMUTATION RULES

To show that the spin operators satisfy the commutation rule

$$a_j a_\ell^+ - a_j^+ a_\ell = \delta_{j\ell}$$

The spin operators are written in the following forms

$$S_+ = (2S)^{\frac{1}{2}} fa, \quad S_- = (2S)^{\frac{1}{2}} a^+ f$$

where

$$f = \left(1 - \frac{a^+a}{2S}\right)^{\frac{1}{2}}, \quad f^2 = 1 - \frac{a^+a}{2S}$$

writing $\varepsilon = [fa, a^+f] = f[a, a^+f] + [f, a^+f]a$

$$= f[a, a^+]f + fa^+[a, f] + [f, a^+]fa + a^+[f, f]a$$

$$= f\alpha f + fa^+\gamma + \gamma^+ fa \qquad \ldots (1)$$

$$[a, f]^+ = (af - fa)^+ = fa^+ - a^+f = [f, a^+]$$

where

$$\alpha = [a, a^+], \quad \gamma = [a, f] \quad \text{or} \quad af - fa = \gamma$$

$$[f^2, a^+] = f[f, a^+] + [f, a^+]f = -\left[\frac{a^+a}{2S}, a^+\right] = \frac{-a^+\alpha}{2S}$$

$$[f^2, a] = f[f, a] + [f, a]f = -\left[\frac{a^+a}{2S}, a\right] = \frac{+\alpha a}{2S}$$

i.e. $f\gamma^+ + \gamma^+ f = \dfrac{-\alpha a^+}{2S}$ $\ldots (4)$

$$f\gamma+\gamma f = \frac{-\alpha a}{2S} \qquad \ldots (4')$$

$$[\gamma,f] = [[a,f],f] = [af-fa,f] = aff-faf$$

$$= -faf+ffa = aff+ffa-2faf = aff+ffa - 2f(fa+\gamma)$$

$$= aff-ffa-2f\gamma = [a,ff] -2f\gamma = \frac{-\alpha a}{2S} -2f\gamma$$

$$\gamma f-f\gamma = \frac{-\alpha a}{2S} - 2f\gamma \text{ or } \gamma f = -\frac{\alpha a}{2S} - f\gamma \qquad \ldots(5)$$

$$f\gamma^+ = \frac{-\alpha a^+}{2S} -\gamma^+ f \Rightarrow \gamma^+ f = \frac{-\alpha a^+}{2S} -f\gamma^+ \qquad \ldots(5')$$

$$\varepsilon = \alpha ff+fa^+\gamma+\gamma^+ fa = \alpha ff+fa^+\gamma-f\gamma^+ a - \frac{\alpha}{2S}a^+a$$

$$= \alpha ff - \frac{\alpha}{2S}a^+a + f(a^+\gamma-\gamma^+a) \qquad \ldots (6)$$

$$a^+\gamma = a^+[a,f] = a^+af-a^+fa \qquad \ldots (7)$$

$$\gamma^+a = fa^+a-a^+fa \qquad \ldots (8)$$

$$a^+\gamma-\gamma^+a = a^+af-fa^+a = 0 \qquad \ldots (9)$$

$$2S\varepsilon = 2S(\alpha ff-\frac{\alpha a^+a}{2S}) = 2S\alpha(1 - \frac{a^+a}{2S})-\alpha a^+a = 2\alpha(S-a^+a)$$

$$= 2(S-a^+a)$$

$$\Leftrightarrow \alpha = 1.$$

APPENDIX B

PADE APPROXIMANTS

The Pade approximants are a particular type of rational fraction approximation to the value of function. The idea is to match the Taylor series expansion as far as possible. For example, we would like to pick an approximation of the form

$$(a+bx)/(c+dx) \qquad \ldots \text{(B1)}$$

so that it would tend to a finite limit as x tends to infinity. We denote the L,M Pade approximant to A(x) by

$$[L/M] = P_L(x)/Q_M(x) \qquad \ldots \text{(B2)}$$

where $P_L(x)$ is a polynomial of degree at most L and $Q_M(x)$ is a polynomial of degree at most M. The formal power series

$$A(x) = \sum_{j=o}^{\infty} a_j x^j \qquad \ldots \text{(B3)}$$

determines the coefficients of $P_L(x)$ and $Q_M(x)$ by the equation

$$A(x)-P_L(x)/Q_M(x) = O(x^{L+M+1}) \qquad \ldots \text{(B4)}$$

Since we can obviously multiply the numerator and denominator by any constant and leave [L/M] unchanged, we impose the normalization condition

$$Q_M(o) = 1.0 \qquad \ldots \text{(B5)}$$

Finally we require that P_L and Q_M have no common factors. If we write the coefficients of $P_L(x)$ and $Q_M(x)$ as

$$\begin{aligned} P_L(x) &= p_o+p_1x+ \ldots + p_1x^L, \\ Q_M(x) &= 1+q_1x + \ldots + q_Mx^M \end{aligned} \qquad \ldots \text{(B6)}$$

then by eqn. (B5) we may multiply eqn.(B4) by $Q_M(x)$, which linearizes the coefficient equations. We can write out eqn.(B4) in more detail as

$$\begin{aligned} a_o &= p_o \\ a_1+a_oq_1 &= p_1 \\ a_2+a_1q_1+a_oq_2 &= p_2 \\ &\vdots \\ a_L+a_{L-1}q_1+\ldots+a_oq_L &= p_L \\ a_{L+1}+a_Lq_1+\ldots+a_{L-M+1}q_M &= 0 \\ a_{L+M}+a_{L+M-1}q_1+\ldots+a_Lq_M &= 0 \end{aligned} \qquad \ldots \text{(B7)}$$

where we define

$$a_n \equiv 0 \text{ if } n<0 \text{ and } q_j \equiv 0 \text{ if } j>m \qquad \ldots \text{(B8)}$$

APPENDIX C

CUBIC LATTICES

Basic features of the simple, body centred, and face centred cubic lattices are given in table below.

Lattice	Simple	Body Centred	Face Centred
Unit cell volume	a^3	a^3	a^3
Nearest-neighbour distance	a	$a\sqrt{3}/2$	$a/\sqrt{2}$
The number of nearest neighbours z	6	8	12
The number of sites per unit cells	1	2	4

Using these data the following sum is readily calculated.

$$J(k) = \frac{1}{Z} \sum_{l=1}^{Z} J_{j\ell} \exp[ik.(R_j - R_\ell)] \qquad \ldots\ C(1)$$

$$= \frac{1}{Z} \sum_{l=1}^{Z} J_{j\ell} \mathrm{Cos}\ k.(R_j - R_\ell)] \qquad \ldots\ C(2)$$

with $R_j = (0,0,0)$, $R_\ell = \{X_\ell, Y_\ell, Z_\ell\}$ ... C(3)

The Reciprocal lattice vector is defined by

$k = \{k_x, k_y, k_z\}$

$k_x = k\mathrm{Cos}\phi\mathrm{Sin}\theta$

$k_y = k\mathrm{Sin}\phi\mathrm{Sin}\theta$

$k_z = k\mathrm{Cos}\theta$

Nearest-neighbour distances are given below

Table (C1) - Nearest-neighbour distances on a simple cubic lattice in units a

ℓ	1	2	3	4	5	6
X	1	-1	0	0	0	0
Y	0	0	1	-1	0	0
Z	0	0	0	0	1	-1

Table (C2) - Nearest-neighbour Distances on a body centred cubic lattice in units a/2

ℓ	1	2	3	4	5	6	7	8
X	1	1	-1	-1	1	1	-1	-1
Y	-1	1	1	-1	-1	1	1	-1
Z	1	1	1	1	-1	-1	-1	-1

Table B3 - Nearest-neighbour Distances on a face centred cubic lattice in units a/2

ℓ	1	2	3	4	5	6	7	8	9	10	11	12
X	1	1	-1	-1	0	0	0	0	1	1	-1	-1
Y	1	-1	1	-1	1	1	-1	-1	0	0	0	0
Z	0	0	0	0	1	-1	1	-1	1	-1	1	-1

The Fourier transform is expressed as follows, for a simple cubic lattice

$$J(k) = \frac{J}{3}[\,\mathrm{Cos}(k_x a) + \mathrm{Cos}(k_y a) + \mathrm{Cos}(k_z a)] \quad \ldots (C4)$$

For a Body centred cubic lattice,

$$J(k) = J\mathrm{Cos}\,\frac{k_x a}{2}\,\mathrm{Cos}\,\frac{k_y a}{2}\,\mathrm{Cos}\,\frac{k_z a}{2}, \quad \ldots (C8)$$

For a face centred cubic lattice,

$$J(k) = \frac{J}{3}[\,\mathrm{Cos}\,\frac{k_x a}{\sqrt{2}} + \mathrm{Cos}\,\frac{k_y a}{\sqrt{2}} + \mathrm{Cos}\,\frac{k_z a}{\sqrt{2}}] \quad \ldots (C6)$$

Introducing the abbreviations,

$\mathrm{Cos}\phi = \alpha$

$\mathrm{Sin}\phi = \beta$

$\mathrm{Cos}\theta = \gamma$

$\mathrm{Sin}\theta = \delta$,

The Fourier transform can be written

$$J(k) = J\{1 - \frac{(ka)^2}{2} + A(\phi,\theta)(ka)^4 - B(\phi,\theta)(ka)^6 + \ldots\} \quad \ldots (C7)$$

where the expansion coefficients are given by, for a simple cubic lattice,

$$A = \frac{1}{72}\{(\alpha\delta)^4 + (\beta\delta)^4 + \gamma^4$$

$$B = \frac{1}{2160}\{(\alpha\delta)^4 + (\beta\delta)^6 + \gamma^6\} \qquad \ldots \text{(C8)}$$

For a body centred cubic lattice,

$$A = \frac{1}{384}\{(\alpha\delta)^4+(\beta\delta)^4+\gamma^4\} + \frac{1}{64}\{(\gamma\delta)^2 + (\alpha\beta)^2\delta^4\}$$

$$B = \frac{1}{2^6,6^1}\{(\alpha\delta)^6 + (\beta\delta)^6+\gamma^6\}$$

$$+ \frac{1}{2^7,4^1}\{\alpha^2\beta^4\delta^6 + (\alpha\delta)^2\gamma^4 + (\beta\delta)^2\gamma^4$$

$$+ \alpha^4\beta^2\delta^6 + \alpha^4\gamma^2\delta^4 + \beta^4\gamma^2\delta^4\}$$

$$+ \frac{1}{2^8,2!}(\alpha\beta\gamma)^2\delta^4; \qquad \ldots \text{(C9)}$$

For a face centred cubic lattice,

$$A = \frac{1}{288}\{(\alpha\delta)^4 + (\beta\delta)^4 + \gamma^4\}$$

$$B = \frac{1}{17280}\{(\alpha\delta)^6+(\beta\delta)^6+\gamma^6\} \qquad \ldots \text{(C10)}$$

APPENDIX D

ON SOME INTEGRATIONS

In the present analysis we use integrals of the form,

$$I_n(\tau) = \int_0^\infty \frac{q^{2n+2}\,dq}{\exp[(1-\eta)\frac{(aq)^2}{\tau}]-1} \qquad \ldots \text{(D1)}$$

where $n = 0,1,2,\ldots,n$ is some parameter such that $\eta \geqslant 0$, τ is a dimensionless temperature defined by

$$\tau = \frac{kT}{2SJ} \qquad \ldots \text{(D2)}$$

By the substitution $(1-\eta)\frac{(aq)^2}{\tau} = x$

we obtain,

$$I_n(\tau) = \frac{1}{2}[a^2(1-\eta)]^{-(n+3/2)}\tau^{n+3/2}\,k_n, \qquad \ldots \text{(D3)}$$

$$k_n = \int_0^\infty \frac{X^{n+\frac{1}{2}}\,dx}{\exp X-1} \qquad \ldots \text{(D4)}$$

$$k_n = \Gamma(n+3/2)\varepsilon(n+3/2) \qquad \ldots \text{(D5)}$$

The Gamma Function

V	$\frac{1}{2}$	1	$\frac{3}{2}$	2	$\frac{5}{2}$	3	$\frac{7}{2}$
$\Gamma(V)$	$\sqrt{\pi}$	1	$\sqrt{\pi}/2$	1	$3\sqrt{\pi}/4$	2	$15\sqrt{\pi}/8$

The Riemann Zeta Function

v	$\frac{3}{2}$	2	$\frac{5}{2}$	3	$\frac{7}{2}$	4	$\frac{9}{2}$
$\varepsilon(v)$	2.612	1.645	1.341	1.202	1.127	1.082	1.055

also use integrals of the form

$$J_n(\tau) = \int_0^\infty dq \int_0^{2\pi} d\phi \int^{\pi} \sin\theta \, d\theta \, \frac{q^{2n+2}}{\exp x-1} \qquad \ldots (D6)$$

where

$$x = \frac{1}{\tau}[(1-\eta)(qa)^2 - zA(\phi,\theta)(qa)^4 + zB(\phi,\theta)(qa)^6 + \ldots] \qquad \ldots (D7)$$

We introduce the substitution

$$\begin{aligned} X &= C(1-Dq^2+Eq^4)q^2, \\ C &= \frac{1}{\tau}(1-\eta)a^2, \\ D &= \frac{zA(\phi,\theta)a^2}{1-\eta} \qquad \ldots (D8) \\ E &= \frac{zB(\phi,\theta)a^4}{1-\eta} \end{aligned}$$

$$Cq^2 = \frac{x}{1-(Dq^2-Eq^4)} \simeq x[1+Dq^2-Eq^4+(Dq^2-Eq^4)^2] \qquad \ldots (D9)$$

$$Cq^2 = x(1 + \frac{D}{C}x + \frac{2D^2-E}{C^2}x^2 + \ldots)$$

$$= x\{1+zA(\phi,\theta)(1-\eta)^{-2}\tau x + [2z^2A^2(\phi,\theta)(1-\eta)^{-4} - zB(\phi,\theta)(1-\eta)^{-3}](\tau x)^2 + \ldots\} \qquad \ldots (D10)$$

There follows the result of integration for the integral J_o,

$$J_o(\tau) = \frac{1}{2}C^{-3/2}\int_0^{2\pi} d\phi \int_0^{\pi} \mathrm{Sin}\theta d\theta \int_0^{\infty} \frac{x^{\frac{1}{2}}f(x)dx}{\exp\ x-1} \quad \ldots \text{(D11)}$$

where

$$f(x) = 1 + \frac{3}{2}zA(\phi,\theta)(1-\eta)^{-2}\tau x + [8z^2A^2(\phi,\theta)(1-\eta)^{-4} - \frac{7}{2}zB(\phi,\theta)(1-\eta)^{-3}](\tau x)^2 + \ldots$$

$$L_1 = \int_0^{2\pi} d\phi \int_0^{\pi} A(\phi,\theta)\mathrm{Sin}\theta d\theta$$

$$L_2 = \int_0^{2\pi} d\phi \int_0^{\pi} A^2(\phi,\theta)\mathrm{Sin}\theta d\theta$$

$$L_3 = \int_0^{2\pi} d\phi \int_0^{\pi} B(\phi,\theta)\mathrm{Sin}\theta d\theta$$

Therefore by virtue of equation (C4) and (C5) the integral J_o becomes

$$J_o(\tau) = C^{-3/2}\{2\pi\Gamma(\tfrac{3}{2})\varepsilon(\tfrac{3}{2}) + \frac{5z}{4}L_1\Gamma(\tfrac{3}{2})\varepsilon(\tfrac{3}{2})(1-\eta)^{-2}\tau$$

$$+ [4z^2L_2(1-\eta)^{-4} - \frac{7z}{4}L_3(1-\eta)^{-3}]\Gamma(\tfrac{7}{2})\varepsilon(\tfrac{7}{2})\tau^2\}$$

For hexagonal close packed lattice, we have

$$\gamma(k) = \frac{1}{Z}\sum_{\ell=1}^{12} \mathrm{Cos}k.R = \frac{1}{Z}\sum_{\ell=1}^{12}\mathrm{Cos}(k_x x_\ell + k_y y_\ell + k_z z_\ell)$$

$$\text{Cos}(k_x x_\ell + k_y y_\ell + k_z z_\ell) = 1 - \frac{(k_x x_\ell + k_y y_\ell + k_z z_\ell)^2}{2!}$$

$$+ \frac{(k_x x_\ell + k_y y_\ell + k_z z_\ell)^4}{4!} - \frac{(k_x x_\ell + k_y y_\ell + k_z z_\ell)^6}{6!}$$

$$\frac{1}{12} \sum_{\ell=1}^{12} \frac{(k_x x_\ell + k_y y_\ell + k_z z_\ell)^2}{2} = \frac{1}{24} D''(\phi,\theta)(ka)^{12}$$

where

$$D''(\phi,\theta) = k_x^2 \sum_{\ell=1}^{12} x_\ell^2 + k_y^2 \sum_{\ell=1}^{12} y_\ell^2 + k_z^2 \sum_{\ell=1}^{12} z_\ell^2$$

From our table

$$2k_y k_x \sum_{\ell=1}^{12} x_\ell z_\ell = 2k_x k_z \sum_{\ell=1}^{12} x_\ell z_\ell = 2k_y k_z \sum_{\ell=1}^{12} y_\ell z_\ell = 0$$

$$\sum_{\ell=1}^{12} \frac{(k_x x_\ell + k_y y_\ell + k_z z_\ell)^4}{4!} = \frac{1}{24} A''(\phi,\theta)(ka)^4$$

$$A''(\phi,\theta) = \sum_{\ell=1}^{12} k_x^4 x_\ell^4 + k_y^4 y_\ell^4 + k_z^4 z_\ell^4 + 6k_x^2 k_y^2 x_\ell^2 y_\ell^2$$

$$+ 6k_y^2 k_z^2 y_\ell^2 z_\ell^2 + 6k_x^2 k_z^2 x_\ell^2 z_\ell^2 + 4k_x^3 k_y x_\ell^3 y_\ell$$

$$+ 4k_x^3 k_z x_\ell^3 z_\ell + 4k_y^3 k_x x_\ell y_\ell^3 + 4k_y^3 k_z y_\ell^3 z_\ell$$

$$+ 4k_z^3 k_x x_\ell z_\ell^3 + 4k_z^3 k_y y_\ell z_\ell^3 \;)$$

$$\sum_{\ell=1}^{12} \frac{(k_x x_\ell + k_y y_\ell + k_z z_\ell)^6}{6!} = \frac{1}{720} B''(\phi,\theta)(ka)^6$$

$$B''(\phi,\theta) = \sum_{\ell=1}^{12}(k_x^6 x_\ell^6 + k_y^6 y_\ell^6 + k_z^6 z_\ell + 7k_z^4 k_y^2 z_\ell^4 y_\ell^2 + 7k_x^4 k_y^2 x_\ell^4 y_\ell^2$$

$$+7k_y^4 k_x^2 y_\ell^4 x_\ell^2 + 7k_x^2 k_z^4 x_\ell^2 z_\ell^4 + 7k_x^4 k_z^2 x_\ell^4 z_\ell^2 + 7k_y^4 k_z^2 y_\ell^4 z_\ell^2$$

$$+4k_x^5 k_y x_\ell^5 y_\ell + 4k_x^5 k_z x_\ell^5 z_\ell + 4k_y^5 k_x x_\ell y_\ell^5 + 4k_y^5 k_z y_\ell^3 z_\ell$$

$$+4k_z^5 k_x x_\ell z_\ell^5 + 4k_z^5 k_y z_\ell^5 y_\ell + 8k_y^3 k_x^3 x_\ell^3 y_\ell^3 + 8k_z^3 k_y^3 z_\ell^3 y_\ell^3$$

$$+8k_z^3 k_x^3 x_\ell^3 z_\ell^3 + 16k_y^3 k_x^2 k_z y_\ell^3 z_\ell x_\ell^2 + 16k_z^3 k_y k_x^2 y_\ell z_\ell^3 x_\ell^2$$

$$+16k_x^3 k_y k_z^2 x_\ell^3 y_\ell z_\ell^2 + 16k_y^2 k_x^3 k_z y_\ell^2 x_\ell^3 z_\ell + 16k_z^3 k_x k_y^2 z_\ell^3 x_\ell y_\ell^2$$

$$+16k_y^3 k_x k_z^2 y_\ell^3 z_\ell^2 x_\ell + 18k_y^2 k_z^2 k_x^2 x_\ell^2 y_\ell^2 z_\ell^2 + 12k_x^4 k_y k_z x_\ell^4 y_\ell z_\ell$$

$$+12k_y^4 k_x k_z y_\ell^4 x_\ell z_\ell + 12k_x k_y k_z^4 x_\ell y_\ell z_\ell^4 + 2k_x^5 k_y x_\ell^5 y_\ell$$

$$+2k_y^5 k_x x_\ell y_\ell^5 + 2k_x^5 k_z x_\ell^5 z_\ell + 2k_z^5 k_x x_\ell z_\ell^5 + 2k_y^5 k_z y_\ell^5 z_\ell$$

$$+2k_z^5 k_y z_\ell^5 y_\ell + 8k_x^4 k_y^2 x_\ell^4 y_\ell^2 + 8k_y^4 k_x^2 x_\ell^2 y_\ell^4 + 8k_x^4 k_z^2 x_\ell^4 z_\ell^2$$

$$+8k_z^4 k_x^2 x_\ell^2 z_\ell^4 + 8k_y^4 k_z^2 y_\ell^4 z_\ell^2 + 8k_z^4 k_y^2 y_\ell^2 z_\ell^4 + 18k_z^4 k_x k_y x_\ell y_\ell z_\ell^4$$

$$+18k_y^4k_xk_zx_\ell z_\ell y_\ell^4 + 18k_x^4k_yk_zx_\ell^4y_\ell z_\ell + 12k_x^3k_y^3x_\ell^3y_\ell^3$$

$$+12k_y^3k_z^3y_\ell^3z_\ell^3 + 12k_x^3k_z^3x_\ell^3z_\ell^3 + 72k_x^2k_y^2k_z^2x_\ell^2y_\ell^2z_\ell^2$$

$$+44k_z^3k_x^2k_yx_\ell^2z_\ell^3y_\ell + 44k_z^3k_y^2k_xy_\ell^2z_\ell^3x_\ell + 44k_y^3k_z^2k_xy_\ell^3z_\ell^2x_\ell$$

$$+44k_x^3k_z^2k_yx_\ell^3z_\ell^2y_\ell + 44k_y^3k_x^3k_zy_\ell^3x_\ell^2z_\ell + 44k_x^3k_y^2k_zx_\ell^3y_\ell^2z_\ell .$$

APPENDIX E

TABLE E1: Thermodynamical quantities of antiferromagnets calculated by the spin wave theory.

	Linear chain	Quadratic Layer	NaCl-type	CsCl-type
$\frac{E_o}{(\frac{N}{2})z\|J\|S}$	S+0,363	S+0,158	S+0.097	S+0.073
$\frac{E_T}{Nz\|J\|S}$	$\frac{\pi}{3}\theta^2$	$\frac{4,808}{\pi}\theta^3$	$\frac{3^{3/2}}{15}\pi^2\theta^4$	$\frac{4\pi^2\theta^4}{15}$
$\frac{S_T}{Nk}$	$\frac{2}{3}\pi\theta$	$\frac{7,212}{\pi}\theta^2$	$\frac{3^{3/2}\pi^2\theta^3}{15}$	$\frac{16}{45}\pi^2\theta^3$
$\frac{M_{so}}{M_\infty/S}$	$5+\frac{1}{2}+(\frac{1}{2\pi})$ x $\log 2\alpha$	S-0.197	S-0,078	S-0.075
$\frac{M_{sT}}{M_\infty/S}$	$(2\pi)^{-\frac{1}{2}}\theta$	$(\frac{1}{\pi}\log\frac{1}{2\alpha})$	$\frac{3^{\frac{1}{2}}}{2}\theta^2$	$\frac{2}{3}\theta^2$
$X_{11}/\frac{N_g^2\mu_o^2}{kT}$	$(\frac{1}{2\alpha})^{\frac{1}{2}}\theta^2$	$(\frac{1}{\pi}\log\frac{1}{2\alpha})\theta^2$	$3^{\frac{1}{2}}\theta^3$	$\frac{4}{3}\theta^3$
$\frac{8\Delta_o}{N_g^2\mu_o^2}$	$(\frac{1}{2\alpha})^{\frac{1}{2}}$	$\frac{1}{\pi}\log\frac{1}{2\alpha}$	finite	0,396
$\frac{8\Delta_T''}{N_g^2\mu_o^2}$	$2(\frac{1}{2\alpha})^{3/2}\theta^2$	$\frac{2}{\pi\alpha}\theta^2$	$\frac{3^{3/2}}{\pi}\frac{1}{(2\alpha)^{\frac{1}{2}}}\theta^2$	$\frac{4}{\pi}\frac{1}{(2\alpha)^{\frac{1}{2}}}\theta^2$
$\frac{C_T}{Nk}$	$\frac{2}{3}\pi\theta$	$\frac{14,424}{\pi}\theta^2$	$\frac{3^{3/2}}{15}\pi^2\theta^3$	$\frac{16}{15}\pi^2\theta^3$