Green's function method for antiferromagnetism

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by

Keum Hwi Lee

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I. INTRODUCTION

Antiferromagnetism is a typical example of a cooperative phenomenon and has therefore been one of the important subjects of statistical mechanics and solid state physics. It is recognized by a well-defined kink in the susceptibility versus temperature curve and by anomalies in the heat capacity and thermal expansion coefficient.

The concept of antiferromagnetism was first put forward theoretically by Néel (1932) in connection with his study of the paramagnetic susceptibility of metals and alloys of transition metals. A few years later, Bizette, Squire, and Tsai (1938) demonstrated that their data on MnO fitted certain predicted features of models of antiferromagnetism. In the early days, Néel employed the expression "paramagnétisme constant" for "antiferromagnetism". The latter term can be traced back to Hulthén's work (1936, 1938).

A statistical theory for antiferromagnetism usually starts from a specific molecular model, and does not inquire very much into its justification. One frequently used model is the Heisenberg model (1928), in which the spins are coupled to each other by exchange interactions. That is, the Hamiltonian of the antiferromagnetic system is assumed to be of the form

\[ H_{\text{ex}} = 2 \sum_{i>j} J_{ij} \vec{S}_i \cdot \vec{S}_j = \sum_{i,j} J_{ij} \vec{S}_i \cdot \vec{S}_j \]

where \( \vec{S}_i \) and \( \vec{S}_j \) are the vector spin operators associated with
the i-th and j-th constituent ions of the crystal, and $J_{ij}$ is the exchange constant. In addition to this exchange interaction, one sometimes needs to take into account other kinds of energy, for instance, anisotropy energy and dipole interaction. Although it is not certain that the Heisenberg model represents a real physical system, it is generally hoped that the statistical theory of this model will explain the observed behavior of antiferromagnetic substances, at least semi-quantitatively. In practice, the exchange coupling parameters are regarded as phenomenological constants, whose values are determined by fitting the theory with a set of experimental results. Then the model can be used to explain other experimental results and thereby correlate a large number of related phenomena.

The crudest approximation in the theory of cooperative phenomena is provided by the so-called molecular field theory, which is equivalent to the well-known Bragg-Williams method (1934) for alloys and regular assemblies. When applied to antiferromagnetism, this gives the Van Vleck theory (1941). This theory gives several successful qualitative predictions including the existence of the transition temperature, specific heat anomaly, susceptibility anomaly, etc., but it has many weak points, such as the failure of the analysis at very low temperatures. Above the transition temperature, the molecular field theory does not predict short-range order. A more refined theory is a quantum mechanical version of the Bethe-Peierls method (1935, 1936), which was first applied to
ferromagnetism by Weiss (1948) and later to antiferromagnetism by Li (1951). This method gives short-range order above the Néel temperature but again fails at very low temperatures.

General experience with cooperative phenomena suggests two ways of making better approximations: the high temperature approximation and the low temperature approximation. The moment expansion method of Heisenberg (1928), or the $1/T$ expansion method developed by Opechowski (1937, 1939), is an analogue of the Bethe-Kirkwood (1938, 1939) expansion method for a regular assembly and belongs to the first category. The most important method for low temperatures is the spin-wave theory, which was developed by Bloch (1930) in order to treat ferromagnetism. Both approximations rely on series expansions, and they suffer from the drawback that their applicability is limited to a narrow range of temperatures where a small number of terms is sufficient. They have not been able to discuss the existence of phase transitions, since it has not been possible to determine the general term in any of these expansions.

Tyablikov (1959) first employed the technique of double-time temperature-dependent Green's functions to the Heisenberg ferromagnet with spin $1/2$. Extension of the theory to higher spin has been achieved by Tahir-Kheli and ter Haar (1962), and by Callen (1963). The application of the theory to the
Heisenberg antiferromagnet has been studied by Pu (1960), Oguchi and Honma (1963), Lines (1963, 1964, 1965), Anderson and Callen (1964), and Lines and Jones (1965, 1966). An important feature of the Green's function theory is that it agrees with the non-interacting spin wave theory at very low temperatures and with the statistical theory at very high temperatures. So there is hope that the results may not be too far from the correct implications of the Heisenberg model over the entire temperature range.

The exact equation of motion for the Green's function involves higher order Green's functions. If a decoupling approximation is made for the higher order functions, a solvable closed system of equations is obtained. The so-called random phase approximation (RPA) is the simplest and most popular decoupling scheme. Callen (1963) and Anderson and Callen (1964) suggested a more satisfactory decoupling scheme from heuristic physical grounds. Although much progress has been made in the direction of Green's function theory, it has not been possible to make a complete study of the Heisenberg model in this way because an essential quantity, the longitudinal or \( z \z \) correlation function of the spins, does not follow directly from the theory, \( z \) being the direction of preferred antiferromagnetic spin alignment. For the Heisenberg ferromagnet, this problem was first solved by Liu (1965) with general spin value using the random phase approximation.
The present work treats the statistical mechanics of the two sublattice model Heisenberg antiferromagnet in a cubic lattice with nearest neighbor interactions using the Green's function technique. The energy spectrum, the sublattice magnetization, the Néel temperature, the transverse spin correlation functions, the perpendicular susceptibility, and the correlation length are investigated for general spin values using the Callen decoupling scheme. In addition to the above mentioned quantities, the longitudinal correlation functions, the energy, and the specific heat are studied for spin 1/2. For spin 1/2, the rotational invariance of susceptibility at and above the Néel temperature, the continuity of susceptibility at the Néel temperature, and the sum rule for spin operators at and above the Néel temperature are shown to hold. It is also shown that the perpendicular susceptibility varies only slightly as the temperature rises from the absolute zero to the Néel temperature while the parallel susceptibility varies from zero to the same value as the perpendicular susceptibility at the Néel temperature. Some results of numerical work for spin 1/2 are also presented.

The two sublattice Heisenberg model with nearest neighbor interactions is one of the simplest possible. It seems to be a valid and useful approximation for insulators and semiconductors. For these reasons, the model has been quite extensively studied by using various methods. It is therefore desirable to study the model by the newly developed Green's
function method so that one can check this method against the older ones. One should attempt to solve more complicated models only if the method proves to be successful. The two sublattice model requires all spins to be divided into two sublattices such that any spin on one sublattice has all its nearest neighbors on the other sublattice. This geometrical restriction is possible in a simple cubic (sc) and body centered cubic (bcc) structure, the two structures considered in the present work. A face centered cubic (fcc) structure cannot be divided into two such sublattices.

The result of the present study reveals very good agreement between the spin-wave theory and the Green's function analysis at low temperatures. The difference comes only in higher order terms in temperature. Some experimental data give very good agreement with the spin-wave theory in the lowest order. For example, Johnson and Nethercot (1959) found that the antiferromagnetic resonance frequency of MnF₂ is within 0.1% of the spin-wave theory result with nearest neighbor interactions. Trapp and Stout (1963) also found very good agreement of their MnF₂ data with lowest order results of the spin-wave theory. At this stage of experimental study of the problem, it is impossible to detect the difference between the spin-wave theory and the present work. But it is to be noted that the present work predicts the decrease of perpendicular susceptibility below the Néel temperature as the temperature rises.
This is the general feature of the perpendicular susceptibility of MnF$_2$ as measured by Trapp and Stout (1963).
II. REVIEW OF EXISTING THEORIES

In theoretical investigations of the properties of solids, two different approaches are widely used. Both of these attempt to describe the behavior of electrons in a solid in terms of one-electron wave functions. In one, the one-electron wave functions are taken to be essentially the same as in the free atom, i.e., each one is strictly localized about some particular atom or ion of the solid, and the atoms or ions interact with each other. The method is analogous to that of Heitler and London (1927) in the theory of molecules. In the other, the collective electron approach, which is originally due to Bloch (1929), the wave functions are not localized and extend throughout the crystal lattice. The Heisenberg model is an application of the Heitler-London method to solids. Since the present work employs the Heisenberg model, only the standard features of the existing theories of this model are reviewed.

A. The Localized Spin Model

The derivation of the Heisenberg Hamiltonian of Eq. (1.1) starts from the localized spin model as follows: The ions in the solid are characterized by an incomplete electron shell whose structure is determined by the Russel-Saunders coupling scheme (Van Vleck, 1932). The orbital angular momenta of the electrons are coupled into \( \mathbf{L} \) and the spin angular momenta into
by the electrostatic interaction. Then $\vec{L}$ and $\vec{S}$ couple into the total angular momentum $\vec{J}$. For a free ion, $J_z$ and $J^2$ are constants of motion of the system. In the presence of a magnetic field $\vec{H}$, the interaction between the electrons in the incomplete shell of an ion and the field is given by (units are used for which $\hbar = c = 1$),

$$H' = -\sum_i (e/2m)\vec{H} \times \vec{p}_i - \sum_i (e/m)\vec{H} \cdot \vec{s}_i,$$

where $e$ is the charge of an electron, $\vec{r}_i$, $\vec{p}_i$ and $\vec{s}_i$ are the position, momentum, and spin vectors of the $i$-th electron, and the summation is taken over all electrons in the shell. By definition of the $\vec{L}$ and $\vec{S}$ operators, $H'$ can be written as

$$H' = (|e|/2m)\vec{H} \cdot (\vec{L} + 2\vec{S}).$$

Taking $\vec{H}$ in the $z$-direction, one obtains

$$H' = (|e|/2m)(L_z + 2S_z) = (|e|/2m)(J_z + S_z).$$

The matrix element of the interaction is, to first order,

$$\langle JJ' | H' | JJ \rangle = (|e|/2m) \langle JJ' | J_z + S_z | JJ \rangle.$$
By the projection theorem for angular momentum, this is equal to

\[(2.5) \langle JJ_z' | H' | JJ_z \rangle = (\frac{|e|}{2m}) \langle JJ_z'| (1 + \frac{S_z J_z}{2J(J+1)}) J_z | JJ_z \rangle \]

\[= \left[ 1 + \frac{J(J+1) - L(L+1) + S(S+1)}{2J(J+1)} \right] (\frac{|e|}{2m}) H_z J_z S_z J_z'. \]

The quantity in the square bracket is called the Landé g-factor and is denoted by $g$. The quantity $(\frac{|e|}{2m})$ is the Bohr magneton $\mu_B$. Therefore the degeneracy in $J_z$ is completely split and the energy levels are equally spaced

\[(2.6) E_{J_z}^1 = g \mu_B H_z. \]

The magnetic moment operator $\vec{\mu}$ is defined by

\[(2.7) H' = -\vec{\mu} \cdot \vec{H}. \]

Therefore, with $\vec{H}$ in the $z$-direction

\[(2.8) \mu_z = - (\frac{|e|}{2m})(L_z + 2S_z) \]

\[= - (\frac{|e|}{2m})(J_z + S_z). \]

The expectation value of $\mu_z$ in the state $|JJ_z\rangle$ is therefore

\[(2.9) \langle \mu_z \rangle = -(|e|/2m) \langle JJ_z | J_z + S_z | JJ_z \rangle \]

\[= -g \mu_B J_z. \]
For a system of $N/2$ free ions per unit volume in thermal equilibrium, the energy levels of different $J_z$ are occupied according to the Boltzmann distribution. The total magnetic moment of the system is therefore

\begin{equation}
M = (N/2) \left[ \sum_{J_z} \langle \mu_z \rangle \exp(-\alpha J_z/J) \right] \left[ \sum_{J_z} \exp(-\alpha J_z/J) \right]^{-1}
= (N/2) g \mu_B J B_J (\alpha)
\end{equation}

where $\alpha = g \mu_B J H / k_B T$, and

\begin{equation}
B_J (\alpha) = \frac{2J+1}{2J} \coth\left(\frac{2J+1}{2J} \alpha\right) - \frac{1}{2J} \coth\left(\frac{1}{2J} \alpha\right)
\end{equation}

is the Brillouin function. This expression gives the magnetic moment of a collection of free ions as a function of temperature and applied field.

For transition metal ions in solids, the orbital angular momentum of the electrons in the incomplete shell is often quenched by the crystalline electric field (Van Vleck, 1932; Fowler and Guggenheim, 1949). In this picture, each ion is regarded as being in a state with total orbital quantum number $L = 0$ and total spin quantum number $S$. Then, for a system of $N/2$ free ions, the total magnetic moment reduces to

\begin{equation}
M = (N/2) g \mu_B S B_S (\alpha)
\end{equation}

by the substitutions of $J = S$ and $L = 0$ from Eqs. (2.10) and (2.11). Actually, the Landé $g$-factor should be 2, since the
absence of any orbital angular momentum is assumed. Nevertheless small amounts of residual orbital angular momentum may be taken into account by allowing \( g \) to take on values slightly different from 2.

**B. Exchange Interactions**

A fundamental problem of coupled spin systems is the origin of the exchange interaction. Heisenberg (1928) was the first to derive the exchange Hamiltonian of the form (1.1). The principle involved in his work may be demonstrated by the following simple problem.

Suppose that there are two atoms a and b that have one electron each and are separated by a distance \( r_{ab} \). The atomic wave functions are designated by \( \psi_a \) and \( \psi_b \) and the energies of the free atoms by \( \epsilon \). In addition, it will be assumed that these states have no orbital angular momentum, so that all of the magnetic moment arises from spin. If one ignores overlap between the spatial atomic orbitals \( \psi_a \) and \( \psi_b \) centered on atoms a and b, and if one further ignores polarization effects of one atom on the other, then one can write approximate antisymmetric wave functions for the two atomic system as

\[
\Psi_I = \left[ \psi_a(1) \psi_b(2) + \psi_a(2) \psi_b(1) \right] \left[ \alpha_1 \beta_2 - \beta_1 \alpha_2 \right],
\]

\[
\Psi_{II} = \left[ \psi_a(1) \psi_b(2) - \psi_a(2) \psi_b(1) \right] \left\{ \alpha_1 \beta_2 + \beta_1 \alpha_2 \right\}.
\]

(2.13)
Here 1 and 2 index the two electrons, and $\alpha$ and $\beta$ are the "up" and "down" spinors, respectively. The first of these is the wave function of the singlet state ($S = 0$), and the other three are the triplet functions ($S = 1$). If electron 1 is on atom a, and electron 2 is on atom b, then the interaction potential for the system can be written of the form

$$V_{ab} = e^2 \left( \frac{1}{r_{ab}} + \frac{1}{r_{12}} - \frac{1}{r_{1b}} - \frac{1}{r_{2a}} \right),$$

where $r_{12}$ is the distance between the electrons, and $r_{1b}$ and $r_{2a}$ are the distances between a given nucleus and the electron on the other atoms. The energies of the two types of state (2.13) are, respectively,

$$E_I = C - J,$$

$$E_{II} = C + J,$$

where

$$C = 2\epsilon + \int |\psi_a(1)|^2 V_{ab} |\psi_b(2)|^2 d\tau_{12}$$

is the sum of the atomic energy and the Coulomb interaction energy and

$$J = \int \psi_a^\alpha(1) \psi_b^\beta(2)V_{ab} \psi_a(2) \psi_b(1) d\tau_{12}$$
is the exchange integral. It is to be noted that $V_{ab}$ in the integrals in Eqs. (2.16) and (2.17) can be replaced by $e^{2/r_{12}}$ if the functions $\Psi_a$ and $\Psi_b$ are orthogonal.

Eq. (2.15) can be cast into a form of the Heisenberg interaction. To do this, one observes that the square of the total spin operator

$$ (S)^2 = (S_1 + S_2)^2 $$

is a constant of motion in each of the states $\Psi_I$ and $\Psi_{II}$, the eigenvalues having the form

$$ S(S + 1) $$ with $S = 0$ and $1$.

If the right hand side of Eq. (2.18) is expanded, it becomes

$$ (S_1)^2 + (S_2)^2 + 2S_1 \cdot S_2. $$

Since $(S_1)^2$ and $(S_2)^2$ are also constants of motion with eigenvalue $3/4$, it follows that $S_1 \cdot S_2$ is also a constant of motion with eigenvalue $-3/4$ or $1/4$ according as $S = 0$ or $1$.

Employing Eq. (2.18), one may write Eq. (2.15) in the operator form

$$ E = C - J(1 - S^2) $$

or, using Eq. (2.20), in the form

$$ E = C + J/2 + 2S_1 \cdot S_2. $$
Hence, apart from an additive constant, the spin-dependent part of exchange interaction of the system can be written as

$$H_{\text{ex}} = \sum_{i,j} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j.$$  

The majority of substances which show antiferromagnetic properties are ionic crystals such as MnO, MnS, MnF₂, etc. In these substances the magnetic ions are separated from each other by anions O, S, F, etc. Neutron diffraction studies on MnO, FeO, CoO and NiO, by Shull et al. (1951a,b) revealed that there exists a strong antiferromagnetic exchange coupling between magnetic ions, which are separated by the intervening large oxygen ions. As will be shown in the following section, the Néel temperature is a measure of the strength of the exchange coupling. Analysis of the experimental data on the Néel temperatures of these substances indicates that antiferromagnetic coupling in such substances arises from a mechanism different from that of the usual direct exchange interaction.

The mechanism of superexchange was proposed by Kramers as early as 1934. Bizette (1946) and Néel (1948) emphasized the importance of this superexchange in antiferromagnetic substances, and Anderson (1950a) presented a detailed theoretical treatment of Kramers' idea and clarified the mechanism of superexchange. The same problem was treated by Van Vleck (1951) using a different method. The main idea is as follows:
Three ions, one oxygen ion and two adjacent magnetic ions, are isolated from the rest for the purpose of the discussion.

Ground and excited states of (MnOMn)\(^{++}\):

\[
\begin{align*}
\text{Mn}^{++} & \quad \text{O}^{2-} & \quad \text{Mn}^{++} \\
\text{d}_1 & \quad \text{pp}' & \quad \text{d}_2 \\
\text{d}_1^1 & \quad \text{p} & \quad \text{d}_2 \\
\text{ground state} & & \text{excited state}
\end{align*}
\]

For simplicity, one considers two electrons occupying the same p-orbital of an O\(^{2-}\) ion and one electron each in a d-orbital of the magnetic ions. In this state, the two electrons in O\(^{2-}\) will form a singlet state, so that there will be no exchange coupling between the magnetic ions M\(_1\) and M\(_2\). One can imagine, however, the possibility of one of the two electrons of the O\(^{2-}\) ion being transferred to one of the two magnetic ions, say M\(_1\), and occupying its s- or d-orbital. In this excited state, the unpaired electron left in O\(^{2-}\) can couple with the electron of the other magnetic ion, M\(_2\). There should also be a strong coupling between the electron transferred to M\(_1\) and the original electron in M\(_1\). Moreover, the two electrons originally belonging to the oxygen ion have opposite spins, so that there will appear an indirect spin coupling between M\(_1\) and M\(_2\) through this excited state. In this way, the super-exchange coupling between magnetic ions separated by a non-magnetic ion can be explained.
Slater (1953) proposed another mechanism of super-exchange: the polarization or deformation of the oxygen ion stabilizes the energy of the antiferromagnetic state of Mn-O-Mn. The following is the main idea. One considers an electron in the charge distribution of other electrons. Due to the intra-atomic exchange effect or Hund's rule effect, the potential energy of the electron is lower when its spin is parallel to the net spin of the other electrons. Therefore, when there is an antiferromagnetic configuration of Mn-O-Mn, in which the spins of one Mn ion point in one direction and those of the other Mn ion in the opposite direction, the electrons of the oxygen ion with plus and minus spins will each be pulled towards that Mn ion which has the same spin direction. In this way, the oxygen ion is polarized and the antiferromagnetic state is stabilized.

Zener (1951) proposed another kind of indirect spin-spin interaction to account for the ferromagnetic properties found in mixed crystals of LaMnO$_3$ and BaMnO$_3$, neither of which is known to show ferromagnetism in itself. These mixed crystals include Mn$^{3+}$ and Mn$^{4+}$ ions, and Zener considered an indirect spin-spin interaction that works between Mn$^{3+}$ and Mn$^{4+}$ by the following mechanism. For simplicity, one oxygen ion and its adjacent two Mn ions are considered. As before, one considers the two paired electrons of O$^{2-}$ and assumes that the one of the two Mn ions has one electron and that the
other has two electrons with spins parallel owing to a strong Hund's rule effect. The state of two Mn ions having parallel spins will be called configuration I.

Ground and excited configurations of (MnOMn)$^{5+}$.

\[
\begin{align*}
\text{Mn}^{3+} & \quad \text{O}^{2-} & \quad \text{Mn}^{4+} & \quad \text{Mn}^{3+} \quad \text{O}^{-} & \quad \text{Mn}^{3+} & \quad \text{Mn}^{4+} \quad \text{O}^{2-} & \quad \text{Mn}^{3+} \\
d_{1}d_{1}' & \quad p & \quad d_{2} & \quad d_{1}d_{1}' & \quad p & \quad d_{2}d_{2}' & \quad d_{1} & \quad p' & \quad d_{2}d_{2}'
\end{align*}
\]

configuration I   configuration II   configuration III

This can change into configuration II by the transfer of an electron of that spin direction from O$^{2-}$ to the right Mn (which had been occupied by one electron). Further, the configuration II can change into another configuration III by the transfer of one of the electrons of the left Mn to the vacant orbital of O$^{2-}$ produced by the first transfer. Configuration I has the same energy as that of configuration III, and therefore a strong resonance will take place between them through the excited configuration II. Thus the ferromagnetic state will be stabilized. For two Mn ions with antiparallel spins, such a resonance is not expected. Therefore, a ferromagnetic spin coupling appears between Mn$^{3+}$ and Mn$^{4+}$. Zener called this type of coupling the "double exchange". He did not study the same kind of exchange for antiferromagnetism.

For metals, Ruderman and Kittel (1954) studied the indirect exchange coupling between magnetic moments of nuclei via their hyperfine interaction with the conduction electrons.
They studied the problem by considering a metal crystal in which all but two of the nuclei are nonmagnetic. The electron wave functions of the perfectly periodic problem will be scattered by the hyperfine interaction with each of the magnetic nuclei. The total wave function seen by one magnetic nucleus will depend on the spin orientation of the other, thus establishing a spin-dependent coupling between the two nuclei. Their final result for the interaction energy between nuclear spins in a metal is of the form

\[ H_{\text{ind.}} = \sum_{i,j} A_{ij} \vec{I}_i \cdot \vec{I}_j \]

where \( \vec{I}_i \) is the spin operator for the i-th nucleus, \( A_{ij} \) is a function of the strength of hyperfine interaction between electrons and nuclei, the effective mass of conduction electron, the spin quantum numbers of nuclei, and the distance between the i-th and j-th nuclei.

By using calculations similar to those of Ruderman and Kittel, Kasuya (1956) was the first to study rigorously the indirect exchange mechanism of antiferromagnetism by Zener's model of ferromagnetism, namely the indirect exchange coupling via conduction electrons. For metals, this mechanism is supposed to play an important role; for rare earth metals, this interaction seems to be almost the only mechanism which can cause ferro- and antiferromagnetism. Kasuya studied in some detail the exchange interaction between a conduction
electron and the magnetic shell electrons of an ions, and the indirect exchange coupling between different ions resulting from it. If one follows Ruderman-Kittel's model, the final result can be put into the form

\[ H_{\text{ind.}} = \sum_{i,j} B_{ij} \vec{J}_i \cdot \vec{J}_j \]

where \( \vec{J}_i \) is the total angular momentum of the \( i \)-th ion, \( B_{ij} \) is the indirect exchange parameter. The strength of the indirect exchange coupling \( B_{ij} \) is an oscillatory function of the distance between ions and is of much longer range than the direct exchange coupling.

C. Molecular Field Theory, Including the Bethe-Peierls-Weiss Theory

The theory of the susceptibility of antiferromagnetic substances which is based on the Weiss molecular field approximation was originated by Néel (1932, 1936a, 1936b), Bitter (1938) and Van Vleck (1941). In this theory one considers two identical sublattices with self interactions and mutual interactions. The simplest model is the Heisenberg model, where the coupling between spins is represented by the Hamiltonian

\[ H = \sum_{\alpha_i, \beta_j} J_{\alpha \beta} \vec{S}_{\alpha i} \cdot \vec{S}_{\beta j} \]

where \( \vec{S}_{\alpha_i} \) and \( \vec{S}_{\beta_j} \) are the spin angular momentum vectors of the \( i \)-th ion in the sublattice \( \alpha \) and the \( j \)-th ion in the sublattice
\( \phi \), respectively, measured in units of \( \hbar \); \( J_{\alpha,1}, \phi \) is the exchange constant; \( \alpha \) and \( \phi \) refer to two sublattices. In low energy states, the spins on sublattice 1 will be primarily in one direction, to be called "up" in the present work; spins on sublattice 2 will be primarily "down". The Hamiltonian (2.26) can be alternatively written as

\[
H = \sum_{i} \left[ \sum_{j} J_{\alpha,1}, \phi \right] \cdot \vec{S}_{\alpha,1}
(2.27)
\]

\[= 2 \sum_{i} \left[ \sum_{j} J_{\alpha,1}, \phi \right] \cdot \vec{S}_{\alpha,1}, \quad (\alpha \neq \phi).\]

Therefore the coupling can be represented by effective fields acting on the ions. The effective field consists of two parts, one coming from other ions in the same sublattice and the other being the contribution from the other sublattice. For the \( i \)-th ion in the sublattice \( \alpha \), the molecular fields are

\[
\overline{H}_{\alpha} = \frac{2}{g \mu_B} \sum_{j} J_{\alpha,1}, \phi \cdot \overline{S}_{\alpha,j}
(2.28)
\]

\[\equiv \frac{2}{g \mu_B} \sum_{j} J_{\alpha,1}, \phi \cdot \left\langle \overline{S}_{\alpha} \right\rangle, \quad (\alpha \neq \phi).\]

The process of replacing the spin operator \( \overline{S}_{\alpha,1} \) by its statistical average \( \left\langle \overline{S}_{\alpha} \right\rangle \) is the essential approximation of this theory. The replacement is equivalent to neglecting the fluctuations of \( \overline{S}_{\alpha,1} \), and since this is not always a good
approximation, some unphysical situations result. Similarly, for the ion $j$ in the sublattice $\beta$, one gets

\[ \mathbf{H}_{\beta} = \frac{2}{g \mu_B} \sum_j J_{\beta j, \beta i} \langle \mathbf{S}_i \rangle, \]

(2.29) \[ \mathbf{H}_{\alpha} = \frac{2}{g \mu_B} \sum_i J_{\alpha j, \alpha i} \langle \mathbf{S}_i \rangle, \ (\alpha \neq \beta). \]

The sublattice magnetizations are given by

\[ \mathbf{M}_\alpha = \frac{N}{2} g \mu_B \langle \mathbf{S}_\alpha \rangle, \]

(2.30) \[ \mathbf{M}_\beta = \frac{N}{2} g \mu_B \langle \mathbf{S}_\beta \rangle, \]

and so the molecular fields may be written as

\[ \mathbf{H}_{\alpha \alpha} = \frac{4}{Ng^2 \mu_B^2} \sum_j J_{\alpha j, \alpha i} \mathbf{M}_\alpha = \lambda' \mathbf{M}_\alpha, \]

(2.31) \[ \mathbf{H}_{\alpha \beta} = \frac{4}{Ng^2 \mu_B^2} \sum_i J_{\alpha i, \beta j} \mathbf{M}_\beta = \lambda \mathbf{M}_\beta, \ (\alpha \neq \beta), \]

\[ \mathbf{H}_{\beta \beta} = \lambda' \mathbf{M}_\beta, \]

\[ \mathbf{H}_{\beta \alpha} = \lambda \mathbf{M}_\alpha, \ (\alpha \neq \beta) \]

with

\[ \lambda' = \frac{4}{Ng^2 \mu_B^2} \sum_i J_{\alpha i, \alpha j}, \]

(2.32) \[ \lambda = \frac{4}{Ng^2 \mu_B^2} \sum_j J_{\alpha j, \beta j}, \ (\alpha \neq \beta). \]
The $\lambda$'s are called the molecular field constants. Hence for an antiferromagnetic crystal, the total effective field is the sum of the external field and the molecular field. Thus, one has

$$\overrightarrow{H}_\alpha = \overrightarrow{H}_0 + \overrightarrow{H}_{m,\alpha} = \overrightarrow{H}_0 - \lambda'\overrightarrow{M}_\alpha - \lambda\overrightarrow{M}_\beta,$$

$$(2.33)$$

$$\overrightarrow{H}_\phi = \overrightarrow{H}_0 + \overrightarrow{H}_{m,\phi} = \overrightarrow{H}_0 - \lambda'\overrightarrow{M}_\phi - \lambda\overrightarrow{M}_\alpha.$$

Therefore the magnitudes of $\overrightarrow{M}_\alpha$ and $\overrightarrow{M}_\phi$ as functions of temperature are given by the coupled equations

$$M_\alpha = |\overrightarrow{M}_\alpha| = (N g \mu_B S/2) B_S (g \mu_B S \overrightarrow{H}_\alpha/k_B T),$$

$$(2.34)$$

$$M_\phi = |\overrightarrow{M}_\phi| = (N g \mu_B S/2) B_S (g \mu_B S \overrightarrow{H}_\phi/k_B T).$$

If there is no external field, $\overrightarrow{M}_\alpha$ and $\overrightarrow{M}_\phi$ are antiparallel to each other as long as $\lambda$ is positive and $\lambda'$ is not too large. (If $\lambda' > \lambda > 0$, each sublattice will divide into further sublattices with antiparallel spins.) So Eq. (2.33) give the same magnitude of sublattice magnetization

$$(2.35) \quad M_\alpha = M_\phi = M = (N g \mu_B S/2) B_S (g \mu_B S (\lambda - \lambda') M/k_B T).$$

Eq. (2.35) has a non-zero solution for $M$ as long as the temperature is less than a critical value $T_N$, known as the Neél temperature, given by

$$(2.36) \quad T_N = (N/2) g^2 \mu_B^2 (\lambda - \lambda') S(S + 1)/3k_B.$$
From Eq. (2.32), one obtains

\[
T_N = \left[ \sum_j J_{\alpha i, \alpha j} - \sum_j J_{\alpha i, \alpha j} \right] 2S(S + 1)/3k_B, \quad (\alpha \neq \beta)
\]

which gives the relationship between the antiferromagnetic-paramagnetic order-disorder transition temperature and the strength of coupling between ions.

At a temperature \( T > T_N \), the system has no net sublattice magnetization unless an external field is applied. In this paramagnetic region, the sublattice magnetizations \( \overrightarrow{M}_1 \) and \( \overrightarrow{M}_2 \) are both parallel to the applied field \( \overrightarrow{H}_o \). At high enough temperatures, the Brillouin function can be approximated by

\[
B_S(\alpha) \longrightarrow \frac{(S + 1)}{3S} \alpha.
\]

Thus, from Eq. (2.34), one obtains

\[
\begin{align*}
M_1 &= \frac{(N/2)}{} \mu_B^2 (H_o - \lambda' M_1 - \lambda M_2) S(S + 1)/3k_B T, \\
M_2 &= \frac{(N/2)}{} \mu_B^2 (H_o - \lambda' M_2 - \lambda M_1) S(S + 1)/3k_B T.
\end{align*}
\]

Solving these equations, one gets

\[
M_1 = M_2
\]

and hence

\[
M_1 \left[ 1 + \frac{(N/2)}{} \mu_B^2 (\lambda + \lambda') S(S + 1)/3k_B T \right] = \frac{(N/2)}{} \mu_B^2 H_o S(S + 1)/3k_B T.
\]
Thus the paramagnetic susceptibility is given by

\[(2.39) \quad \chi = \frac{M_1 + M_2}{H_0} = \frac{2M_1}{H_0} = C/(T + \Theta)\]

with

\[(2.40) \quad C = N s^2 \mu_B^2 (S + 1)/3k_B,\]

\[(2.41) \quad \Theta = C(\lambda + \lambda')/2 = (\lambda + \lambda') T_N/(\lambda - \lambda'),\]

where \(C\) is called the Curie constant. If there are nearest neighbor interactions only, \(\lambda'\) vanishes and hence

\[(2.42) \quad \Theta = T_N.\]

In real noncubic materials, there is almost always a direction of preferred spin orientation, or easy magnetization. A complete Hamiltonian for the spin energies contains a corresponding anisotropy energy. One defines parallel and perpendicular susceptibilities for an external field applied parallel or perpendicular to the preferred spin orientation. In an isotropic material it is still possible to calculate the response to small external fields parallel or perpendicular to the (accidental) direction of spin orientation assuming only small changes in spin direction and magnitude.

The susceptibility below the Néel point can be calculated by expanding \(B_S(\alpha)\) of Eq. (2.34) in powers of \(H_0\) and retaining the first order term only. To calculate the parallel
susceptibility, it is essential to assume that the effective molecular fields $\mathbf{H}_m,\alpha$ and $\mathbf{H}_m,\phi$ in Eq. (2.33) are, respectively, parallel and antiparallel to $\mathbf{H}_0$ in order to obtain a consistent solution; otherwise, except in the case where they are equal in magnitude and make the same angle with $\mathbf{H}_0$, Eq. (2.34) cannot be solved. One gets

$$M_1 - M = M - M_2, \tag{2.43}$$

$$\chi_\parallel = (M_1 - M_2) / H_0$$

$$= \frac{3S B^i(\alpha)}{S + 1} \left[ T + (\lambda + \lambda')3S B^i(\alpha)/2(S+1) \right]^{-1}$$

with $\alpha = g\mu_B S(\lambda - \lambda')\hbar/k_B T$.

This susceptibility vanishes at $T = 0$, increases with rising temperature, and becomes equal to Eq. (2.39) above the Néel point. When the applied external field $\mathbf{H}_0$ is perpendicular to the preferred alignment direction of spins, $\mathbf{M}_i$ and $\mathbf{M}_2$ have the same magnitude and incline symmetrically to $\mathbf{H}_0$. The torque on, say, $\mathbf{M}_1$ must vanish:

$$0 = \mathbf{M}_1 \times (\mathbf{H}_0 + \mathbf{H}_m,1)$$

$$= \mathbf{M}_1 \times (\mathbf{H}_0 - \lambda'\mathbf{M}_1 - \lambda\mathbf{M}_2)$$

$$= M_1 H_0 \cos \phi - \lambda M_1^2 \sin (2\phi),$$
\( \phi \) being the inclination angle of \( \overrightarrow{M} \)'s from the unperturbed preferred alignment direction. From Eq. (2.44), it follows that

\[
(2.45) \quad 2 \mathcal{M}_1 \sin \phi = H_0 / \lambda.
\]

Since the left hand side is the total magnetization, one gets the perpendicular susceptibility

\[
(2.46) \quad \chi_p = 1 / \lambda = \text{constant}.
\]

It is to be noted that Eqs. (2.39) and (2.46) give the same susceptibility at the Neel temperature.

The internal energy of the system can be shown (Mattis, 1965) to be

\[
(2.47) \quad U = \langle H \rangle = - (N/2) \left[ 3k_B T / 4S(S+1) \right] \left[ 2S k(T) / \mathcal{M}(0) \right]^2 \text{ for } T < T_N
\]

\[ = 0 \quad \text{for } T > T_N. \]

And hence the discontinuity in the specific heat at the Neel temperature is given by

\[
(2.48) \quad \Delta C \bigg|_{T_N} = 5Nk_B S(S+1) / [S^2 + (S+1)^2].
\]

Among many authors who extended the original molecular field approach, Néel (1948) and Anderson (1950b), as well as Smart (1953), recognized the importance of the next nearest neighbors for the Neel point and the susceptibility; Kittel
(1951), Nagamiya (1951), Yosida (1951), Keffer and Kittel (1952), Gorter and Haantjes (1952), Ubbink (1953), Wangsness (1952, 1953a,b) and many others treated problems including anisotropy, Bitter (1938), Garret (1951a,b) and the Leiden workers under Gorter (1951, 1953) considered the case in which the applied magnetic field is of the order of, or greater than, the Weiss molecular field.

Li (1951) applied the Bethe-Peierls-Weiss (BPW) method to antiferromagnetism. The basic assumption of the method is that a cluster of \((n + 1)\) ions, i.e., a central ion \(\alpha_1\) and its neighbors, is statistically represented by the operator

\[
(2.49) \quad \hat{\phi}_{\text{cluster}} = \exp \left[ -2J \sum_{j=1}^{n} \vec{S}_{\alpha_1} \cdot \vec{S}_j - g\mu_B H_0 S_{\alpha_1}^z - g\mu_B H_x \sum_{j=1}^{n} S_j^z \right] \left( j \neq \alpha \right)
\]

where \(H_0\) is an external field and \(H_x\) is the internal field representing the effect of outer ions on the ion \(\alpha_1\), which is to be determined in a self-consistent manner. Taking two kinds of cluster, one being centered on an ion of the sublattice 1, the other on the sublattice 2, and assuming different internal fields \(H_1\) and \(H_2\) in place of \(H_x\), the statistical average of the spin on a given type of ion is calculated in two ways. Equating these expressions, one obtains two equations to be solved for \(H_1\) and \(H_2\). For vanishing external field, one of the possible solutions is identically zero, which corresponds to the disordered state, but another non-trivial solution appears
below the critical point. The values of the transition points have been calculated by Li. He also succeeded in showing that one- and two-dimensional lattices will not be ordered. Oguchi and Obata (1953) proposed a modified operator for (2.49) and obtained somewhat higher critical points, but their modification brought a failure of the theory for ferromagnetism.

D. High Temperature Approximations

The most systematic approximation from the high temperature side is the 1/T expansion method developed by Opechowski (1937, 1939), which is an analogue of the Bethe-Kirkwood expansion method for a regular assembly.

The principle of the 1/T expansion method is to calculate the partition function by expanding exp(- $\beta H$) in powers of $\beta$. The calculation of interested quantities then reduces to the computation of the traces of various products of spin operators. This calculation is elementary in principle though extremely tedious for higher order terms. In this method, the determination of the critical point is necessarily an extrapolation. The most critical fact is that 1/T expansion converges much slower for the antiferromagnetic case than for the ferromagnetic case (Nagamiya et al., 1955). Several modifications of this method have been tried.
E. Low Temperature Approximations

The statistical properties at low temperatures are determined by the quantum states at the bottom of energy spectrum. So the low-temperature theory always requires more detailed analysis of the quantum states of the whole system than the high-temperature theories. In the high-temperature theories, it is possible to treat the constituent units as nearly independent because of the high degeneracy of the quantum states. Thus, at low temperatures, one meets essentially a many-body problem, which is usually solved by finding the approximate normal modes.

One of the best examples of a successful low-temperature theory is the spin-wave theory of Bloch (1930) for ferromagnetism. Bethe (1931) gave a detailed mathematical theory of the spin-wave in a linear chain, in which he succeeded in treating states involving any number of reversed spins. Hulthén (1936) corrected some errors in Bethe's calculation and solved the problem giving an exact value for the ground state energy. He was also the first to apply to antiferromagnetism the semi-classical method of spin-waves due to Heller and Kramers (1934). Anderson (1952) re-examined the Heller-Kramers-Hulthén theory and showed that the spin-wave method can be used to give a reasonable approximation to the ground state of an antiferromagnetic array. Although the
theory is still not satisfactory, the spin-wave method is, at present, the most reasonable treatment feasible for low temperatures.

The basis of the spin-wave approximation is the fact that at sufficiently low temperatures the interaction between the spin deviations may be neglected. For, at sufficiently low temperatures, one can expect that the average number of spin deviations in the crystal is very small compared to the total numbers of ions in the crystal. The approach is based on approximating the magnetic spin system by a system of harmonic oscillators. There are two ways of doing this, one being the Heller-Kramers method due to Bloch, and the other the Holstein-Primakoff method (1940). In the first method, one observes that the commutation rule

\[(2.50) \quad [S^x, S^y] = iS^z = is\]

is, if $S^z$ is nearly constant, approximately equivalent to the relation which would hold between $S^x$ and $S^y$ if they were canonically conjugate variables. Also, the expansion

\[(2.51) \quad S^z = [S(S + 1) - (S^x)^2 - (S^y)^2]^{1/2} = S - \frac{(S^x)^2 + (S^y)^2}{2S} - S\]
is valid in the same approximation. The Holstein-Primakoff method consists in writing the spin operators in the following forms:

\[ S^+ = S^x + iS^y = (2S)^{1/2}(1 - \frac{n}{2S})^{1/2}a, \]

\[ S^- = S^x - iS^y = (2S)^{1/2}a^+(1 - \frac{n}{2S})^{1/2}, \]

\[ S^z = S - n \]

where the operators \( a^+ \) and \( a \), called the creation and annihilation operators of the "spin deviation", satisfy the commutation rule

\[ [a, a^+] = 1, \]

and the spin deviation is defined by

\[ a^+a = n. \]

It is easy to show the equivalence of the two formalisms in the limit of

\[ (n/2S) \ll 1, \]

which holds at sufficiently low temperatures, in which region the spin-wave theory holds rigorously. In fact, in the limit of (2.55), Eq. (2.52) can be written as

\[ S^+ = (2S)^{1/2}a, \]

\[ S^- = (2S)^{1/2}a^+, \]
so that

\[ S^z = (1/2) [S^+, S^-] = S. \]

The last expression is nothing but Eq. (2.50), and one also observes that

\[ (2.57) \quad S^- S^+ = (S^x)^2 + (S^y)^2 - S^z \]

\[ = (S^x)^2 + (S^y)^2 - s. \]

The left hand side is 2Sn in the same approximation so that the expansion of Eq. (2.51) follows.

To illustrate the content of the theory, only the isotropic coupling between neighboring spins is assumed to exist, so that the Hamiltonian reads

\[ (2.58) \quad H = 2J \sum_{i,j} \vec{S}_{1i} \cdot \vec{S}_{2(i+j)} \]

where \( \vec{S} \) is a vector between neighboring spins. The Holstein-Primakoff transformation to creation and annihilation operators of the spin deviations in two sublattices is defined by

\[ (2.59) \]

\[ s^+_{1i} = (2S)^{1/2} \left[ 1 - \left( a^+_{1i} a^-_{1i} / 2S \right) \right]^{1/2} a^+_{1i}, \]

\[ s^-_{1i} = (2S)^{1/2} a^+_{1i} \left[ 1 - \left( a^+_{1i} a^-_{1i} / 2S \right) \right]^{1/2}, \]

\[ s^+_{2j} = (2S)^{1/2} a^+_{2j} \left[ 1 - \left( a^+_{2j} a^-_{2j} / 2S \right) \right]^{1/2}, \]

\[ s^-_{2j} = (2S)^{1/2} \left[ 1 - \left( a^+_{2j} a^-_{2j} / 2S \right) \right]^{1/2} a^-_{2j}. \]
where the spin-deviation operators satisfy

\[
[a_{\alpha_i}, a_{\alpha_j}^+] = \delta_{\alpha\beta} \delta_{ij},
\]

\[
[a_{\alpha_i}, a_{\alpha_j}] = [a_{\alpha_i}^+, a_{\alpha_j}^+] = 0,
\]

\( S_i \)'s being the Kronecker deltas. From Eq. (2.59), it is easy to show that

\[
(s_{\alpha_i}^z)^2 = (s - a_{\alpha_i}^+ a_{\alpha_i})^2,
\]

and hence

\[
s_{11}^z = s - a_{11}^+ a_{11},
\]

\[
-s_{2j}^z = s - a_{2j}^+ a_{2j},
\]

the signs being chosen on physical grounds. The spin-wave operators are defined by the Fourier components of the spin-deviation operators

\[
b_{1k} = (2/N)^{1/2} \sum_i a_{1i} \exp(i \vec{k} \cdot \vec{r}_i),
\]

\[
b_{1k}^+ = (b_{1k})^+ = (2/N)^{1/2} \sum_i a_{1i}^+ \exp(-i \vec{k} \cdot \vec{r}_i),
\]

\[
b_{2k} = (2/N)^{1/2} \sum_j a_{2j} \exp(-i \vec{k} \cdot \vec{r}_j),
\]

\[
b_{2k}^+ = (2/N)^{1/2} \sum_j a_{2j}^+ \exp(i \vec{k} \cdot \vec{r}_j),
\]
where \( \vec{a}_i \) is the position vector of the \( i \)-th site of sublattice \( \alpha \) and the wave number vector \( \vec{k} \) runs over \( N/2 \) points in the first zone of the reciprocal space of the lattice, \( N \) being the total number of sites. In terms of these new variables, the Hamiltonian (2.58) reads

\[
H = -NzJS^2 + zJS \sum_{\vec{k}} \gamma_k \left[ (b^+_1 b^+_2 + b^-_1 b^-_2) + (b^+_1 b^-_1 + b^+_2 b^-_2) \right]
+ H'
\]

with

\[
\gamma_k = (1/z) \sum_{\vec{S}} \exp(i \vec{k} \cdot \vec{S}) = \gamma_{-k},
\]

where \( z \) is the number of nearest neighbors, and \( H' \) contains all terms of higher than the second power of the spin-deviation operators. A canonical transformation is defined by

\[
\begin{align*}
b^+_1 &= c^{+}_k \cosh \xi_k + \tilde{d}^{+}_k \sinh \xi_k, \\
b^+_2 &= c^{+}_k \sinh \xi_k + \tilde{d}^{+}_k \cosh \xi_k
\end{align*}
\]

with \( \xi_k \) such that

\[
\tanh(2 \xi) = -\gamma_k.
\]
These new creation and annihilation operators satisfy the commutation rules

\[ [c_k, c_{k'}^+] = [\tilde{d}_k, \tilde{d}_{k'}^+] = \delta_{kk'}, \]

\[ [c_k, \tilde{d}_{k'}^+] = [c_{k'}, \tilde{d}_k^+] = 0. \]

Except for the higher order term \( H' \), the Hamiltonian is easily diagonalized by this transformation, so that it leads to

\[ (2.67) \]

\[ H = -NzJS(S+1) + H' + \sum_k [\omega_k (c_k^+ c_k + 1/2) + \omega_k (\tilde{d}_k^+ \tilde{d}_k + 1/2)] \]

with the normal frequency of the spin-wave

\[ (2.68) \]

\[ \omega_k = (2zJS) (1 - \gamma_k^2)^{1/2}. \]

In Eq. (2.67) the first term, \(-NzJS(S+1)\), can be regarded as the energy of spins perfectly aligned, if the magnitude of a spin at rest is taken as \([S(S+1)]^{1/2}\) instead of \(S\). There is zero-point motion of the spins, due to the uncertainty coming from the non-commutability of spin components, so that a certain zero-point energy has to be added to the naively obtained lowest energy. Neglecting the higher order term \( H' \), one can show that the zero-point energy is given by

\[ (2.69) \]

\[ E_0 = \langle H \rangle_0 = -NzJS(S+1) + \sum_k \omega_k. \]
One can express $E_0$ in terms of a constant $c$ (Appendix A) defined by

$$(2.70) \quad E_0 = -NzJS^2(1 + c/S).$$

From Eq. (2.66), it follows that

$$(2.71) \quad c = (2/N) \sum_k \left[ 1 - (1 - \gamma_k^2)^{1/2} \right].$$

A striking feature of the theory of antiferromagnetism is the departure of the sublattice magnetic moment at absolute zero from the value $(g\mu_B SN/2)$, which corresponds to the elementary picture of a saturated sublattice. From Eqs. (2.61), (2.62), and (2.65) one gets

$$(2.72) \quad M_{1,op} = g\mu_B \sum_{i=1}^2 S_{i,1}^z$$

$$= g\mu_B SN/2 - g\mu_B \sum_k (c_k^+ c_k \cosh 2\delta_k + d_k^+ d_k \sinh 2\delta_k + \text{off-diagonal terms}).$$

At absolute zero $<c_k^+ c_k> = 0$, so if one uses Eq. (2.66), it follows that

$$(2.73) \quad g\mu_B SN/2 - M_1(0) = g\mu_B SN/2 - <M_{1,op} >$$

$$= (g\mu_B/2) \sum_k [(1 - \gamma_k^2)^{-1/2} - 1].$$
Defining a constant $c'$ (Appendix A) by

$$M_1(0) = (N/2) \mathcal{g} \mu_B (S - c'/2),$$

one gets

$$c' = (2/N) \sum_k [ (1 - y_k^2)^{-1/2} - 1 ].$$

At positive temperatures

$$\langle c^+_k c^-_k \rangle = \langle d^+_k d^-_k \rangle = 1 / [ \exp(\omega_k) - 1 ],$$

so, noting that $d_k^+ d^-_k = d^+_k d^-_k + 1$, one gets

$$M_1(0) - M_2(T) = \mathcal{g} \mu_B \sum_k (1 - y_k^2)^{-1/2} [ \exp(\omega_k) - 1 ]^{-1}.$$

The parallel and perpendicular susceptibilities can also be calculated and the results are

$$\chi^p(T) = (\mathcal{g} \mu_B)^2 \sum_k \left\{ \frac{2}{N} \sum_k \frac{\exp(\omega_k)}{[\exp(\omega_k) - 1]^2} \right\},$$

$$\chi^\perp(T) = (\mathcal{g} \mu_B)^2 (N/4zJ).$$

The spin-wave theory so far discussed is based on the simplification of neglecting the interactions between spin-waves. There are two kinds of interaction: one is the kinematical interaction which arises from the fact that more than $(2S + 1)$ units of reversed spin cannot be attached to the same
ion simultaneously, the other is the dynamical interaction which represents the non-diagonal part $H'$ of the Hamiltonian in its basic set of states. The simplification of neglecting the interactions is not valid if the concentration of spin-wave quanta is increased. So one expects that the approximation of non-interacting spin-waves becomes poor when the temperature is raised. Several authors, including Kubo (1952), Ziman (1952, 1953), Oguchi (1960), and Liu (1966), have investigated the problem.
III. REVIEW OF GREEN'S FUNCTIONS

In this review, the properties of the temperature-dependent, double-time causal Green's function are studied extensively in relation to the present work. More general treatments of the problem may be found in the standard review articles and books, such as those by Zubarev (1960), Bonch-Bruevich and Tyablikov (1962), Kadanoff and Baym (1962), and Parry and Turner (1964).

A. Causal Green's Functions and Time Correlation Functions

For a system with a time independent Hamiltonian $H$, the causal Green's function for a pair of operators $A$ and $B$ is defined as follows:

\begin{align}
G_{AB}(t) &= -i \langle T A(t) B(0) \rangle \\
A(t) &= \exp(iHt) A \exp(-iHt);
\end{align}

where $A(t)$ is the Heisenberg representation for the operator $A$. T is the time ordering operator of Dyson, which is defined in the usual way so that

\begin{align}
T A(t) B(0) &= \theta(t) A(t) B(0) + \theta(-t) B(0) A(t)
\end{align}
with

\[(3.4) \quad \theta(t) = \begin{cases} 
1 & \text{for } t > 0 \\
0 & \text{for } t < 0
\end{cases} \]

in case of the Bose operators A and B which are used in the present work; the single angular bracket denotes an average with respect to the canonical density matrix of the system

\[(3.5) \quad \langle \cdot \cdot \cdot \rangle = \text{Tr}(\varphi \cdot \cdot \cdot)\]

where

\[(3.6) \quad \varphi = \exp(-\beta H)/\text{Tr} [\exp(-\beta H)], \quad \beta = (1/k_B T).\]

The equation of motion for \(G_{AB}(t)\) is derived easily from the definition of \(G_{AB}(t)\) and the equation of motion for the operator \(A(t)\) as follows:

\[(3.7) \quad i(d/dt)G_{AB}(t) = i(d/dt)[\langle A(t)B(0) \rangle - i\varphi(-t)\langle B(0)A(t) \rangle] \]
\[= \theta'(t) \langle A(t)B(0) \rangle + \theta'(-t) \langle B(0)A(t) \rangle \]
\[+ (-1) \langle T [A'(t)B(0)] \rangle \]
\[= S(t) \langle [A(t), B(0)] \rangle - i \langle T [A(t), B(t)] B(0) \rangle \]

since

\[(3.8) \quad \theta'(t) = (d/dt)\left[ \int_{-\infty}^{t} S(t') dt' \right] = S(t).\]
(3.9) \[ i(d/dt)A(t) = [A(t), H(t)] \].

The following time correlation functions play an important role in statistical mechanics and will be necessary for the present work.

\[ F_{AB}(t) = \langle A(t)B(0) \rangle, \]
\[ F_{BA}(-t) = \langle B(0)A(t) \rangle. \]

(3.10)

It can be shown that the second definition in Eq. (3.10) is consistent with the first in the case of statistical equilibrium. For one has, from the definition, that

\[ F_{AB}(t) = Tr \{ \exp(-\gamma H) \exp(iHt) A \exp(-iHt) B \} / Tr[\exp(-\gamma H)] \]
\[ = Tr \{ \exp(-\gamma H) A \exp(iHt) B \exp(iHt) \} / Tr[\exp(-\gamma H)] \]
\[ = \langle A(0)B(-t) \rangle. \]

B. Spectral Representations

The spectral representation of the time correlation functions is obtained by considering the eigenfunctions \( |m\rangle \) and eigenvalues \( E_m \) of the Hamiltonian \( H \),

\[ (3.12) \quad H |m\rangle = E_m |m\rangle. \]
From the definitions, the time correlation functions in (3.10) can be written as

\[ F_{AB}(t) = \frac{\sum_m \langle m \mid \exp(-\beta H) \exp(iHt) A \exp(-iHt) B \mid m \rangle}{\sum_m \langle m \mid \exp(-\beta H) \mid m \rangle} \]

\[ = \left( \frac{1}{Q} \right) \sum_{m,n} \langle m \mid A \mid n \rangle \langle n \mid B \mid m \rangle \exp(-\beta E_m + iE_m t - iE_n t), \]

(3.14)

\[ F_{BA}(-t) = \left( \frac{1}{Q} \right) \sum_{m,n} \langle m \mid B \mid n \rangle \langle n \mid A \mid m \rangle \exp(-\beta E_m - iE_m t + iE_n t) \]

with

(3.15) \[ Q = \sum_m \exp(-\beta E_m). \]

By introducing the notation

(3.16) \[ J_{AB}(\omega) = \left( \frac{2\pi}{Q} \right) \sum_{m,n} \langle m \mid A \mid n \rangle \langle n \mid B \mid m \rangle \exp(-\beta E_m) \delta(E_m - E_n + \omega). \]

Eqs. (3.13) and (3.14) can be written as

(3.17) \[ F_{AB}(t) = \int_{-\infty}^{\infty} \left( \frac{d\omega}{2\pi} \right) J_{AB}(\omega) \exp(-i\omega t), \]

(3.18) \[ F_{BA}(-t) = \int_{-\infty}^{\infty} \left( \frac{d\omega}{2\pi} \right) \exp(-\beta \omega) J_{AB}(\omega) \exp(-i\omega t). \]
From Eqs. (3.15) and (3.16), the last equation can be written as

\[(3.19) \quad F_{BA}(-t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} J_{BA}(-\omega) \exp(-i\omega t),\]

or, by change of the integration variable,

\[(3.20) \quad F_{BA}(-t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} J_{BA}(\omega) \exp(i\omega t),\]

which again shows the self-consistency of the definition in Eq. (3.10). Thus, from Eqs. (3.18) and (3.19), the following identity holds:

\[(3.21) \quad \int_{-\infty}^{\infty} d\omega J_{BA}(\omega) \exp(i\omega t) = \int_{-\infty}^{\infty} d\omega \exp(i\omega) J_{AB}(-\omega) \exp(i\omega t).\]

From Eqs. (3.17) and (3.18), it follows that

\[(3.22) \quad \langle A(t)B(0) \rangle = \langle B(0)A(t + 1\beta) \rangle.\]

The time Fourier component, \(G_{AB}(\omega)\), of the causal Green's function \(G_{AB}(t)\) is defined by

\[(3.23) \quad G_{AB}(\omega) = \int_{-\infty}^{\infty} dt G_{AB}(t) \exp(i\omega t), (\omega \text{ real}).\]
Using Eqs. (3.3), (3.17), (3.18), and integrating, one can write Eq. (3.23) as

\[ (3.24) \quad G_{AB}(\omega) = \int_{-\infty}^{\infty} \left( \frac{d\omega^\prime}{2\pi} J_{AB}(\omega^\prime) \right) \left[ \frac{1}{\omega-\omega^\prime + i\epsilon} - \frac{\exp(-\beta\omega^\prime)}{\omega-\omega^\prime - 1\epsilon} \right] \]

with \( \epsilon = 0^+. \)

Using the symbolical identity

\[ (3.25) \quad \frac{1}{\omega-\omega^\prime \pm i\epsilon} = P \frac{1}{\omega-\omega^\prime} \mp i\pi \delta(\omega-\omega^\prime), \]

one can write Eq. (3.24) alternatively as

\[ (3.26) \quad G_{AB}(\omega) = \int_{-\infty}^{\infty} \frac{d\omega^\prime}{2\pi} \left[ 1 - \exp(-\beta\omega^\prime) \right] J_{AB}(\omega^\prime) \cdot \left[ P \frac{1}{\omega-\omega^\prime} - i\pi \frac{1 + \exp(-\beta\omega^\prime)}{1 - \exp(-\beta\omega^\prime)} \delta(\omega-\omega^\prime) \right], \]

where \( P \) means Cauchy's principal value of the integral. It follows, from Eq. (3.26), that

\[ \text{Re} \ G_{AB}(\omega) = (1/2\pi) \ P \int_{-\infty}^{\infty} \frac{d\omega^\prime}{2\pi} \left[ 1 - \exp(-\beta\omega^\prime) \right] \frac{J_{AB}(\omega^\prime)}{\omega-\omega^\prime}, \]

\[ (3.27) \quad \text{Im} \ G_{AB}(\omega) = -(1/2) \left[ 1 + \exp(-\beta\omega) \right] J_{AB}(\omega), \]

\[ \text{Re} \ G_{AB}(\omega) = (1/\pi) \ P \int_{-\infty}^{\infty} \frac{d\omega^\prime}{2\pi} \left[ 1 - \exp(-\beta\omega^\prime) \right] \frac{\text{Im} \ G_{AB}(\omega^\prime)}{[1 + \exp(-\beta\omega^\prime)](\omega^\prime - \omega)}. \]
C. Analytic Continuation of Green's Functions

The time-development operator \( \exp(-iHt) \) bears a strong formal similarity to the weighting factor \( \exp(-\beta H) \) that occurs in the canonical ensemble average. Indeed, for \( t = -i\beta \), the two are the same. By definition,

\[
G_{AB}(t) = -i \langle TA(t)B(0) \rangle
\]

(3.28) \[
= \begin{cases} 
-1 \langle A(t)B(0) \rangle & \text{for } t > 0 \\
-1 \langle B(0)A(t) \rangle & \text{for } t < 0.
\end{cases}
\]

Now

(3.29) \[-1 \langle A(t)B(0) \rangle = \frac{\text{Tr} \left[ \exp(-\beta H) \exp(iHt) A \exp(-iHt) B \right]}{\text{Tr} \left[ \exp(-\beta H) \right]} \]

is an analytic function for complex values of the time arguments in the region \( 0 > (\text{Im } t) > -\beta \). This analyticity follows directly from the assumption that the \( \exp(-\beta H) \) factor is sufficient to guarantee the absolute convergence of the trace for real time. Similarly the function \(-1 \langle B(0)A(t) \rangle\) is an analytic function in the region \( 0 < (\text{Im } t) < \beta \). To complete the definition of the Green's functions in the time domain \( 0 \leq \text{it} \leq \beta \), the definition of the time-ordering operator \( T \) is extended to mean "1 x t" ordering when the time is imaginary. The "further" down the imaginary axis a time is, the "later" it is. Then the Green's functions are well defined in the interval \( 0 \leq (\text{it}) \leq \beta \), and similarly in the interval...
0 \geq (it) \geq -\varepsilon$. Thus, the Green's function in the imaginary time domain can be defined as

\begin{equation}
G_{AB}(t) = \begin{cases} 
\langle A(t)B(0) \rangle \text{ for } (it) > 0 \\
\langle B(0)A(t) \rangle \text{ for } (it) < 0 
\end{cases}
\end{equation}

or

\begin{equation}
G_{AB}(\tau) = \langle TA(\tau)B(0) \rangle \text{ with } \tau = (it).
\end{equation}

The above argument is equivalent to the following replacements:

\begin{equation}
t \longrightarrow (-i\tau),
\end{equation}

\begin{equation}
G_{AB}(t) \longrightarrow -iG_{AB}(\tau) = -i \langle TA(\tau)B(0) \rangle.
\end{equation}

From the relation (3.22), by substituting $t = 0$, one gets

\[ \langle A(0)B(0) \rangle = \langle B(0)A(1\varepsilon) \rangle. \]

This is just the relationship between two boundary values of $G_{AB}(\tau)$:

\begin{equation}
G_{AB}(\tau = 0) = G_{AB}(\tau = 1\varepsilon).
\end{equation}

D. Periodic Property of Green's Functions of Imaginary Time Argument

In the imaginary time domain, the causal Green's function is defined as

\begin{equation}
G_{AB}(\tau) = \langle TA(\tau)B(0) \rangle, \quad -\varepsilon \leq \tau \leq \varepsilon.
\end{equation}
where $A(\tau) = [\exp(\tau H) A \exp(-\tau H)]$ and $T$ is the $\tau$-ordering operator. From the definition, for $\tau > 0$, one observes that

\begin{equation}
G_{AB}(\tau) = \langle B(0)A(\tau) \rangle
\end{equation}

\begin{equation}
= \frac{1}{Q} \text{Tr} [\exp(-\beta H) B \exp(\tau H - \beta H) A \exp(-\tau H + \beta H)]
\end{equation}

\begin{equation}
= \frac{1}{Q} \text{Tr} [\exp(-\beta H) \exp(\tau H) A \exp(-\tau H) B]
\end{equation}

\begin{equation}
= G_{AB}(\tau).
\end{equation}

And, for $\tau < 0$, one has

\begin{equation}
G_{AB}(\tau + \beta) = G_{AB}(\tau).
\end{equation}

From Eqs. (3.34) and (3.35) it follows that $G_{AB}(\tau)$ is a periodic function of period $\beta$, and the definition of $G_{AB}(\tau)$ can be extended outside the range $(-\beta, \beta)$. Actually, Eq. (3.32) is a particular case of this periodicity. This periodicity guarantees the following expansion:

\begin{equation}
G_{AB}(\tau) = \frac{1}{\beta} \sum_n G_{AB}(n) \exp(-i \omega_n \tau), \quad \omega_n = \frac{2\pi n}{\beta},
\end{equation}

\begin{equation}
G_{AB}(n) = \int_0^\beta G_{AB}(\tau) \exp(i \omega_n \tau) = \int_{-\beta}^{\beta_4} G_{AB}(\tau) \exp(i \omega_n \tau).
\end{equation}
The equation of motion for $G_{AB}(\tau)$ can be derived from the definition as follows:

\[(3.37)\]

\[
\frac{d}{d\tau} G_{AB}(\tau) = (\frac{d}{d\tau}) \left[ \Theta(\tau) \langle A(\tau)B(0) \rangle + \Theta(-\tau) \langle B(0)A(\tau) \rangle \right]
\]

\[
= \Theta'(\tau) \langle A(\tau)B(0) \rangle + \Theta'(-\tau) \langle B(0)A(\tau) \rangle
\]

\[
+ \langle T A'(\tau)B(0) \rangle
\]

\[
= S(\tau) \langle [A, B] \rangle + G_{AB}(\tau)
\]

where $A' = (\frac{d}{d\tau})A(\tau)$.

The analytic continuation of the equation of motion for $A(t)$ gives the equation of motion for $A(\tau)$:

\[(3.38)\]

\[
i(\frac{d}{dt})A(t) = [A(t), H(t)] \rightarrow (\frac{d}{d\tau})A(\tau) = [H(\tau), A(\tau)].
\]

Thus, the equation of motion for $G_{AB}(\tau)$ reads

\[(3.39)\]

\[
(\frac{d}{d\tau})G_{AB}(\tau) = S(\tau) \langle [A, B] \rangle + G_{AB}(\tau)
\]

\[
= S(\tau) \langle [A, B] \rangle + \langle T [H(\tau), A(\tau)] B \rangle.
\]

E. Green's Functions with a Periodic Perturbation

The reaction of a quantum-mechanical system with a time-independent Hamiltonian $H$, when an external perturbation $H_t$ is switched on, is considered in the following. The total Hamiltonian $H'$ is

\[(3.40)\]

\[
H' = H + H_t.
\]
where the second term is a time-dependent perturbation which is switched on adiabatically. It will be assumed to be very small and of the form

\[ H_t = \sum_{\alpha} \exp(\varepsilon t) \exp(-i\Omega t) V_\alpha \]

with \( \varepsilon = 0^+ \) so that

\[ H_t \bigg|_{t=-\infty} = 0, \]

and \( V_\alpha \) is an operator which does not explicitly depend on the time.

Now, the average value of the operator \( A \) is

\[ \langle A \rangle' = \text{Tr}(\varphi' A) \]

where \( \varphi' \) is a statistical operator satisfying the equation of motion

\[ i\frac{d}{dt} \varphi' = [H', \varphi'] = [H + H_t, \varphi'] \]

and the initial condition

\[ \varphi' \bigg|_{t=\infty} = \varphi = (1/\Omega) \exp(-\varphi H). \]

For Eq. (3.44), a solution of the form

\[ \varphi' = \varphi + \Delta\varphi \]
is desired. Then Eq. (3.44) reads

\begin{equation}
1 \frac{d}{dt} \Delta \varphi = [H, \Delta \varphi] + [H_t, \varphi],
\end{equation}

\begin{equation}
\Delta \varphi(t) \bigg|_{t=-\infty} = 0
\end{equation}

neglecting the higher order term \([H_t, \Delta \varphi]\).

Defining the operator

\begin{equation}
\Delta \varphi_1(t) = \exp(iHt) \Delta \varphi \exp(-iHt)
\end{equation}

and taking into account that \(\varphi\) and \(H\) commute, one finds

\begin{equation}
1 \frac{d}{dt} \Delta \varphi_1(t) = \exp(iHt) [H_t, \varphi] \exp(-iHt),
\end{equation}

\begin{equation}
\Delta \varphi_1(-\infty) = 0.
\end{equation}

So, after integration, one gets

\begin{equation}
\Delta \varphi(t) = -i \int_{-\infty}^{t} \exp(iHt' - iHt) [H_t', \varphi] \exp(-iHt' + iHt) \, dt'.
\end{equation}

Thus, the average value of the operator \(A\) is given by

\begin{equation}
\langle A \rangle' = \text{Tr}(\varphi A) + \text{Tr} [\Delta \varphi(t), A]
\end{equation}

\begin{equation}
= \langle A \rangle - i \text{Tr} \left[ \int_{-\infty}^{t} dt' \, \exp(iHt' - iHt) [H_t', \varphi] \exp(-iHt' + iHt), A \right]
\end{equation}

\begin{equation}
= \langle A \rangle + i \sum_{\alpha} \exp(-i\Omega t + it) \int_{-\infty}^{0} dt' \langle [V_\alpha(t'), A] \rangle \exp(-i\Omega t' + it')
\end{equation}

where \(V_\alpha(t) = \exp(iHt) V_\alpha \exp(-iHt)\).
Since $H'$ is time-dependent, one must be more careful in defining the Green's functions. At $t = -\infty$, the system has the unperturbed Hamiltonian $H$, and the subsequent motion is described by the time development operator $U(t, -\infty)$ which satisfies the equation of motion

\[(3.52) \quad i(\partial/\partial t) U(t, t') = H' U(t, t')\]

and the boundary condition

\[(3.53) \quad U(t, t) = 1.\]

In terms of $U(t, t')$, the Green's function is defined as

\[(3.54) \quad G_{AB}(t) = -i \text{Tr}[\rho(-\infty)U(-\infty, t)AU(t, 0)BU(0, -\infty)] \text{ for } t > 0\]
\[= -i \text{Tr}[\rho(-\infty)U(-\infty, 0)BU(0, t)AU(t, -\infty)] \text{ for } t < 0,\]

where $\rho(-\infty)$ is the density operator at $t = -\infty$ and is identical to the $\rho$ in Eq. (3.6). From the properties of density operator and time development operator, one observes that the above definition is consistent with that of the unperturbed system as given in Eq. (3.1).

It is straightforward to derive the equation of motion of $G_{AB}'(t)$ by use of the properties of $U(t, t')$ as given in Eqs. (3.52) and (3.53). The equation is

\[(3.55) \quad i(d/dt)G_{AB}'(t) = S(t)\langle A, B \rangle' - i \langle T [A(t), H'(t)]B(0) \rangle\]
where \( A(t) \) is the Heisenberg representation of the operator \( A \),

\[
A(t) = U(-\infty, t) A U(t, -\infty),
\]

and

\[
\langle [A, B] \rangle' = \text{Tr} [\varphi(-\infty) U(-\infty, t) [A, B] U(t, -\infty)]
\]

\[
= \text{Tr} ( \varphi' [A, B] )
\]

is the average of \([A, B]\) under perturbation as given in Eq. (3.43). The last step of Eq. (3.57) follows from the property of density operator,

\[
\varphi' = U(t, -\infty) \varphi(-\infty) U(-\infty, t).
\]

The same procedure as that of Eqs. (3.37)-(3.39) gives the equation of motion for \( G_{AB}'(\tau) \), the Green's function of imaginary time argument:

\[
(\frac{d}{d\tau}) G_{AB}'(\tau) = \delta(\tau) \langle [A, B] \rangle ' + \langle T [H'(\tau), A(\tau)] B(0) \rangle.
\]
IV. GREEN'S FUNCTION THEORY OF THE HEISENBERG ANTIFERROMAGNET

In this chapter Callen's work (1963) and Liu's work (1965) for ferromagnetism are extended to antiferromagnetism. Callen invented a decoupling scheme which is more desirable than the conventional random phase approximation for the zeroth order equation of motion for Green's functions. To calculate the longitudinal correlation functions by Liu's method, a perturbation calculation is necessary. A satisfactory extension of the Callen's decoupling scheme to first order equations is found. The sublattice magnetization, energy spectrum, Néel temperature, transverse correlation functions, perpendicular susceptibility, and correlation length are calculated for the general spin value $S$. The longitudinal correlation functions and parallel susceptibility are calculated for $S = 1/2$. For $S = 1/2$ and $T > T_N$, the rotational invariance of correlation functions and susceptibilities are shown, and the energy and specific heat are calculated.

A. Green's Functions for the Heisenberg Antiferromagnet

The problem to be considered is the statistical mechanics of the antiferromagnetic spin system described by the Heisenberg type interaction with isotropic exchange. In the low energy states, the lattice is divided into two sublattices with opposite magnetic moments, and all the nearest neighbors
of a spin belong to the other sublattice. The Hamiltonian for the model is

\[ (4.1) \quad H = \sum_{\alpha, \beta} J_{\alpha \beta} \vec{S}_{\alpha} \cdot \vec{S}_{\beta} \]

where \( \vec{S}_{\alpha} \) is the spin operator (in units of \( \hbar \)) for the ion at site \( \alpha \) of sublattice \( \alpha \); \( J_{\alpha \beta} \) is the exchange constant between ions at sites \( \alpha \) and \( \beta \) and is assumed to be a function only of the distance between ions. As usual, it is assumed that the self-exchange terms vanish. Thus, one assumes that

\[ (4.2) \quad J_{\alpha \alpha} = 0 \text{ and } J_{\alpha \beta} = J_{\beta \alpha}. \]

At this point the interaction is not restricted to nearest neighbors, but such a restriction will be made in a later stage of the calculation.

With the completely isotropic Hamiltonian (4.1) an antiferromagnetic state is degenerate, since the common direction of the resulting antiparallel magnetic moments of the two sublattices is arbitrary. This degeneracy cannot be removed by an external field. For a not too large external field, the spins would arrange themselves antiferromagnetically in a plane perpendicular to the external field, but the direction of the spins in the plane would still be arbitrary. In any real antiferromagnetic crystal this degeneracy is removed by the anisotropy which plays a much more important role here than in the ferromagnetic case. The anisotropy must be
introduced in the form of an effective anisotropy field which, however, is quite different from the corresponding ferromagnetic anisotropy field. It must be such that the spins on sublattice 1 are preferentially oriented in the +z direction, say, and those on sublattice 2 in the -z direction. This can be achieved by introducing a hypothetical field \( h = g \mu_B H_m \) pointing in the +z direction at the sites of sublattice 1, and in the -z direction at those of sublattice 2. The Hamiltonian becomes

\[
(4.1a) \quad H_a = H - h \left[ \sum_i S_{1i}^z - \sum_j S_{2j}^z \right].
\]

As will be shown in Section G, the algebra turns out to be exactly the same whether one uses (4.1) or (4.1a) when \( h \) is not too large. For this reason, (4.1) will be used for the analysis below the Néel temperature.

The causal Green's functions to be used in this section are defined as follows:

\[
(4.3) \quad G_{\alpha_1, \beta_1}(\tau) = \langle S_{\alpha_1}^{+} ; \exp(a S_{\beta_1}^{Z}) S_{\beta_1}^{-} \rangle = \langle T S_{\alpha_1}^{+}(\tau) \exp(a S_{\beta_1}^{Z}) S_{\beta_1}^{-} \rangle
\]

where \( \tau \) is the imaginary time variable \( \tau = (i\tau) \); \( T \) is the \( \tau \)-ordering operator defined in a previous section; \( a \) in the
exponent is a parameter; $S_{\alpha_1}^\tau(\tau)$ is the imaginary time version of the Heisenberg operator $S_{\alpha_1}^\tau(t)$ so that

\begin{equation}
(4.4) \quad S_{\alpha_1}^\tau(\tau) = \exp(\tau H) S_{\alpha_1}^\tau \exp(-\tau H)
\end{equation}

and

\begin{equation}
(4.5) \quad S_{\alpha_1}^\tau = S_{\alpha_1}^x \pm i S_{\alpha_1}^y.
\end{equation}

As shown in Eq. (3.39), the equation of motion for the Green's function is

\begin{equation}
(4.6) \quad \left(\frac{d}{d\tau}\right) G_{\alpha_1, \beta_1}(\tau) = \mathcal{S}(\tau) \left< \left[ S_{\alpha_1}^+, \exp(aS_{\beta_1}^z) S_{\beta_1}^- \right] \right> + \left< T \left[ H(\tau), S_{\alpha_1}^\tau(\tau) \right] \exp(aS_{\beta_1}^z) S_{\beta_1}^- \right>
\end{equation}

where

\begin{equation}
(4.7) \quad \theta_{\alpha_1}(a) = \left< [S_{\alpha_1}^+, \exp(aS_{\beta_1}^z) S_{\beta_1}^-] \right>.
\end{equation}

Noting that

\begin{align*}
[H(\tau), S_{\alpha_1}^\tau(\tau)] &= \left[ \exp(\tau H) H \exp(-\tau H), \exp(\tau H) S_{\alpha_1}^\tau \exp(-\tau H) \right] \\
&= \exp(\tau H) [H, S_{\alpha_1}^\tau] \exp(-\tau H)
\end{align*}
and the commutation relations

\[ [S_{\varphi}^+ J, S_{\varphi 1}^+] = 0, \]

\( [S_{\varphi}^-, S_{\varphi 1}^+] = -2 \sum \delta S_1^+ S_{\varphi 1}^z, \)

\[ [S_{\varphi}^z, S_{\varphi 1}^+] = \sum \delta S_1^+ S_{\varphi 1}^z, \]

one can reduce the last term of Eq. (4.6) as follows:

\( [H, S_{\varphi 1}^+] = 2 \sum_j \sum_{\chi_1, \chi_k} (s_{\chi_1}^+ s_{\chi_k}^z - s_{\chi_1}^z s_{\chi_k}^+). \)

Thus, from Eqs. (4.6) and (4.9), the equation of motion for the Green's function is given by

\[
\frac{\partial}{\partial \tau} \mathcal{G}^\alpha_{\chi_1, \varphi J}(\tau) = \mathcal{S}(\tau) \mathcal{S}_{\varphi} \mathcal{S}_1 \mathcal{G}^\alpha_{\chi_1}(\alpha) \\
+ 2 \sum_{\chi_k, \chi_1, \chi_k} \mathcal{T}[\mathcal{S}_{\chi_1}^+(\tau) \mathcal{S}_{\chi_k}^z(\tau) - \mathcal{S}_{\chi_1}^z(\tau) \mathcal{S}_{\chi_k}^+(\tau)] \exp(\alpha S_{\varphi}^z) S_{\varphi}^-.
\]

B. The Decoupling Approximation

As shown above, the equation of motion for the Green's function contains higher order Green's functions. The equations of motion for these Green's functions contain even higher order Green's functions. Thus the exact treatment of the equations of motion involves the solution of an infinite set of coupled equations for an infinite number of Green's
functions. Approximate solutions can be obtained by a de-
coupling procedure, in which the higher order Green's functions
on the right of Eq. (4.10) are expressed in terms of lower
order Green's functions so that Eq. (4.10) can be explicitly
solved for $G_{\alpha_1,\gamma_1}(\tau)$.

Two decoupling approximations have been studied by several
authors: the random phase approximation (RPA) and the Callen
decoupling approximation (CDA). In the random phase approx-
imation, the fluctuations of $S_{\alpha_1}^z$ are ignored, and the operator
$S_{\alpha_1}^z$ is replaced by its average value:

\begin{equation}
\langle T S_{\alpha_1}^z(\tau) S_{\tau \mathbf{k}}^+(\tau) B \rangle \rightarrow \langle S_{\alpha_1}^z(\tau) \rangle \langle T S_{\tau \mathbf{k}}^+(\tau) B \rangle.
\end{equation}

This approximation results in a disagreement with the low-
temperature theory and gives a constant perpendicular sus-
ceptibility below the Néel temperature (Lines, 1964).

Callen's approximation takes into account the fluctuations
of the operator around its statistical average, and it gives
better agreement with the low-temperature theory and a
slightly temperature-dependent perpendicular susceptibility.

For ferromagnetism, an investigation by Tahir-Kheli (1963)
revealed that the optimum decoupling to obtain agreement
with all available rigorous series-expansion results is Callen
decoupling with an additional inhomogeneous term. This
additional term is particularly large for $S = 1/2$, but for
other spin values its contribution is significant only in the vicinity of the Curie temperature.

In the present work, the Callen decoupling scheme is used. For ferromagnetism, Callen gives a heuristic argument from physical grounds to choose a proper decoupling scheme. If one tries to extend the argument to antiferromagnetism, an ambiguity comes in from the fact that there are two sublattices. The following is the corresponding argument for antiferromagnetism.

In the special case of $S = 1/2$, one has

\begin{align}
(4.12) & \quad S_{\alpha_1}^Z = S - S_{\alpha_1}^- S_{\alpha_1}^+, (S = 1/2), \\
(4.13) & \quad S_{\alpha_1}^Z = \frac{1}{2} (S_{\alpha_1}^+ S_{\alpha_1}^- - S_{\alpha_1}^- S_{\alpha_1}^+), \\
(4.14) & \quad S_{\alpha_1}^Z = - S + S_{\alpha_1}^+ S_{\alpha_1}^-, (S = 1/2),
\end{align}

or multiplying the first of these by an arbitrary parameter $b_{\alpha_1}$, the second by $(1 - b_{\alpha_1})$, and adding

\begin{equation}
(4.15) \quad S_{\alpha_1}^Z = b_{\alpha_1} S + \frac{1}{2} (1 - b_{\alpha_1}) S_{\alpha_1}^+ S_{\alpha_1}^- - \frac{1}{2} (1 + b_{\alpha_1}) S_{\alpha_1}^- S_{\alpha_1}^+, (S = 1/2).
\end{equation}

So far $b_{\alpha_1}$ is entirely arbitrary. One may choose it to depend on the lattice site $\alpha_1$ or some other lattice site appearing in the three spin Green's function. But, for convenience, the subscript $\alpha_1$ is attached to denote the possible dependence
on some lattice site. The Green's functions \( \langle S_{\alpha_1}^+ S_{\alpha_1}^- S_{\beta_1}^+ ; B \rangle \) and \( \langle S_{\alpha_1}^- S_{\alpha_1}^+ S_{\beta_1}^+ ; B \rangle \) are reasonably decoupled in the symmetric forms:

\begin{equation}
\langle S_{\alpha_1}^+ S_{\alpha_1}^- S_{\beta_1}^+ ; B \rangle \quad 1 \neq j \quad \longrightarrow \quad \langle S_{\alpha_1}^+ S_{\alpha_1}^- \rangle \langle S_{\beta_1}^+ ; B \rangle + \langle S_{\alpha_1}^- S_{\beta_1}^+ \rangle \langle S_{\alpha_1}^+ ; B \rangle,
\end{equation}

\begin{equation}
\langle S_{\alpha_1}^- S_{\alpha_1}^+ S_{\beta_1}^+ ; B \rangle \quad 1 \neq j \quad \longrightarrow \quad \langle S_{\alpha_1}^- S_{\alpha_1}^+ \rangle \langle S_{\beta_1}^+ ; B \rangle + \langle S_{\alpha_1}^- S_{\beta_1}^+ \rangle \langle S_{\alpha_1}^+ ; B \rangle,
\end{equation}

where the relation

\begin{equation}
\langle S_{\alpha_1}^+ S_{\beta_1}^+ \rangle = 0
\end{equation}

is used since \( S_{\alpha_1}^+ S_{\beta_1}^+ \) is not diagonal in the total z component of the spin. Thus, the identity (4.15) together with Eqs. (4.16) and (4.17) leads to

\begin{equation}
\langle S_{\alpha_1}^+ S_{\beta_1}^+ ; B \rangle \quad 1 \neq j \quad \longrightarrow \quad \langle S_{\alpha_1}^+ \rangle \langle S_{\beta_1}^+ ; B \rangle - b_{\alpha_1} \langle S_{\alpha_1}^- S_{\beta_1}^+ \rangle \langle S_{\alpha_1}^+ ; B \rangle.
\end{equation}

If \( b_{\alpha_1} \) is chosen as unity, the result corresponds to decoupling on the basis of identity (4.12); \( b_{\alpha_1} = 0 \) corresponds to decoupling on the basis of identity (4.13); \( b_{\alpha_1} = -1 \) corresponds to decoupling on the basis of the identity (4.14). Thus a suitable choice of \( b_{\alpha_1} \) may provide a correction to the random
phase approximation. Some physical criterion is required to select the proper value for $b_{\alpha_1}$.

The operator $S_{\alpha_1}^- S_{\alpha_1}^+$ in (4.12) represents the deviation of $S_{\alpha_1}^z$ from $S$. The operator $S_{\alpha_1}^+ S_{\alpha_1}^-$ in (4.14) represents that of $S_{\alpha_1}^z$ from $-S$. The operators $S_{\alpha_1}^- S_{\alpha_1}^+$ and $S_{\alpha_1}^+ S_{\alpha_1}^-$ are treated approximately in deriving Eq. (4.19). It is to be noted that the random phase approximation neglects these terms. It therefore seems reasonable to use Eq. (4.12) when $\langle S_{\alpha_1}^z \rangle \approx S$ and Eq. (4.14) when $\langle S_{\alpha_1}^z \rangle \approx -S$. Similarly, the operator $(S_{\alpha_1}^+ S_{\alpha_1}^- - S_{\alpha_1}^- S_{\alpha_1}^+)/2$ in Eq. (4.13) represents the deviation of $S_{\alpha_1}^z$ from zero; and it therefore is reasonable to use Eq. (4.13) as the basis of decoupling when $\langle S_{\alpha_1}^z \rangle \approx 0$.

All the above observations are contained in the choice

$$\text{(4.20) } b_{\alpha_1} = \frac{\langle S_{\alpha_1}^z \rangle}{S}, \ (S = 1/2),$$

or

$$\text{(4.21) } b_{\alpha_1} = -\frac{\langle S_{\alpha_1}^z \rangle}{S}, \ (S = 1/2),$$

where

$$\text{(4.22) } \alpha_1^\pm = \begin{cases} 2 & \text{for } \alpha = 1, \\ 1 & \text{for } \alpha = 2. \end{cases}$$

The ambiguity between Eqs. (4.20) and (4.21) arises from the fact that there are two sublattices in an antiferromagnet. Anderson and Callen (1964) claims that the first choice results in some internal inconsistency. The present work does not
produce any inconsistency with the first choice but the algebra is more complicated when an external d.c. field is applied to the system. For calculations of a.c. response one expects $b_{\alpha 1}$ to be $i$-dependent or $j$-dependent, $j$ being the other lattice site appearing in the higher order Green's function together with $i$. Without external field, the two choices, Eq. (4.20) or (4.21), are identical. The parameter $b_{\alpha 1}$ is taken to be

$$b_{\alpha 1} = -\frac{\langle S^z_{\sigma j} \rangle}{S} \text{ for } S = 1/2$$

which is the same as the Anderson-Callen decoupling for the higher order Green's function of an unperturbed system, and reduces to the Callen decoupling in ferromagnetism for the special case of nearest neighbor interactions. The final result is

$$\langle S^z_{\alpha 1} S^z_{\sigma j} ; B \rangle_{\alpha \neq j} \rightarrow \langle S^z_{\alpha 1} \rangle \langle S^z_{\sigma j} ; B \rangle + \frac{\langle S^z_{\alpha 1} \rangle}{S} \langle S^+_{\alpha 1} S^+_\sigma j \rangle \langle S^+_\alpha 1 ; B \rangle$$

for $S = 1/2$.

The author has carried out calculations based on Eq. (4.20) as well as (4.23). Only the latter are reported here. A posteriori advantages of Eq. (4.23) include continuity of correlation functions and susceptibility at the Néel temperature, and above the Néel temperature rotational invariance
of correlation functions and susceptibility and the validity of sum rule for spin operators.

To generalize the choice for $b_{\alpha_1}$ to higher spin, Eqs. (4.12) and (4.14) are replaced by

\begin{align}
(4.25) & \quad S_{\alpha_1}^z = S(S + 1) - (S_{\alpha_1}^z)^2 - S_{\alpha_1}^- S_{\alpha_1}^+, \\
(4.26) & \quad S_{\alpha_1}^z = -S(S + 1) + (S_{\alpha_1}^z)^2 + S_{\alpha_1}^+ S_{\alpha_1}^-,
\end{align}

with Eq. (4.13) unchanged

\begin{equation}
(4.27) \quad S_{\alpha_1}^z = \frac{1}{2} (S_{\alpha_1}^+ S_{\alpha_1}^- - S_{\alpha_1}^- S_{\alpha_1}^+).
\end{equation}

Decoupling as before, and neglecting the fluctuations of $(S_{\alpha_1}^z)^2$, one finds in this case as well,

\begin{equation}
(4.28) \quad \langle S_{\alpha_1}^z S_{\phi j}^+; B \rangle_{i \neq j} \rightarrow \langle S_{\alpha_1}^z \rangle \langle S_{\phi j}^+; B \rangle - b_{\alpha_1} \langle S_{\alpha_1}^- S_{\phi j}^+ \rangle \langle S_{\alpha_1}^+; B \rangle.
\end{equation}

The parameter $b_{\alpha_1}$ is deduced by the following requirements:

(a) For $S = 1/2$, $b_{\alpha_1}$ should reduce to $-\langle S_{\phi j}^z \rangle/S$.

(b) For $\langle S_{\alpha_1}^z \rangle = 0$, $b_{\alpha_1}$ should vanish. This follows from the fact that the identity (4.13) retains its interpretation for arbitrary $S$.

(c) For $\langle S_{\alpha_1}^z \rangle = \pm S$, one expects that $S_{\alpha_1}^z$ should have the form $S_{\alpha_1}^z = \pm(S - n_\alpha)$, where $n_\alpha$ is a deviation which is of order unity rather than of order $S$. 
Requirement (c) implies that \( b_\alpha <S^-_1 S^+_j> \) should be of order unity, rather than of order \( S_1 \), at low temperatures. 

Now \( <S^-_1 S^+_1>/2S \) is the approximate spin deviation as one can see from Eq. (2.57), so that \( <S^-_1 S^+_1> \) is of order \( 2S \); similarly \( <S^-_1 S^+_j> \) will be of order \( 2S \) if \( i \) and \( j \) are closely coupled. The choice

\[
(4.29) \quad \frac{1}{2S} \frac{<S^Z_i>}{S} = -\frac{<S^Z_\alpha I>}{2S^2}
\]

satisfies all the physical requirements above. Thus, for general \( S \), one has

\[
(4.30) \quad <S^Z_\alpha I S^+;B>_{i\neq j}
\]

\[
\rightarrow <S^Z_\alpha S^+;B> - (<S^Z_i>/2S^2) <S^-_1 S^+_1> <S^+_1;B>.
\]

C. Solution of Equations for the Green's Functions

The equation of motion for the Green's function

\[
G^a_{\alpha i, \beta j}(\tau)
\]

is given by Eq. (4.40):

\[
(4.31) \quad (d/d\tau) G^a_{\alpha i, \beta j}(\tau) = \Sigma(\tau) \Sigma_{\alpha\beta} \Sigma_{ij} \Theta_{\alpha i}(a)
\]

\[
+2 \sum_{i,j,k} <S^Z_i S^+_j; \exp(aS^Z_j) S^-_{\alpha k}> - <S^Z_\alpha S^+_j; \exp(aS^Z_j) S^-_{\alpha k}>]
\]

\[
\exp(aS^Z_j) S^-_{\alpha k} >
\]
with

\[ \Theta_{\alpha_1}(a) = \langle [S^{+}_{\alpha_1}, \exp(a S_{\alpha_1}^{z}) S^{-}_{\alpha_1}] \rangle. \]

After decoupling by (4.30), noting that

\[ \langle S^{z}_{\alpha_1}(\tau) \rangle = (1/Q) \text{Tr}[\exp(-\varphi H) \exp(\tau H) S^{z}_{\alpha_1} \exp(-\tau H)] \]

\[ = (1/Q) \text{Tr}[\exp(-\varphi H) S^{z}_{\alpha_1}] \]

\[ = \langle S^{z}_{\alpha_1} \rangle \]

and defining

\[ \psi_{\alpha_1, \gamma k}(\tau, a) = \langle \exp[a S^{z}_{\alpha_1}(\tau)] S^{-}_{\alpha_1}(\tau) S^{+}_{\gamma k}(\tau) \rangle \]

\[ = \langle \exp(a S^{z}_{\alpha_1}) S^{-}_{\alpha_1} S^{+}_{\gamma k} \rangle \]

\[ = \psi_{\alpha_1, \gamma k}(a). \]

one can write Eq. (4.31) as

\[ (d/d\tau) G^{a}_{\alpha_1, \beta j}(\tau) = \Delta(\tau) \sum_{\alpha \phi} S_{\alpha \phi} S^{+}_{1 j} \Theta_{\alpha_1}(a) \]

\[ -2 \sum_{\gamma k} J_{\alpha_1, \gamma k} \left\{ \langle S^{z}_{\alpha_1} \rangle \left[ 1 - \psi_{\gamma k, \alpha_1(0)}/2S^{2} \right] G^{a}_{\gamma k, \beta j}(\tau) \right\} \]

\[ = \psi_{\alpha_1, \gamma k}(0)/2S^{2} \].
These equations are a set of coupled equations for various pairs \((\nu_1, \nu_j)\) and \((\gamma_k, \nu_j)\). The periodicity of the Green's functions guarantees the expansion given in Eq. (3.36):

\[
G_{\alpha_1, \beta j}(\tau) = \frac{1}{\beta} \sum_n G_{\alpha_1, \beta j}(n) \exp(-i\omega_n \tau),
\]

\[
G_{\alpha_1, \beta j}(n) = \int_0^\beta d\tau G_{\alpha_1, \beta j}(\tau) \exp(i\omega_n \tau)
\]

After the transformation (4.35), Eq. (4.34) leads to

\[
-i\omega_n G_{\alpha_1, \beta j}(n) = \Theta_{\alpha_1} \Theta_{\beta j}(a)
\]

\[
-2 \sum_{\gamma k} \langle \nu_1 \nu_j \nu_{\gamma k} \rangle \left[ 1 - \nu_{\gamma k, \nu_1(0)/2s^2} \right] G_{\nu_{\gamma k}, \beta j}(n)
\]

\[
- \langle \nu_{\nu_{\gamma k}} \nu_j(0)/2s^2 \rangle G_{\nu_{\nu_{\gamma k}}, \beta j}(n)
\]

Translational invariance dictates consideration of the spatial Fourier transforms:

\[
G_{\alpha_1, \beta j}(n) = (2/N) \sum_{\vec{k}} G_{\alpha_\nu}(\vec{k}, n) \exp(i\vec{k} \cdot \vec{\nu}_1 - i\vec{k} \cdot \vec{\beta}_j),
\]

\[
G_{\alpha_\nu}(\vec{k}, n) = \sum_{\nu j} G_{\alpha_1, \beta j}(n) \exp(-i\vec{k} \cdot \vec{\nu}_1 + i\vec{k} \cdot \vec{\beta}_j);
\]
\[ J_{\alpha i, \beta j} = (2/N) \sum_{k} J_{\alpha \beta}(k) \exp(-i\vec{k} \cdot \vec{R}_{i} + i\vec{k} \cdot \vec{R}_{j}), \]

(4.38)

\[ J_{\alpha \beta}(k) = \sum_{i-j} J_{\alpha i, \beta j} \exp(i\vec{k} \cdot \vec{R}_{i} - i\vec{k} \cdot \vec{R}_{j}); \]

\[ \psi_{\alpha i, \beta j}(0) = (2/N) \sum_{k} \psi_{\alpha}(k, 0) \exp(-i\vec{k} \cdot \vec{R}_{i} + i\vec{k} \cdot \vec{R}_{j}), \]

(4.39)

\[ \psi_{\alpha \beta}(k, 0) = \sum_{i-j} \psi_{\alpha i, \beta j}(0) \exp(i\vec{k} \cdot \vec{R}_{i} - i\vec{k} \cdot \vec{R}_{j}); \]

where \( N/2 \) is the number of magnetic ions in each sublattice; \( \vec{k} \cdot \vec{R} \) denotes the dot product \( \vec{k} \cdot \vec{R}_{i} \) with \( \vec{R}_{i} \) being the position vector of the site \( i \) in sublattice \( \alpha \).

From the reasons discussed in the introduction, only nearest neighbor interactions are assumed from now on. This effect comes in \( J_{\alpha i, \beta j} \), so that one gets

(4.40) \[ J_{\alpha i, \beta j} = \sum_{\vec{s}(\alpha \pm 1)} \sum_{j(\pm 2)} J \]

where \( \vec{s} \) is a nearest neighbor vector. Eqs. (4.37) and (4.39) are unchanged, but Eq. (4.38) leads to

\[ J_{11}(\vec{k}) = J_{22}(\vec{k}) = 0, \]

(4.41) \[ J(\vec{k}) = J_{12}(\vec{k}) = J_{21}(\vec{k}) = J \sum_{\vec{s}} \exp(i\vec{k} \cdot \vec{s}), \]

\[ J = (2/N) \sum_{k} \exp(-i\vec{k} \cdot \vec{s}), \]
and if there exists a center of symmetry for the lattice

\[(4.42) \quad J(\vec{k}) = J(-\vec{k}).\]

It is convenient to define \( \gamma(\vec{k}) \), a function of \( \vec{k} \) and lattice structure, by

\[(4.43) \quad \gamma(\vec{k}) = \left( \frac{1}{z} \right) \sum_{\vec{r}} \exp(i\vec{k} \cdot \vec{r}) = \gamma(-\vec{k}),\]

\( z \) being the number of nearest neighbors. For simple cubic structure, \( \gamma(\vec{k}) \) is of the form

\[(4.44) \quad \gamma(\vec{k}) = \left( \frac{1}{3} \right) \left[ \cos(k_x a) + \cos(k_y a) + \cos(k_z a) \right],\]

and for the body centered cubic structure,

\[(4.45) \quad \gamma(\vec{k}) = \cos(k_x a/2) \cos(k_y a/2) \cos(k_z a/2),\]

where \( a \) is the smallest period of the structure in the \( x \)-, \( y \)-, and \( z \)-directions. It is evident that

\[(4.46) \quad \gamma(0) = 1 \text{ and } J(\vec{k}) = J(0) \gamma(\vec{k}) = 2J \gamma(\vec{k}).\]

The translational invariance implies that \( \Theta_{x_1}(a) \) and \( \langle S_{x_1}^z \rangle \) are independent of \( i \):

\[
\Theta_{x_1}(a) = \langle [S_{x_1}^+, \exp(aS_{x_1}^z)] S_{x_1}^- \rangle = \Theta_s(a), \quad \Theta_s(0) = 2m_s,
\]

\[(4.47) \quad \langle S_{x_1}^z \rangle = m_s,\]
where \( m_\alpha \) is the sublattice magnetization per spin in the sublattice \( \alpha \).

After the spatial Fourier transformation, Eq. (4.36) leads to

\[
- 1 \omega_n g^{\alpha_\beta}_{\chi, \phi}(\overline{k}, n) = \sum_{\chi} g_{\chi}(a)
\]

\[
+ 2m_\gamma \left[ J(0) - \frac{J(0)}{2S^2} \frac{2}{N} \sum_{k'} \gamma(\overline{k}^\prime) \gamma(\overline{k}^\prime, 0) \right] g^{\alpha}_{\chi}(\overline{k}, n)
\]

\[
- 2m_\gamma \left[ J(\overline{k}) - \frac{J(0)}{2S^2} \frac{2}{N} \sum_{k'} \gamma(\overline{k}^\prime - \overline{k}) \gamma(\overline{k}^\prime, 0) \right] g^{\alpha}_{\chi}(\overline{k}, n)
\]

with \( \alpha \neq \gamma \). It is convenient to define \( A(\overline{k}) \) by

\[
A(\overline{k}) = 2m_\gamma \left[ J(\overline{k}) - \frac{1}{2S^2} \frac{2}{N} \sum_{k'} \gamma(\overline{k}^\prime - \overline{k}) \gamma(\overline{k}^\prime, 0) \right] (\alpha \neq \gamma).
\]

It can be shown (Appendix B) that

\[
\frac{1}{N} \sum_{k'} \gamma(\overline{k}^\prime - \overline{k}) \gamma(\overline{k}^\prime, 0) = \gamma(\overline{k}) \frac{1}{N} \sum_{k'} \gamma(\overline{k}^\prime) \gamma(\overline{k}^\prime, 0),
\]

so that, noting that \( m_1 = - m_2 = m \), one has

\[
A_1(\overline{k}) = - A_2(\overline{k}) = A(\overline{k})
\]

where

\[
A(\overline{k}) = \gamma(\overline{k}) A(0) = \gamma(\overline{k}) 2mJ(0) \left[ 1 - \frac{1}{2S^2} \frac{2}{N} \sum_{k'} \gamma(\overline{k}^\prime) \gamma(\overline{k}^\prime, 0) \right].
\]
The solution of Eq. (4.48) is

\[ G_{11}(\bar{k},n) = -\frac{\Theta_1(a)}{\Delta(\bar{k},n)} [A(0) + i\omega_n], \]

\[ G_{21}(\bar{k},n) = \frac{\Theta_1(a)}{\Delta(\bar{k},n)} A(\bar{k}), \]

(4.54)

\[ G_{12}(\bar{k},n) = -\frac{\Theta_2(a)}{\Delta(\bar{k},n)} A(\bar{k}), \]

\[ G_{22}(\bar{k},n) = \frac{\Theta_2(a)}{\Delta(\bar{k},n)} [A(0) - i\omega_n], \]

with

(4.55) \[ \Delta(\bar{k},n) = (\omega_k - i\omega_n)(\omega_k - i\omega_n), \]

(4.56) \[ \omega_k = [A^2(0) - A^2(\bar{k})]^{1/2} = A(0) [1 - \gamma^2(\bar{k})]^{1/2}. \]

Eq. (4.54) can, alternatively, be written as

(4.57)

\[ G_{11}(\bar{k},n) = \frac{\Theta_1(a)}{2} \left\{ \left[ 1 + \frac{A(0)}{\omega_k} \right] \frac{1}{\omega_k - i\omega_n} + \left[ 1 - \frac{A(0)}{\omega_k} \right] \frac{1}{-\omega_k - i\omega_n} \right\}, \]

\[ G_{21}(\bar{k},n) = -\frac{\Theta_1(a) A(\bar{k})}{2\omega_k} \left\{ \frac{1}{\omega_k - i\omega_n} - \frac{1}{-\omega_k - i\omega_n} \right\}, \]

\[ G_{12}(\bar{k},n) = \frac{\Theta_2(a) A(\bar{k})}{2\omega_k} \left\{ \frac{1}{\omega_k - i\omega_n} - \frac{1}{-\omega_k - i\omega_n} \right\}, \]

\[ G_{22}(\bar{k},n) = \frac{\Theta_2(a)}{2} \left\{ \left[ 1 - \frac{A(0)}{\omega_k} \right] \frac{1}{\omega_k - i\omega_n} + \left[ 1 + \frac{A(0)}{\omega_k} \right] \frac{1}{-\omega_k - i\omega_n} \right\}. \]
The Green's functions in the r-representation are found by

\[(4.58) \quad G^a_{\kappa}(\vec{r}, \tau) = \langle 1/\phi \rangle \sum_n G^a_{\kappa}(\vec{r},n) \exp(-i\omega_n \tau), \quad \omega_n = (2\pi n/\phi).\]

Since it can be shown (Appendix C) that

\[(4.59) \quad \frac{1}{\phi} \sum_n \exp(-i\omega_n \tau)\frac{\exp(i\omega_k \tau)}{1 - \exp(i\beta\omega_k)} = \frac{\exp(i\omega_k \tau)}{1 - \exp(\beta\omega_k)}.

Eq. (4.57) leads to

\[(4.60) \quad G^a_{11}(\vec{r}, \tau) = \frac{\Theta_1(a)}{2} \left\{ \left[ 1 + \frac{A(0)}{\omega_k} \right] \frac{\exp(-\omega_k \tau)}{1 - \exp(-\beta\omega_k)} + \left[ 1 - \frac{A(0)}{\omega_k} \right] \frac{\exp(\omega_k \tau)}{1 - \exp(\beta\omega_k)} \right\},\]

\[G^a_{21}(\vec{r}, \tau) = -\frac{\Theta_1(a)A(\vec{r})}{2\omega_k} \left[ \frac{\exp(-\omega_k \tau)}{1 - \exp(-\beta\omega_k)} - \frac{\exp(\omega_k \tau)}{1 - \exp(\beta\omega_k)} \right],\]

\[G^a_{12}(\vec{r}, \tau) = \frac{\Theta_2(a)A(\vec{r})}{2\omega_k} \left[ \frac{\exp(-\omega_k \tau)}{1 - \exp(-\beta\omega_k)} - \frac{\exp(\omega_k \tau)}{1 - \exp(\beta\omega_k)} \right],\]

\[G^a_{22}(\vec{r}, \tau) = \frac{\Theta_2(a)}{2} \left\{ \left[ 1 - \frac{A(0)}{\omega_k} \right] \frac{\exp(-\omega_k \tau)}{1 - \exp(-\beta\omega_k)} + \left[ 1 + \frac{A(0)}{\omega_k} \right] \frac{\exp(\omega_k \tau)}{1 - \exp(\beta\omega_k)} \right\}.

One notes that

\[(4.61) \quad \frac{\Theta_1(0)}{2} = \langle [S^+_{11}, S^-_{11}] \rangle = 2m_1 = -2m_2 = -\Theta_2(0),\]
which follows from the periodicity of Green's functions in the imaginary time argument. One observes from Eq. (4.60) that

\[(4.63)\quad G_{12}(\vec{k}, \tau) = G_{12}^0(\vec{k}, \tau),
G_{22}(\vec{k}, \tau^-) = G_{11}^0(\vec{k}, \tau^+),
\]

\[(4.64)\quad G_{12}^0(\vec{k}, \tau^-) = G_{12}^0(\vec{k}, \tau^+) = G_{12}^0(\vec{k}, \tau^-) = G_{21}^0(\vec{k}, \tau^-).\]

From definitions given in Eqs. (4.3), (4.33), (4.37), and (4.39), it follows that

\[(4.65)\quad \psi_{\alpha}(\vec{k}, a) = G_{\alpha\alpha}^\alpha(\vec{k}, \tau = \tau^-);\]

and, in particular, Eq. (4.63) guarantees that

\[(4.66)\quad \psi_{12}(\vec{k}, 0) = \psi_{21}(\vec{k}, 0).\]

Eq. (4.65), together with Eq. (4.56) defining \(\omega_k\), and Eq. (4.47) defining \(\theta(a)\), are the basic equations of the theory. They must, however, be augmented by an explicit relationship between \(\psi\) and \(\theta\), and it is this step which complicates the problem for \(S > 1/2\).
From definitions, one gets

\[ T(\tau = 0^-) = \frac{2}{N} \sum_k G^0_{\kappa\kappa}(\vec{k}, \tau = 0^-) \]

\[ = \langle s_{\alpha_1}^- s_{\alpha_1}^+ \rangle \]

\[ (4.67) \]

\[ = S(S + 1) - \langle (s_{\alpha_1}^z)^2 \rangle - m_\alpha \]

\[ = 1/2 - m_\alpha \text{ for } S = 1/2, \]

\[ G^0_{\kappa\kappa}(\tau = 0^+) = \frac{2}{N} \sum_k G^0_{\kappa\kappa}(\vec{k}, \tau = 0^+) \]

\[ = \langle s_{\alpha_1}^+ s_{\alpha_1}^- \rangle \]

\[ (4.68) \]

\[ = S(S + 1) - \langle (s_{\alpha_1}^z)^2 \rangle + m_\alpha \]

\[ = 1/2 + m_\alpha \text{ for } S = 1/2. \]

Thus, for the case of \( S = 1/2 \), \( \frac{N}{2} G^0_{11}(\tau = 0^-) \) and \( \frac{N}{2} G^0_{22}(\tau = 0^+) \) can be interpreted as the total number of spin reversals in each sublattice. Then \( G^0_{11}(\vec{k}, 0^-) \) and \( G^0_{22}(\vec{k}, 0^+) \) are the occupation numbers of elementary excitation of wave vector \( \vec{k} \) in each sublattice. This interpretation is no longer quite so evident for \( S > 1/2 \) because of the additional term \( \langle (s_{\alpha_1}^z)^2 \rangle \) in Eqs. \( (4.67) \) and \( (4.68) \). From symmetry one expects occupation numbers to be equal in pairs, corresponding to the two sublattices, and in fact Eq. \( (4.64) \) confirms it.
Since

\[(4.69) \quad \Theta_1(0) = 2m_1 = - 2m_2 = - \Theta_2(0) = 2m \text{ for } S = 1/2,\]

Eqs. (4.65) and (4.69) determine \(\psi_{12}(k,0) = \psi_{21}(k,0)\) as a function of \(m\), and Eq. (4.67) or (4.68) provides a requirement of self-consistency which determine \(m\).

D. Relationship of \(\Theta_\alpha(\alpha)\) to \(m_\alpha\)

By exploiting the functional dependence of \(\Theta_\alpha(\alpha)\) and the quantity

\[(4.70) \quad \psi_{\alpha\phi}(\alpha) = \langle \exp(\alpha S_1^{Z_{\alpha}}) \rangle \]

on the parameter \(\alpha\), both \(\Theta_\alpha(\alpha)\) and \(\psi_{\alpha\phi}(\alpha)\) can be explicitly related to \(m_\alpha\) for arbitrary \(S\), in close analogy with the case of \(S = 1/2\). This approach is originally due to Callen (1963).

It is convenient to introduce the quantity

\[(4.71) \quad \Omega_\alpha^{\alpha}(\alpha) = \langle \exp(\alpha S_1^{Z_{\alpha}}) \rangle \]

and the notation

\[(4.72) \quad D = (d/\alpha a).\]
Then it can be shown (Callen, 1963) that

\[(4.73)\]
\[
\Theta_\alpha(a) = \langle [S_{\alpha_1}^+, \exp(as_{\alpha_1}^Z) S_{\alpha_1}^-] \rangle
\]
\[= [S(S + 1)(e^{-a} - 1) + (e^{-a} + 1)D - (e^{-a} - 1)D^2] \Omega_\alpha(a)\]

\[(4.74)\]
\[
\bar{\psi}_{\alpha_1}(a) = \langle \exp(as_{\alpha_1}^Z) S_{\alpha_1}^- S_{\alpha_1}^+ \rangle
\]
\[= [S(S + 1) - D - D^2] \Omega_\alpha(a) .\]

It is to be observed from Eq. (4.57) or (4.60) that the Green's function is a product of two functions, one of which depends only on \(k\) and the other only on \(a\). The same is true for \(\varphi_{\alpha_1}(k,a)\), according to Eq. (4.65). Hence by defining

\[(4.75)\]
\[
\varphi_{\alpha_1}(k) = \frac{G_{\alpha_1}^a(k, \tau = 0^-)}{\Theta_\alpha(a)}\]

which is independent of \(a\), \(\varphi_{\alpha_1}(k,a)\) is cast into a convenient form:

\[(4.76)\]
\[
\psi_{\alpha_1}(k,a) = \varphi_{\alpha_1}^a(k, 0^-)
\]
\[= \Theta_\alpha(a) \varphi_{\alpha_1}(k) .\]
The self-consistency requirement on Green's functions is now contained in the condition

$$
\varphi_{\alpha\varphi}(a) = (2/N) \sum_k G_{\alpha\varphi}(\vec{k}, 0^-)
$$

(4.77)

$$
= \Phi(a) \Phi_{\alpha\varphi}
$$

with

(4.78) \[ \Phi_{\alpha\varphi} = (2/N) \sum_k \Phi_{\alpha\varphi}(\vec{k}), \]

and it is evident that

$$
\Phi_{21} = \Phi_{12} = 0
$$

(4.79)

$$
\varphi_{12}(a) = \varphi_{21}(a).
$$

Explicit expressions for the quantity \( \Phi_{\alpha\varphi}(\vec{k}) \) are given by

(4.80)

\( \Phi_{11}(\vec{k}) = \frac{1}{2} \left[ 1 + \frac{A(0)}{\omega_k} \right] N(\omega_k) + \frac{1}{2} \left[ 1 - \frac{A(0)}{\omega_k} \right] N(-\omega_k), \)

\( \Phi_{12}(\vec{k}) = -\frac{1}{2} \frac{A(\vec{k})}{\omega_k} \left[ N(\omega_k) - N(-\omega_k) \right], \)

\( \Phi_{21}(\vec{k}) = -\Phi_{12}(\vec{k}), \)

\( \Phi_{22}(\vec{k}) = \frac{1}{2} \left[ 1 - \frac{A(0)}{\omega_k} \right] N(\omega_k) + \frac{1}{2} \left[ 1 + \frac{A(0)}{\omega_k} \right] N(-\omega_k). \)
with

\[(4.81) \quad N(\omega_k) = \left[ \exp(\beta \omega_k) - 1 \right]^{-1}. \]

Since

\[2N(\omega_k) + 1 = \coth(\beta \omega_k/2), \]

Eq. (4.80) can, alternatively, be written as

\[\Phi_{11}(E) = \frac{1}{2} \left[ -1 + \coth(\beta \omega_k/2)A(0)/\omega_k \right], \]

\[(4.82) \quad \Phi_{21}(E) = -\Phi_{12}(E) = \coth(\beta \omega_k/2)A(E)/2\omega_k, \]

\[\Phi_{22}(E) = \frac{1}{2} \left[ -1 - \coth(\beta \omega_k/2)A(0)/\omega_k \right]. \]

Because of Eq. (4.79), the condition (4.77) leads to only two equations

\[(4.83) \quad \overline{\Phi}_{\alpha \alpha}(a) = \Theta_\alpha(a) \Phi_{\alpha \alpha} \quad (\alpha = 1, 2) \]

which should determine \(\Theta_\alpha(a)\), and hence \(m_\alpha = \Theta_\alpha(0)/2\).

But it is more convenient to determine \(\Theta_\alpha(a)\), and thence to find \(\Theta_\alpha(a)\) by Eq. (4.73). In fact, from Eqs. (4.73), (4.74), and (4.83), it follows that

\[\left[ S(s + 1) - D - D^2 \right] \Theta_\alpha(a) \]

\[= \Phi_{\alpha}[S(s + 1)(e^{-a} - 1) + (e^{-a} + 1)D - (e^{-a} - 1)D^2]\Theta_\alpha(a)\]
or

\[(4.84)\]
\[D^2 \Omega_\alpha(a) + \frac{(1 + \phi_\alpha)e^a + \phi_\alpha}{(1 + \phi_\alpha)e^a - \phi_\alpha} D \Omega_\alpha(a) - S(S + 1) \Omega_\alpha(a) = 0\]

with the two boundary conditions

\[(4.85)\]
\[\Omega_\alpha(0) = 1\]

\[(4.86)\]
\[\left[ \prod_{p = -S}^{S} (D - p) \Omega_\alpha(a) \right]_{a = 0} = 0.\]

The first condition follows from the definition \((4.71)\), and

the second comes from the well-known operator identity

\[(4.87)\]
\[\left[ \prod_{p = -S}^{S} (S^z_{\alpha 1} - p) \right] = 0.\]

Callen gives the solution:

\[(4.88)\]
\[\Omega_\alpha(a) = \frac{(\phi_\alpha)^{2S+1}e^{-S} - (1 + \phi_\alpha)^{2S+1}(S+1)e^a}{[(\phi_\alpha)^{2S+1} - (1 + \phi_\alpha)^{2S+1}][(1 + \phi_\alpha)e^a - \phi_\alpha]}\]

from which the sublattice magnetization \(m_\alpha\) and the quantity \(\Theta_\alpha(a)\) can be obtained by differentiation.
For example, \(m_\alpha = \langle S_{\alpha 1}^Z \rangle \) is given by

\[
(4.89) \quad m_\alpha = [D \mathcal{O}_\alpha(a)]_{a = 0} = \frac{(S - \Phi_\alpha)(1 + \Phi_\alpha)^{2S+1} + (S + 1 + \Phi_\alpha)(\Phi_\alpha)^{2S+1}}{(1 + \Phi_\alpha)^{2S+1} - (\Phi_\alpha)^{2S+1}}.
\]

It is observed, from Eq. (4.82), that

\[
(4.90) \quad \Phi_{11} = -(1 + \Phi_{22}).
\]

The substitution of Eq. (4.90) into Eq. (4.88) gives

\[
(4.91) \quad \mathcal{O}_2(a) = \mathcal{O}_1(-a),
\]

so that \(m_2 = [D \mathcal{O}_2(a)]_{a = 0} = -[D \mathcal{O}_1(a)]_{a = 0} = -m_1\) as expected.

For \(S = 1/2\), it is not necessary to go through the above procedure with parameter \(a\), and the calculation simplifies as mentioned at the end of the previous section.

E. Energy Spectrum, Sublattice Magnetization, and Transverse Correlation Functions

The energy spectrum is given by Eq. (4.56):

\[
(4.92) \quad \omega_k = A(0)[1 - \gamma^2(k)]^{1/2} = 2SJ(0)R[1 - \gamma^2(k)]^{1/2}
\]
where

\[ R = \frac{(m/S)}{1 - (1/2S^2)(2/N) \sum_{k'} \gamma(k') \psi(k',0)} \]  

(4.93)

is the renormalization factor for energy spectrum. \( R = (m/S) \) is the result of decoupling by RPA, while \( R = 1 \) corresponds to non-interacting spin-wave theory.

The sublattice magnetization is given by Eq. (4.89):

\[ m_s = \frac{(S - \phi_n)(1 + \phi_n)^{2S+1} + (S + 1 + \phi_n)(\phi_n)^{2S+1}}{(1 + \phi_n)^{2S+1} - (\phi_n)^{2S+1}} \]

(4.94)

\[ m_s \bigg|_{S = 1/2} = 1/2(1 + \phi_n) \]

with

\[ \phi_n = \frac{(2/N) \sum_k \phi_{11}(\vec{k})}{(1/N) \sum_k \phi_{22}(\vec{k})} = (1/N) \sum_k \left[ \frac{-1 + \coth(\phi_n/2)A(0)/\omega_k}{1 - \coth(\phi_n/2)A(0)/\omega_k} \right]. \]

(4.95)

In the subsequent calculations, it is convenient to introduce the Fourier transform of spin operators by

\[ \vec{S}_{\alpha,k} = \sum_{\alpha} \vec{S}_{\alpha,1} \exp(-i\vec{k} \cdot \vec{r}) \],

(4.96)

\[ \vec{S}_{\alpha,1} = (2/N) \sum_k \vec{S}_{\alpha,k} \exp(i\vec{k} \cdot \vec{r}). \]
Then, from Eqs. (4.3), (4.35), (4.37), (4.75), and (4.82), one gets

\begin{align}
(4.97) \quad \langle S^\alpha_{\alpha, -k} S^\alpha_{\alpha, k} \rangle &= (N/2) G^{0}_{\beta, \alpha} (\vec{k}, 0^-) = (N/2) \Theta_{\alpha}(0) \Phi_{\alpha}(\vec{k}) \\
(4.98) \quad \langle S^\alpha_{\alpha, -k} S^\alpha_{\alpha, k} \rangle &= (N/2) G^{0}_{\alpha, \alpha} (-\vec{k}, 0^+).
\end{align}

Explicit expressions for Eqs. (4.97) and (4.98) are

\begin{align}
(4.99) \quad \langle S^\alpha_{\alpha, -k} S^\alpha_{\alpha, k} \rangle &= m(N/2) \left[ \coth(\beta \omega_k/2) A(0)/\omega_k - 1 \right], \\
(4.100) \quad \langle S^\alpha_{\alpha, -k} S^\alpha_{\alpha, k} \rangle &= \langle S^\alpha_{\alpha, -k} S^\alpha_{\alpha, k} \rangle = -m(N/2) \coth(\beta \omega_k/2) A(\vec{k})/\omega_k, \\
\langle S^\alpha_{\alpha, -k} S^\alpha_{\alpha, k} \rangle &= m(N/2) \left[ \coth(\beta \omega_k/2) A(0)/\omega_k + 1 \right].
\end{align}

From Eqs. (4.3), (4.35), (4.37), and (4.75), it follows that

\begin{align}
(4.101) \quad \langle S^\alpha_{\alpha, -k} S^\alpha_{\alpha, k} \rangle &= \langle S^\alpha_{\alpha, -k} S^\alpha_{\alpha, k} \rangle, \\
\langle S^\alpha_{\alpha, -k} S^\alpha_{\alpha, k} \rangle &= \langle S^\alpha_{\alpha, -k} S^\alpha_{\alpha, k} \rangle = \langle S^\alpha_{\alpha, -k} S^\alpha_{\alpha, k} \rangle, \\
\langle S^\alpha_{\alpha, -k} S^\alpha_{\alpha, k} \rangle &= \langle S^\alpha_{\alpha, -k} S^\alpha_{\alpha, k} \rangle.
\end{align}
and explicit expressions turn out to be

$$(4.102) \langle S_{\alpha}^{-} S_{\beta}^{+} \rangle = (2/N)^{2} \sum_{k} \exp(-i\mathbf{k} \cdot \mathbf{a} + i\mathbf{k} \cdot \mathbf{b}) \langle S_{\alpha}^{-}, -k S_{\beta}^{+}, k \rangle$$

with $\langle S_{\alpha}^{-}, -k S_{\beta}^{+}, k \rangle$ given in Eq. (4.99), as expected from the definition of Fourier transform of spin operators. For the pairing of the same lattice site or nearest neighbors, Eq. (4.102) reduces to

$$(4.103)$$

$$\langle S_{11}^{-} S_{11}^{+} \rangle = m(2/N) \sum_{k} \left\{1 - \gamma^{2}(\mathbf{k}) \right\}^{-1/2} \coth(\beta \omega_{k}/2) - 1$$

$$\langle S_{21}^{-} S_{21}^{+} \rangle = m(2/N) \sum_{k} \left\{1 - \gamma^{2}(\mathbf{k}) \right\}^{-1/2} \coth(\beta \omega_{k}/2) + 1$$

$$\langle S_{12}^{-} S_{21}^{+} \rangle = \langle S_{21}^{-} S_{12}^{+} \rangle$$

$$= (1/z) \sum_{k} \langle S_{11}^{-} S_{12}^{+} \rangle$$

$$= - m(2/N) \sum_{k} \frac{\gamma^{2}(\mathbf{k})}{[1 - \gamma^{2}(\mathbf{k})]^{1/2}} \coth(\beta \omega_{k}/2).$$

Since from Eqs. (4.76) and (4.82)

$$\psi(\mathbf{k}, 0) = \psi_{12}(\mathbf{k}, 0) = \psi_{21}(\mathbf{k}, 0)$$

(4.104)

$$= \Theta_{1}(0) \phi_{12}(\mathbf{k})$$

$$= - m \coth(\beta \omega_{k}/2) A(\mathbf{k}) / \omega_{k},$$
one finds

\begin{equation}
(4.105) \\
R = \left(\frac{m}{S}\right) \left[ 1 + \left(\frac{m}{2S^2}\right) \frac{2(\frac{r}{k})}{2/N} \frac{\gamma^2(\frac{r}{k})}{1 - \gamma^2(\frac{r}{k})} \coth(\beta\omega_k/2) \right].
\end{equation}

Thus, for arbitrary spin \( S \), temperature \( T \), and nearest neighbor interaction \( J \), the quantities \( \omega_k \), \( m \), and the correlation functions are completely determined via a set of coupled equations: Eqs. (4.92), (4.94), (4.101), and (4.105).

For \( S = 1/2 \), these equations are

\begin{equation}
(4.106) \\
\omega_k = 2mzJ \left[ 1 + 2m(2/N) \sum_k \frac{\gamma^2(\frac{r}{k})}{1 - \gamma^2(\frac{r}{k})} \coth(\beta\omega_k/2) \right],
\end{equation}

\[ m = \frac{1}{2}(1 + \phi_{11}), \]

\[ \phi_{11} = \frac{1}{2} \left[ (2/N) \sum_k \frac{1}{1 - \gamma^2(\frac{r}{k})} \coth(\beta\omega_k/2) - 1 \right], \]

and

\[ \langle S_{1i}^- S_{1i}^+ \rangle = 2m \phi_{11}, \]

\[ \langle S_{2i}^- S_{2i}^+ \rangle = 2m(\phi_{11} - 1), \]

\begin{equation}
(4.107) \\
\langle S_{1i}^- S_{2(1+i)}^+ \rangle = \langle S_{2i}^- S_{1(1+i)}^+ \rangle \\
= -m(2/N) \sum_k \frac{\gamma^2(\frac{r}{k})}{1 - \gamma^2(\frac{r}{k})} \coth(\beta\omega_k/2).
\end{equation}
Calculations of $m$ and $R$ have been carried out according to Eqs. (4.105) and (4.106), and results are shown in Figs. 1, 2, 3, and 4.

1. Properties at the Neel temperature

Just below the Neel temperature the average sublattice magnetization $m_\alpha$ is vanishingly small, and $\Phi_\alpha$ becomes very large since

$$\omega_k \to 0 \quad \text{as} \quad m \to 0$$

and

$$\coth(\beta \omega_k/2) \to \infty \quad \text{as} \quad m \to 0$$

so that

$$\Phi_\alpha = \frac{1}{N} \sum_k \left[ -1 + \frac{\coth(\beta \omega_k/2)}{[1 - \gamma^2(k)]^{1/2}} \right] \to +\infty$$

as $m \to 0$.

For convenience, $\Phi_{11}$ will be discussed from now on:

$$\Phi = \Phi_{11} = \frac{2}{N} \sum_k \Phi_{11}(k).$$

A new quantity $P$ is defined by

$$P = (S/m)^2$$

$$= \left[ 1 + \frac{m/2s^2}{(2/N) \sum_k \gamma^2(k)} \frac{\gamma^2(k)}{[1 - \gamma^2(k)]^{1/2}} \coth(\beta \omega_k/2) \right].$$
Fig. 1. Sublattice magnetization per spin for simple cubic structure ($S = 1/2$)
Fig. 2. Sublattice magnetization per spin for body centered cubic structure ($S = 1/2$).
Fig. 3. Energy spectrum renormalization factor for simple cubic structure (S = 1/2).
Fig. 4. Energy spectrum renormalization factor for body centered cubic structure ($S = 1/2$).
ENERGY RENORMALIZATION FACTOR (R)

TEMPERATURE (T/Tm)

0.0

0.5

1.0

0.5

1.0
so that $\omega_k$ is given by

$$ (4.110) \quad \omega_k = 2mzNP \left[ 1 - \gamma^2(k) \right]^{1/2}. $$

Assuming $P \rightarrow P_N$, a positive finite constant, as $T \rightarrow T^+_N$, one gets

$$ \frac{m}{2} \frac{2/N}{\sum_k \frac{\gamma^2(k)}{[1 - \gamma^2(k)]^{1/2}}} \coth(\beta \omega_k/2) $$

$$ \rightarrow \frac{k_B T_N}{ZJP_N} (I_o - 1) $$

where

$$ (4.111) \quad I_o = \frac{2/N}{\sum_k [1 - \gamma^2(k)]^{-1}} \quad \text{(Appendix A)}. $$

Hence it follows that

$$ (4.112) \quad P_N = 1 + \frac{k_B T_N}{2zJP_N S^2} (I_o - 1). $$

When $\phi \rightarrow \infty$, one sees from Eq. (4.94) that

$$ (4.113) \quad m = S(S + 1)/3\phi + O(\phi^{-2}), $$

and Eq. (4.95) gives

$$ (4.114) \quad m\phi = \frac{m}{2} \frac{2/N}{\sum_k \frac{\coth(\beta \omega_k/2)}{[1 - \gamma^2(k)]^{1/2}} - 1} $$

$$ \rightarrow \frac{k_B T_N I_o}{2zJP_N}. $$
Eqs. (4.113) and (4.114) lead to

\[(4.115) \quad (k_B T_N / 2zJ) = S(S + 1)P_N / 3I_o, \]

so that

\[(4.116) \quad P_N = 1 + (S + 1)(I_o - 1) / 3I_o S \]

and

\[(4.117) \quad (k_B T_N / 2zJS) = [(S + 1) / 3I_o] [1 + (S + 1)(I_o - 1) / 3I_o S]. \]

Thus, one gets

\[(4.118) \quad (k_B T_N / 2zJS)_{S=1/2} = (2 - 1/I_o) / 2I_o, \]

\[(4.119) \quad (k_B T_N / 2zJS) \rightarrow \infty \rightarrow [(S + 1) / 3I_o] [1 + (I_o - 1) / 3I_o]. \]

The molecular field theory result is given by Eq. (2.37)

\[(4.120) \quad (k_B T_N / 2zJS) = (S + 1) / 3, \]

and the RPA result (Lines, 1964) is

\[(4.121) \quad (k_B T_N / 2zJS) = (S + 1) / 3I_o, \]

which can be obtained from the present result by putting \( P = 1 \).

Close to but below the Néel temperature, \( P \) is given by

\[(4.122) \quad P_N = 1 + (S + 1)(I_o - 1) / 3SI_o. \]
With this $P_N$, the limiting values of correlation functions are, from Eqs. (4.99) and (4.100), given by

$$\langle S_{1,-k}^- S_{2,k}^- \rangle = \langle S_{2,-k}^- S_{1,k}^- \rangle = \langle S_{1,-k}^+ S_{2,k}^- \rangle = \langle S_{2,-k}^+ S_{1,k}^- \rangle$$

(4.123)

$$= \frac{k_B T_N}{zJ P_N [1 - \gamma^2(k)]},$$

and

$$\langle S_{1,-k}^- S_{2,k}^+ \rangle = \langle S_{2,-k}^- S_{1,k}^+ \rangle = \langle S_{1,-k}^+ S_{2,k}^+ \rangle = \langle S_{2,-k}^+ S_{1,k}^+ \rangle$$

(4.124)

$$= -\frac{k_B T_N \gamma(k)}{zJ P_N [1 - \gamma^2(k)]}.$$

2. Ground state properties

In the limit of $T \rightarrow 0^+$, it is evident that

$$\coth(\beta \omega_k/2) \rightarrow 1.$$ 

So, from Eqs. (4.92), (4.94), (4.95), and (4.105), it follows that

(4.125) \[ \phi_o = (1/2) \left[ \frac{(2/N) \sum_k}{1 - \gamma^2(k)} \right]^{1/2} - 1 \] = $c'/2$,

$$P_o = \left[ 1 + \left( \frac{m/2s^2}{2/N} \right) \sum_k \frac{\gamma^2(k)}{[1 - \gamma^2(k)]^{1/2}} \right]$$

(4.126)

$$= 1 + \left( \frac{m}{2s^2} \right) (c + c'),$$
with \( c \) and \( c' \) as given in Eqs. (2.71) and (2.75). The limiting values of correlation functions are easily obtained.

For \( S = 1/2 \), \( m_0 \), \( P_0 \), and \( R_0 \) have the values

\[
m_0 = 1/2(1 + c') \approx 0.433 \text{ for s.c.}
\]

\[
\approx 0.448 \text{ for b.c.c.},
\]

\[
P_0 = 1 + (c + c')/(1 + c'),
\]

\[
R_0 = 2m_0 P_0 \approx 1.055 \text{ for s.c.}
\]

\[
\approx 1.047 \text{ for b.c.c.}
\]

The values of \( c \) and \( c' \) are given in Appendix A.

For general \( S \), since \( \Phi_0 \) is less than 0.08, \( m_0 \) can be expanded into a power series in \( \Phi_0 \),

\[
m_0 = S - \Phi_0 + 0(\Phi_0^2) = S - c'/2 + 0(c'^2)
\]
in agreement with the non-linear spin-wave theory (Oguchi, 1960; Liu, 1966) to first order in the small quantity \( c' \).

Also,

\[
P_0 = 1 + \left( m_0 / 2S^2 \right) (c + c')
\]

\[
(4.133) = 1 + \left( 1/2S \right) (1-c/2S) (c + c') + 0(c'^3)
\]

\[
= 1 + \left( c + c'/2S \right) + 0(c'^2),
\]

\[
R_0 = \frac{m_0 P_0}{S}
\]

\[
(4.134) = \left( 1 - c'/2S \right) \left( 1 + c/2S + c'/2S \right) + 0(c'^2)
\]

\[
= 1 + c/2S + 0(c'^2)
\]

in agreement with the non-linear spin-wave theory to first order in the small quantities \( c \) and \( c' \).

3. Low temperature properties

To study the low temperature properties, the quantities of interest are expanded in powers of a reduced temperature, \( (k_B T / 2zJ) \) or \( (k_B T / 2zJS) \). From Eqs. (4.92) and (4.95), \( \omega_k \) and \( \phi \) are given by

\[
(4.135) \quad \omega_k = 2mzJP \left[ 1 - \gamma^2(\kappa) \right]^{1/2},
\]
\[ \phi = \phi_0 + (\Phi - \phi_0) \]
\[ (4.136) \]
\[ = \frac{c'}{2} + \frac{1}{2N} \sum_{\vec{k}} \frac{1}{[1 - \gamma^2(\vec{k})]^{1/2}} \frac{1}{[\exp(\beta \omega_\vec{k}) - 1]}. \]

In the infinite lattice limit, the sum over \( \vec{k} \) can be replaced by an integration over the first Brillouin zone in \( \vec{k} \) space. At very low temperatures, a significant contribution comes from small values of \( k \), so that the integral can be extended over the entire \( \vec{k} \) space:

\[ (4.137) \quad \frac{2}{N} \sum_{\vec{k}} \rightarrow \frac{1}{8\pi^3} \int_0^\infty 4\pi k^2 \, dk \]

where the volume of the crystal is taken as unity for simplicity. For very small \( k \), one can show that

\[ (4.138) \quad [1 - \gamma^2(\vec{k})]^{1/2} \rightarrow \gamma k \]

where \( \gamma \) is a constant depending on the crystal structure.

With this limiting value, Eq. (4.136) leads to

\[ (4.139) \quad \phi = \frac{c'}{2} + \frac{1}{2\pi^2 \gamma^2 (\text{mP})^2} \left( k_B T / 2zJ \right)^2 \int_0^\infty \frac{x \, dx}{e^x - 1} + \ldots \ldots \]

The integral can be expressed in terms of Riemann's Zeta-function (Whittaker and Watson, 1952) through the relation

\[ (4.140) \quad \int \frac{z^{x-1} \, dz}{e^z - 1} = \Gamma(x) \zeta(x). \]
and $\phi$ reduces to

\[(4.141) \quad \phi = c'/2 + \frac{\tilde{\sigma}(2)}{2 \pi^2 \gamma^3(mP)^2} \left( k_B T/2zJ \right)^2 + \ldots \ldots \ldots \cdot \]

From Eqs. (4.109), (4.126), and (4.136), it follows that

\[(4.142) \quad (2S^2/m)(P - 1) = \frac{2}{N} \sum \frac{\gamma^2(k)}{[1 - \delta^2(k)]^{1/2}} \coth(\beta \omega_k/2) \]

\[= c + c' + \frac{c}{\pi^2 \gamma^3(mP)^2} \left( k_B T/2zJ \right)^2 \]

\[= \frac{6}{\pi^2 \gamma^3(mP)^4} \left( k_B T/2zJ \right)^4 + \ldots \ldots \ldots \cdot \]

For $S = 1/2$, the sublattice magnetization is

\[(4.143) \quad m = \frac{1}{3} (1 + 2\phi)^{-1} \]

\[= \frac{1}{3} \left[ 1 - c' + c'^2 - (1 - 2c') \frac{\tilde{\sigma}(2)}{\pi^2 \gamma^3(mP)^2} \left( k_B T/2zJ \right)^2 \right. \]

\[+ \frac{\tilde{\sigma}(2)}{\pi^4 \gamma^6(mP)^2} \left( k_B T/2zJ \right)^2 + \ldots \ldots \ldots \cdot \]
The last term is a new term that does not appear in the non-linear spin-wave theory. For $S = 1$, 

\[(4.144)\]

\[m = (1 + 2 \phi)/(1 + 3 \phi + 3 \phi^2)\]

\[= 1 - \phi'/(2 + 3 \phi^3/8 - (1 - 9 \phi'^2/4) \frac{\varphi'(2)}{2 \pi^2 \gamma^3(mP)^2} (k_B T/2zJ)^2\]

\[+ (9 \phi'^2/4) \frac{\varphi'^2(2)}{\pi^2 \gamma^6(mP)^4} (k_B T/2zJ)^4 + \cdots \cdots \cdot\]

The additional term contains a factor $\phi' \sim 0.15$. For general spin $S$, 

\[(4.145)\]

\[m = S - \phi + O(\phi^{2S+1})\]

\[= S - \phi'/(2 - 9 \phi'^2/4) \frac{\varphi'(2)}{2 \pi^2 \gamma^3(mP)^2} (k_B T/2zJ)^2\]

\[+ O(\phi'^{2S+1}) + O(\phi'^{2S}k_B^2T^2) + O(\phi'^{2S-1}k_B^4T^4) + \cdots \cdots \cdot\]

Thus, it is easily seen that the additional term becomes very small when $S$ is large. This means that the present work is in better agreement with the interacting spin-wave theory as $S$ increases.
If one ignores the additional terms in \( m \) and solves for \( R \) by iteration, one finds

\[
R \approx 1 + \frac{c}{2S} - \frac{c + 2c'}{S} \frac{\zeta(2)}{2 \pi^2 \gamma S^3} (k_B T/2zJS)^2
\]

\[
- 2 \left[ 1 - \frac{3(3c + c')}{4S} \right] \left[ \frac{\zeta(2)}{2 \pi^2 \gamma S^3} \right]^2 (k_B T/2zJS)^4
\]

\[
- 6 \left( 1 - \frac{2c + c'}{S} \right) \frac{\zeta(4)}{2 \pi^2 \gamma S^3} (k_B T/2zJS)^4 + \cdots.
\]

The two middle terms are new. The \( T^2 \) term is proportional to \( (c + 2c') \), so to lowest order it may be ignored, except at very low temperatures. The ratio between the last two terms is

\[
\frac{3(1 - \frac{2c + c'}{S}) \zeta(4)}{2 \pi^2 \gamma S^3} \left[ 1 - \frac{3(3c + c')}{4S} \right]^2 \zeta(2)
\]

\[
\sim 0(S) \gg 1
\]

when \( S \) is large. So the spin-wave interaction term dominates the new term. The quantity \( R \) corresponds to the energy renormalization factor in the non-linear spin-wave theory. The factor there (Liu, 1966) is

\[
1 + \frac{c}{2S} - \frac{6 \zeta(4)}{2 \pi^2 \gamma S^3} (k_B T/2zJS)^4 + \cdots.
\]
The appearance of additional terms that do not appear in spin-wave theory is a general feature of the Green's function theory (Callen, 1963; Anderson and Callen, 1964). The same kind of extra term appears in ferromagnetism (Callen, 1963). But it is to be remembered that the extra term becomes less important as $S$ increases. Further, at this stage of experimental study of the antiferromagnetic systems, it is impossible to detect any quantity of the order of the extra term.

F. Perpendicular Susceptibility

Using the Kubo method (1957) for the linear response function and taking $z$ to be the direction of preferred antiferromagnetic spin alignment, one can write the perpendicular susceptibility of the system in terms of spin correlation functions as

$$\chi_i = (g/\mu_B)^2 \int_0^\beta <T S_i^z(\tau) S_i^z(0)> d\tau$$

where

$$\overrightarrow{S}_0 = \sum_{\alpha 1} \overrightarrow{S}_{\alpha 1} = \overrightarrow{S}_{1,0} + \overrightarrow{S}_{2,0}.$$
Since it can easily be shown that

(4.150) \[[H, S^x_o] = 0,\]

the susceptibility leads to

(4.151)

\[
\chi_\perp = (g\mu_B)^2 \beta \left< S^x_o S^x_o \right>
\]

\[
= (g\mu_B)^2 \beta \left( \left< S^+_o S^-_o \right> + \left< S^-_o S^+_o \right> \right) / 4
\]

\[
= (g\mu_B)^2 \beta \left( \left< S^+_{1,0} S^-_{1,0} \right> + \left< S^+_{1,0} S^-_{2,0} \right> + \left< S^+_{2,0} S^-_{1,0} \right> + \left< S^+_{2,0} S^-_{2,0} \right> \right)
\]

\[
+ \left< S^-_{2,0} S^+_{1,0} \right> + \left< S^-_{1,0} S^+_{2,0} \right> + \left< S^-_{1,0} S^+_{1,0} \right> + \left< S^-_{2,0} S^+_{2,0} \right> \right) / 4.
\]

Putting Eqs. (4.99) and (4.100) into Eq. (4.151), one gets

\[
\chi_\perp = (N/4)(g\mu_B)^2 \beta
\]

(4.152)

\[
[\lim_{k \to 0} \frac{1 - \gamma(k)}{1 - \gamma^2(k)}]^{1/2} \coth\left(\beta\omega_k/2\right)
\]

\[
= (g\mu_B)^2 N / 4zJP
\]
where

\[
\tag{4.153} P = \left[ 1 + \left( \frac{m}{2S^2} \right) \frac{1}{2N} \sum_{k} \frac{\gamma^2(k)}{1 - \frac{1}{2} \gamma^2(k)} \coth \left( \frac{\omega B \gamma}{2} \right) \right].
\]

From Eqs. (4.116) and (4.126), one finds

\[
\tag{4.154}
\begin{align*}
P_o &= 1 + \frac{m_o}{2S^2} (c + c'), \\
P_N &= 1 + (S + 1) (I_0 - 1) / 3I_0 S;
\end{align*}
\]

the difference between \(P_o\) and \(P_N\) turns out to be very small, so that \(\chi_\perp\) varies only slightly from \(T = 0\) to \(T = T_N\). As one can easily see from Eqs. (2.32), (2.46), and (2.79), both the molecular field theory and the non-interacting spin-wave theory predict constant perpendicular susceptibility which is equal to that of Eq. (4.152) with \(P = 1\). This means that the RPA should give a constant value for \(\chi_\perp\) as was indeed found by Lines (1964). But the present work gives a slightly temperature-dependent \(\chi_\perp\), which is also the case for the interacting spin-wave theory (Oguchi, 1960; Liu, 1966).

At low temperatures, from Eqs. (4.142) and (4.145), one finds that

\[
\tag{4.155} P = 1 + \left( 1 - \frac{c'}{2S} \right) (c + c') / 2S
\]

\[
+ \left( 1 - \frac{c + 2c'}{2S} \right) \frac{\zeta(2)}{2 \pi^2 \gamma^2 S} \left( k_B T / 2JmP \right)^2 + \ldots .
\]
so that

\[ \chi_1 = \frac{\langle \mathcal{M}_B \rangle^2}{4zJ} \left[ 1 - \frac{c + c'}{2S} \right] + \left(1 - \frac{c + 2c'}{2S} \right) \frac{\zeta(2)}{2 \pi^2 \chi_S^3} \left( k_B T / 2zJm \right)^2 + \cdots \]

(4.156)

The temperature independent term is the same as the result of interacting spin-wave theory, while the \( T^2 \) term gives a deviation of order \( c/S \).

G. Analysis Above the Néel Temperature

In real antiferromagnetic crystals, there still exists short range order even above the Néel temperature. In the absence of any external field, a proper way of treating the problem is to introduce a fictitious field \( H_m \) pointing in the \( +z \) direction at the sites of sublattice 1, and in the \( -z \) direction at those of sublattice 2 (Van Kranendonk and Van Vleck, 1958), and to take the limit of vanishing \( H_m \) at the end of calculation. The model Hamiltonian is

\[ (4.157) \quad H = \sum_{i,j} J_{ij} \vec{s}_i \cdot \vec{s}_j - h \left[ \sum_i s_i^z - \sum_j s_j^z \right] \]

with

\[ (4.158) \quad h = g \mu_B H_m. \]
The symmetry between the two sublattices still exists. So one has

\[ m_1 = -m_2 \]

(4.159)

\[ = m, \]

(4.160) \[ \psi_{12}(\bar{k},0) = \psi_{21}(\bar{k},0) \]

\[ = \psi(\bar{k},0). \]

The explicit calculation turns out to be exactly the same as that with the isotropic Hamiltonian (4.1), except for the replacements

\[ A_1(0) \rightarrow h + A_1(0), \]

\[ A_2(0) \rightarrow -h + A_2(0), \]

or equivalently

(4.161) \[ A(0) \rightarrow h + A(0) \]

since \[ A_1(\bar{k}) = -A_2(\bar{k}) \]

\[ = A(\bar{k}). \]

The replacement (4.161) means another replacement

\[ \omega_k = \left[ A^2(0) - A^2(\bar{k}) \right]^{1/2} \]

(4.162)

\[ \rightarrow \omega_k = \left\{ [h + A(0)]^2 - A^2(\bar{k}) \right\}^{1/2}. \]
For example, the spatial transforms of Green's functions are, instead of Eq. (4.60), given by

\[
G_{11}^{\alpha}(k,\tau) = \frac{\Theta_1(a)}{2} \left( 1 + \frac{h + A(0)}{\omega_k} \right) \frac{e^{-\omega_k \tau}}{1 - e^{-\beta\omega_k}}
\]

\[
+ \left[ 1 - \frac{h + A(0)}{\omega_k} \right] \frac{e^{\omega_k \tau}}{1 - e^{\beta\omega_k}}
\]

\[
G_{21}^{\alpha}(k,\tau) = -\frac{\Theta_1(a)A(k)}{2\omega_k} \left[ \frac{e^{-\omega_k \tau}}{1 - e^{-\beta\omega_k}} - \frac{e^{\omega_k \tau}}{1 - e^{\beta\omega_k}} \right],
\]

(4.163)

\[
G_{12}^{\alpha}(k,\tau) = \frac{\Theta_2(a)A(k)}{2\omega_k} \left[ \frac{e^{-\omega_k \tau}}{1 - e^{-\beta\omega_k}} - \frac{e^{\omega_k \tau}}{1 - e^{\beta\omega_k}} \right],
\]

\[
G_{22}^{\alpha}(k,\tau) = \frac{\Theta_2(a)}{2} \left( 1 - \frac{h + A(0)}{\omega_k} \right) \frac{e^{-\omega_k \tau}}{1 - e^{-\beta\omega_k}}
\]

\[
+ \left[ 1 + \frac{h + A(0)}{\omega_k} \right] \frac{e^{\omega_k \tau}}{1 - e^{\beta\omega_k}}
\]

with \(\omega_k\) defined in Eq. (4.162). Special attention must be paid to the fact that

(4.164) \(\omega_k \neq A(0) \left[ 1 - \gamma^2(k) \right]^{1/2}\),
even though the relation

\[(4.165) \quad A(\vec{k}) = \gamma(\vec{k})A(0)\]

is still true.

The correlation functions are given by

\[(4.166)\]
\[\langle S^-_{\alpha_1}, -k S^+_{\beta_1}, k \rangle = m(N/2) \left[ \frac{h + A(0)}{\omega_k} \coth(\beta \omega_k/2) - 1 \right],\]

\[\langle S^-_{\alpha_1}, -k S^+_{\beta_1}, k \rangle = \langle S^-_{\alpha_2}, -k S^+_{\beta_2}, k \rangle = -m(N/2) \frac{A(\vec{k})}{\omega_k} \coth(\beta \omega_k/2),\]

\[\langle S^-_{\alpha_2}, -k S^+_{\beta_2}, k \rangle = m(N/2) \left[ \frac{h + A(0)}{\omega_k} \coth(\beta \omega_k/2) + 1 \right],\]

and

\[(4.167) \quad \langle S^-_{\alpha_1} S^+_{\beta_2} \rangle = (2/N)^2 \sum_k \langle S^-_{\alpha_1}, -k S^+_{\beta_2}, k \rangle \exp(-i \vec{k} \cdot \vec{r}_1 + i \vec{k} \cdot \vec{r}_2),\]

and the identities in Eq. (4.100) hold. It turns out that

\[(4.168) \quad A(0) = 2mJ(0) \left[ 1 + \frac{mA(0)}{2S^2} \sum_k \frac{\gamma^2}{\omega_k} \coth(\beta \omega_k/2) \right],\]

\[(4.169) \quad \omega_k = \left[ \left[ h + A(0)(1 + \gamma) \right] \left[ h + A(0)(1 - \gamma) \right] \right]^{1/2}\]

where, for brevity, one has written that

\[(4.170) \quad \gamma(\vec{k}) = \gamma.\]
The sublattice magnetization \( m \) is given by the Callen's relation (4.94) with

\[
\Phi = (1/2) \left[ (2/N) \sum_k \frac{h + A(0)}{\omega_k} \coth(\beta \omega_k/2) - 1 \right].
\]

To investigate the properties above the Neél point, it is very convenient to introduce an order parameter \( x \):

\[
x = \lim_{h \to 0} \frac{m}{h},
\]

since \( m \to 0 \) in the limit of \( h \to 0 \) for \( T > T_N \). One easily sees that

\[
\coth(\beta \omega_k/2) \to \frac{2}{\beta \omega_k}
\]

in the same limit. Another quantity \( a \) is defined from \( A(0) \):

\[
a = \lim_{h \to 0} \frac{A(0)}{hx} [A(0)/hx]
\]

\[
= \lim_{h \to 0} \frac{A(0)}{m}.
\]

For \( T > T_N \), one can write

\[
\omega_k = h \left\{ [1 + ax(1 + \gamma)][1 + ax(1 - \gamma)] \right\}^{1/2},
\]

\[
a = 2zJ \left[ 1 + (ax^2/S^2) \sum_k \frac{k_B T_0^2}{(1 + ax)^2 - (ax\gamma)^2} \right].
\]
\begin{equation}
\phi \rightarrow (1/h)(2/N) \sum_k \frac{k_B T (1 + ax)}{(1 + ax)^2 - (ax\gamma)^2}.
\end{equation}

It can be shown (Appendix D) that
\begin{equation}
x \rightarrow \infty \text{ as } T \rightarrow T^+_N.
\end{equation}

The correlation functions are given by
\begin{equation}
\langle S_{1}^{-}, k S_{1}^{+} \rangle = (N/2) \frac{2k_B T x (1 + ax)}{(1 + ax)^2 - (ax\gamma)^2},
\end{equation}
\begin{equation}
\langle S_{1}^{-}, k S_{2}^{+} \rangle = \langle S_{2}^{-}, k S_{1}^{+} \rangle = -(N/2) \frac{2k_B T x^2 \gamma}{(1 + ax)^2 - (ax\gamma)^2},
\end{equation}
\begin{equation}
\langle S_{2}^{-}, k S_{2}^{+} \rangle = \langle S_{1}^{-}, k S_{1}^{+} \rangle.
\end{equation}
\begin{equation}
\langle S_{a_{1}}^{-} S_{a_{j}}^{+} \rangle = (2/N)^2 \sum_k \langle S_{a_{1}}^{-}, k S_{a_{j}}^{+} \rangle \exp(-i \vec{k} \cdot \vec{x} + i \vec{k} \cdot \vec{\phi} \cdot \vec{j}).
\end{equation}

From Eq. (4.151), the perpendicular susceptibility is given by
\begin{equation}
\chi_{\perp} = (g/\mu_B)^2 \lim_{k \rightarrow 0} \left( \langle S_{1}^{-}, k S_{1}^{+} \rangle + \langle S_{1}^{-}, k S_{2}^{+} \rangle \right)
= (g/\mu_B)^2 N x / (1 + 2ax).
\end{equation}

At \( T = T^+_N \), \( x \rightarrow \infty \), so that one gets
\begin{equation}
\chi_{\perp} = (g/\mu_B)^2 N / 2a_N = (g/\mu_B)^2 N / 4zJ_P N.
\end{equation}
Thus the perpendicular susceptibility is continuous at the Néel temperature. The correlation functions reduce to

\[
\langle S^-_1, -kS^+_1, k \rangle \rightarrow \frac{(N/2)(2k_B T_N/a)}{(1 - \gamma^2)},
\]

(4.183)

\[
\langle S^-_1, -kS^+_2, k \rangle \rightarrow -\frac{(N/2)(2k_B T_N/a) \gamma}{(1 - \gamma^2)},
\]

which are continuous with the lower temperature phase values as given in Eqs. (4.123) and (4.124).

H. The Correlation Length

As discussed in Appendix D, the equation for the order parameter is given by

\[
S(S + 1)/3 = \frac{(2k_B T/N) \sum (1 + ax)}{k (1 + ax)^2 - (ax \gamma)^2}.
\]

(4.184)

At very high temperatures, one expects

\[
x \propto (1/k_B T).
\]

(4.185)

Then one has

\[
a = 2zJ \left[ 1 + \frac{(ax^2/S^2)(2/N) \sum k_B T \gamma^2}{k (1 + ax)^2 - (ax \gamma)^2} \right]
\]

\[
\rightarrow 2zJ
\]
and \((ax)\) is small. In fact, from Eq. (4.184) \(x\) can be written as

\[(4.187) \quad x = \frac{S(S + 1)}{3k_BT} + O(T^{-2}).\]

At lower temperatures, \(x\) can be expanded in powers of \((1/T)\).

When \(x\) is large and \(k\) is small, it follows from Eq. (4.179) that

\[(4.188) \quad \langle S_{1,-k}^-, S_{1,k}^- \rangle \equiv (Nk_BT/a) \frac{1}{(2/ax) + (1 - \gamma^2)} \]

\[= (Nk_BT/a) \frac{1}{(2/ax) + \gamma^2 k^2} \]

\[= (Nk_BT/a \gamma^2) \frac{1}{k^2 + k^2} \]

where \(\gamma\), defined in Eq. (4.138), is a constant depending on the crystal structure and \(K\) is defined by

\[(4.189) \quad K^2 = \frac{2}{ax} \gamma^2.\]

The correlation function is given by Eq. (4.180):

\[(4.190) \quad \langle S_{1i}^- S_{1j}^+ \rangle = \frac{(2k_BT/a \gamma^2)(2/N)}{k^2 + K^2} \sum_k \exp(-ik \cdot \vec{i} + ik \cdot \vec{j}) \]

for large \(|\vec{i} - \vec{j}|\). It is evident that the most significant contribution of the summation comes from the smallest \(k\) and
the factor inside the summation sign vanishes if one takes \( k \to \infty \). So the argument given for Eq. (4.137) applies, and the summation can be replaced by an integration without much loss of accuracy. In this case, it can be shown that

\[
(4.191) \quad \left(\frac{2}{N}\right) \sum_k \frac{e^{-ik \cdot (\vec{i} - \vec{j})}}{k^2 + k^2} = \frac{e^{-K|\vec{i} - \vec{j}|}}{4\pi |\vec{i} - \vec{j}|},
\]

so that

\[
(4.192) \quad \langle S_{\vec{i} \vec{j}}^- S_{\vec{i} \vec{j}}^+ \rangle = \left(\frac{k_B T}{2\pi a^2}\right) e^{-K|\vec{i} - \vec{j}|}. 
\]

Thus the quantity

\[
(4.193) \quad \frac{1}{\xi} = \left(\frac{a^2 \gamma^2}{2}\right)^{1/2}
\]

can be interpreted as a correlation length between two spins. And the square root of the order parameter \( x \) is proportional to the correlation length between two spins in the long wave length limit. As the temperature is lowered to the Néel point the correlation length becomes infinite, i.e., long-range ordering commences at the Néel temperature. At very high temperatures, the correlation length decreases as \( T^{-1/2} \).

Van Hove (1954) studied the nature of spin correlation functions related to neutron diffraction in ferromagnetic crystal. For temperatures above the Curie point but not too high, and for two spins far apart, his result is similar to Eq. (4.192).
I. Longitudinal Correlation Functions

The longitudinal correlation functions of two spins play an important role in the statistical mechanics of antiferromagnetism. Unfortunately, they do not follow directly from the theory as developed to this point. Liu (1965) was the first to carry out the task for ferromagnetism in the random phase approximation. In this section, his work is extended to antiferromagnetism in the framework of the Callen decoupling scheme. It is shown that, when a small a.c. field is applied to the system, the wavelength- and frequency-dependent part of the sublattice magnetizations are proportional to Fourier transform of a two-time longitudinal correlation functions of the spins. As shown in a similar problem by Kawasaki and Mori (1961) and Mori and Kawasaki (1962), the a.e. part of the sublattice magnetizations can be solved by the equation of motion method with the Callen decoupling scheme. Thus the longitudinal correlation functions are obtained by taking the inverse Fourier transform of the latter result.

In contrast with ferromagnetism, one needs to calculate four correlation functions. To this end, it is necessary to use two different perturbation terms in the Hamiltonian, so that each choice gives two correlation functions.
The perturbed Hamiltonian to be used is

\[(4.194)\quad H_\alpha' = H + H_\alpha \exp(\varepsilon t - i\omega t), \alpha = 1 \text{ or } 2, \varepsilon = 0^+,\]

where the first term \(H\) is the unperturbed Hamiltonian (4.5) and the second term is a perturbation:

\[H_\alpha = -f \sum_i S^Z_{i\alpha} \exp(i\vec{q} \cdot \vec{x}) \tag{4.195}\]

\[= -f S^Z_{\alpha, -q}\]

where \(f\) is a small parameter proportional to the amplitude of a fictitious a.c. field which is applied to one sublattice only. It is evident that

\[(4.196)\quad H_\alpha = 0, H_\alpha' = H \text{ at } t = -\infty.\]

From the discussions in Eqs. (3.40)--(3.51), one gets

\[\langle S^Z_{\phi j} \rangle_\alpha = \text{Tr}(\phi_\alpha^i S^Z_{\phi j}) \tag{4.197}\]

\[= m_{\phi} + f \exp(\varepsilon t - i\omega t) \phi_j^x(\omega) + O(f^2)\]

with

\[(4.198)\quad \phi_j^x(\omega) = -i \int_{-\infty}^{\infty} \langle [S^Z_{\phi, -q}(t'), S^Z_{\phi j}(0)] \exp(\varepsilon t' - i\omega t') dt'.\]
It is convenient to define the Fourier components of \( \sigma^\xi_j(\omega) \) by

\[
(4.199) \quad \sigma^\xi_j(\overrightarrow{q}, \omega) = \sum_j \sigma^\xi_j(\omega) \exp(-i\overrightarrow{q} \cdot \overrightarrow{r}_j).
\]

then

\[
(4.200) \quad \sigma^\xi(\overrightarrow{q}, \omega) = -\frac{i}{\hbar} \int_{-\infty}^{\infty} \langle [S^Z_{\alpha}, -q(t')], S^Z_{\beta, q}(0) \rangle \exp(\varepsilon t' - i\omega t') \, dt'.
\]

As shown in Eqs. (3.12)--(3.21), the two spin correlation functions in Eq. (4.200) have the following spectral representations:

\[
(4.201) \quad \langle S^Z_{\alpha, -q}(t)S^Z_{\beta, q}(0) \rangle = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} J_{\xi}(\overrightarrow{q}, \omega) \exp(-\omega t),
\]

where

\[
(4.202) \quad J_{\xi}(\overrightarrow{q}, \omega) = 2\pi \sum_{m,n} \phi_m <m| S^Z_{\alpha, -q} |n> <n| S^Z_{\beta, q} |m> \delta(E_m - E_n + \omega)
\]

and the sums are taken over the complete set of eigenstates of the unperturbed Hamiltonian \( H \). By Eqs. (3.17) and (3.18), it follows after a simple integration that

\[
(4.203) \quad \langle [S^Z_{\alpha, -q}(t), S^Z_{\beta, q}(0)] \rangle = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} J_{\xi}(\overrightarrow{q}, \omega') (1 - e^{-\omega'}) e^{-i\omega't}.
\]
In later calculations, it is more convenient to work in the imaginary time formalism. A Green's function is defined by

\begin{equation}
G^{Z}_{\alpha\beta}(\vec{q},\tau) = \langle T S^{Z}_{\alpha,-\vec{q}}(\tau) S^{Z}_{\beta,q}(0) \rangle.
\end{equation}

As discussed in Eqs. (3.33)-(3.36), the periodic property of the Green's function guarantees the validity of the expansion

\begin{equation}
G^{Z}_{\alpha\beta}(\vec{q},\tau) = \sum_{n} G^{Z}_{\alpha\beta}(\vec{q},n) \exp(-i\omega_{n}\tau) \quad \text{with} \quad \omega_{n} = \left(\frac{2\pi n}{\beta}\right).
\end{equation}

By use of Eqs. (4.202) and (4.205), and after integration, \( G^{Z}_{\alpha\beta}(\vec{q},n) \) can be expressed in terms of the spectral representation as follows:

\begin{equation}
G^{Z}_{\alpha\beta}(\vec{q},n) = \int_{0}^{\beta} d\tau \, G^{Z}_{\alpha\beta}(\vec{q},\tau) \exp(i\omega_{n}\tau)
\end{equation}

\begin{equation}
\quad = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \, J_{\omega'}(\vec{q},\omega') \frac{1 - e^{-\beta\omega'}}{\omega' - i\omega_{n}}.
\end{equation}

with \( J_{\omega'}(\vec{q},\omega') \) defined in Eq. (4.202). If one defines

\begin{equation}
S^{Z}_{\beta}(\vec{q},n) = G^{Z}_{\alpha\beta}(\vec{q},n),
\end{equation}
then, by comparison with Eq. (4.204), one finds

\[ \sigma_\phi^\infty(\vec{q}, \omega) = S_\phi^\infty(\vec{q}, i\omega + \epsilon), \quad \epsilon = 0^+. \]

Hence \( \sigma_\phi^\infty(\vec{q}, \omega) \) and \( S_\phi^\infty(\vec{q}, n) \) are related by analytic continuation. In the following \( S_\phi^\infty(\vec{q}, n) \)'s are calculated by the equation of motion method with the Callen decoupling. Then, by use of Eq. (3.24), it follows from Eqs. (4.207) and (4.208) that

\[ J_\phi(\vec{q}, \omega) = \frac{1}{e^{-\beta\omega} - 1} \left[ S_\phi^\infty(\vec{q}, -i\omega + \epsilon) - S_\phi^\infty(\vec{q}, -i\omega - \epsilon) \right] . \]

Putting this result into Eq. (4.201), one gets the dynamical zz correlation functions of the spins.

The calculation is carried out in the following. For simplicity, only the case of \( S = 1/2 \) is considered. The general spin problem is, in principle, the same as the spin 1/2 case except that the algebra is more complex. It is convenient to work in the imaginary time formalism. Eqs. (4.208) and (4.209) suggest the proper analytic continuation to be adopted for the frequency. This, together with the discussions in Eqs. (3.28)–(3.31), gives an appropriate set of analytic continuations

\[ t \longrightarrow -i\tau, \]

\[ \omega \longrightarrow i(\omega_n - \epsilon), \]

\[ G_{\alpha\beta}(t) \longrightarrow -iG_{\alpha\beta}(\tau). \]
Under this analytic continuation, the Hamiltonian becomes

\[(4.212) \quad H' = H + H_\omega \exp(i \omega t) \quad \rightarrow \quad H'_\omega = H + H_\omega \exp(-i \omega \tau),\]

and the equation of motion for the Green's function is given by Eq. (3.59).

For spin 1/2, it suffices to use the Green's function of the form (4.3) with the parameter \(a = 0\). The Green's function to be used is

\[(4.213) \quad G_{\xi, \xi'}^{ij}(\tau) = \langle S^{+}_{\xi} S^{-}_{\xi'} \rangle^{\xi}, \]

\[= \langle T S^{+}_{\xi}(\tau) S^{-}_{\xi'}(0) \rangle^{\xi}. \]

Here it is to be understood that \(a\) is zero, so the explicit \(a\)-dependence index has been dropped. \(\xi\) is the perturbation index of Eq. (4.194). One must note that the average is taken with the perturbed density matrix \(\varrho^{\xi}\), and this is denoted by a prime. As given in Eq. (3.58), the equation of motion for the Green's function is

\[(4.214) \quad \frac{d}{d\tau} G_{\xi, \xi'}^{ij}(\tau) = 2 \Sigma(\tau) \Sigma_{\xi} \xi' S^{z}_{1j} \langle S^{z}_{\xi} \rangle^{\xi}, \]

\[+ \langle T [H^{\xi}_{\omega}(\tau), S^{+}_{\xi}(\tau)] S^{-}_{\xi'}(0) \rangle. \]
where one can see the origin of the first term from the relation

\[ G_{\alpha_1}^\pi(0) = \langle [S_{\alpha_1}^+, \exp(0) S_{\alpha_1}^-] \rangle^{\pi} \]

(4.215)

\[ = 2 \langle S_{\alpha_1}^z \rangle^{\pi}. \]

This is the essential simplification of the algebra for spin 1/2 case, and for the general spin problem, the quantity \( G_{\alpha_1}^\pi(\alpha) \) should be carried through the rest of the calculation.

As shown in Eq. (4.210), to calculate the longitudinal correlation functions, one needs to calculate the first order quantity \( S_{\alpha}^\pi(\vec{q}, n) \) in the presence of the perturbation. The decoupling scheme must be extended accordingly. That is, there arises the problem of how to take the first order quantity in small parameter \( f \) from the right hand side of Eq. (4.30). It is trivial for the first term, i.e., one takes

\[ \left[ \langle S_{\alpha_1}^z \rangle \langle S_{\beta,j}^+ ; B \rangle \right]^{(1)} \]

(4.216)

\[ = \langle S_{\alpha_1}^z \rangle^{(1)} \langle S_{\beta,j}^+ ; B \rangle + \langle S_{\alpha_1}^z \rangle \langle S_{\beta,j}^+ ; B \rangle^{(1)}. \]

The second term of Eq. (4.30) has its origin as a refinement to the random phase approximation, and the factor \( \langle S_{\alpha_1}^- S_{\beta,j}^+ \rangle / 2S^2 \) is of different character than the first. One might expect this factor to be small compared to unity. So the second of
Eq. (4.30) combined with its first order term \(\langle S_{\alpha_1}^- S_{\beta j}^+ \rangle^{(1)} / 2s^2\) might bring little physical consequence as far as one works to the first order Green's functions in small parameter \(f\). For this reason, the following procedure is adopted and it gives not only simpler algebra, but also many desirable physical results for \(S = 1/2\):

\[
\begin{align*}
[\langle S_{\alpha_1}^Z \rangle \langle S_{\alpha_1}^- S_{\beta j}^+ \rangle \langle S_{\alpha_1}^+ \rangle]^{(1)} & = [\langle S_{\alpha_1}^Z \rangle^{(1)} \langle S_{\alpha_1}^+ \rangle + \langle S_{\alpha_1}^Z \rangle \langle S_{\alpha_1}^+ \rangle^{(1)}] \langle S_{\alpha_1}^- S_{\beta j}^+ \rangle.
\end{align*}
\]

After decoupling by the extended Callen decoupling to the first order quantities, Eq. (4.214) leads to

\[
(a/d\tau) \langle G_{\alpha_1, \beta j}^{\tilde{\tau}}(\tau) \rangle = 2 \bar{\Sigma}(\tau) \Sigma_\rho \sum_1 [\langle S_{\alpha_1}^Z \rangle^{(1)} \langle 1 - 2 \gamma_{\rho, \gamma_{\alpha_1}} \rangle G_{\alpha_1, \beta j}^{\tilde{\tau}}(\tau)]
\]

One obtains the following expansions in powers of \(f\):

\[
(a/d\tau) \langle G_{\alpha_1, \beta j}^{\tilde{\tau}}(\tau) \rangle = \langle G_{\alpha_1, \beta j}(\tau) \rangle + f \langle G_{\alpha_1, \beta j}(\tau) \rangle + O(f^2),
\]
(4.220) \[ m_{\alpha} (\tau) = m_{\alpha} + f \exp(-i\omega_n \tau) S_{\alpha_1} (n) + O(f^2), \]

where the first terms are the quantities considered before, but without \( a \)-dependence. The form of the second term in the latter equation is guaranteed from its real time representation given in Eq. (3.51).

The unperturbed equation has already been solved and discussed in the preceding sections. The first order equation is

\[
(4.221) \quad \frac{d}{d\tau} G_{\alpha_1, \alpha_1, \phi, j} (\tau) = 2 \delta(\tau) \sum_{\alpha} \sum_{j} \exp(-i\omega_n \tau) S_{\alpha_1} (n) \\
- \delta_{\alpha} \exp(-iq_{\alpha} \cdot \tau - i\omega_n \tau) G_{\alpha_1, \phi, j} (\tau) \\
- 2 \sum_{\gamma_k \alpha_1} \sum_{\gamma_k} \exp(-i\omega_n \tau) [S_{\alpha_1} (n)(1-2 \psi_{\gamma_k, \alpha_1}) G_{\gamma_k, \phi, j} (\tau) ] \\
- S_{\gamma_k} (n)(1-2 \psi_{\alpha_1, \gamma_k}) G_{\alpha_1, \phi, j} (\tau) \\
- 2 \sum_{\gamma_k \alpha_1} \sum_{\gamma_k} [m_{\gamma}(1-\psi_{\gamma_k, \alpha_1}) G_{\gamma_k, \phi, j} (\tau) ] \\
- m_{\gamma}(1-\psi_{\alpha_1, \gamma_k}) G_{\alpha_1, \phi, j} (\tau), \gamma \neq \alpha.
\]
By making the transformation

$$G^\xi_{\gamma 1, \rho 1, \phi 1}(\tau) = \frac{1}{\beta} \sum_{m} G^\xi_{\gamma 1, \rho 1, \phi 1}(m) \exp(-i\omega_m \tau),$$

(4.222)

$$G^\xi_{\gamma 1, \rho 1, \phi 1}(m) = \int_{\tau}^{t} d\tau G^\xi_{\gamma 1, \rho 1, \phi 1}(\tau) \exp(i\omega_m \tau)$$

one obtains from Eq. (4.221) that

(4.223)

$$-i\omega_m G^\xi_{\gamma 1, \rho 1, \phi 1}(m) = 2 \sum_{\gamma} \sum_{1j} S^\xi_{\gamma 1}(n)$$

$$- \sum_{\gamma} \exp(\text{i}\mathbf{q} \cdot \mathbf{1}) G_{\gamma 1, \phi 1}(m-n)$$

$$- 2 \sum_{\gamma} J_{\gamma 1, \gamma k} \left[ S^\xi_{\gamma 1}(n)(1 - 2\gamma_k, \gamma 1) G_{\gamma k, \phi 1}(m-n) - S^\xi_{\gamma 1}(n)(1 - 2\gamma_k, \gamma 1) G_{\gamma 1, \phi 1}(m-n) \right]$$

$$- 2 \sum_{\gamma} J_{\gamma 1, \gamma k} \left[ m_{\gamma}(1 - 2\gamma_k, \gamma 1) G^\xi_{\gamma k, \phi 1}(m) - m_{\gamma}(1 - 2\gamma_k, \gamma 1) G^\xi_{\gamma 1, \phi 1}(m) \right],$$
where the transformation (4.35) is used for the zeroth order Green's functions. The following spatial Fourier transformations are made for the first order quantities:

\( (4.224) \)

\[
G_{1;\alpha_1,\alpha_j}(m) = (2/N)^2 \sum_{k_1,k_2} G_{1;\alpha_1}(k_1,k_2,m) \exp(ik_1 \cdot \alpha_1 - ik_2 \cdot \alpha_j).
\]

\[
G_{1;\alpha_1}(k_1,k_2,m) = \sum_{j_1,j_2} G_{1;\alpha_1,j}(m) \exp(-ik_1 \cdot \alpha_1 + ik_2 \cdot \alpha_j),
\]

\[
S_{\alpha_1}(n) = (2/N) \sum_k S_{\alpha}(k,n) \exp(ik \cdot \alpha_1),
\]

\( (4.225) \)

\[
S_{\alpha}(k,n) = \sum_1 S_{\alpha_1}(n) \exp(-ik \cdot \alpha_1).
\]

The linear response of the perturbation guarantees that

\( (4.226) \)

\[
S_{\alpha}(k,n) = \sum_{k,q} S_{\alpha}(q,n),
\]

so Eq. (4.225) reduces to

\[
S_{\alpha_1}(n) = (2/N) S_{\alpha}(q,n) \exp(1q \cdot \alpha_1),
\]

\( (4.227) \)

\[
S_{\alpha}(q,n) = \sum_1 S_{\alpha_1}(n) \exp(-1q \cdot \alpha_1).
\]
For the zeroth order quantities, the transformations in Eqs. (4.37)–(4.39) are made. Then Eq. (4.223) leads to

\[-1 \omega m G^e_{11; \kappa} (\vec{k}_1, \vec{k}_2, m) = 2 \delta_{k_2, k_1} S^e_{\kappa, q} (\vec{q}, n)\]

\[-(N/2) \delta_{k_2, k_1} A^{(0)} f_{\kappa, q} (\vec{k}_2, m-n)\]

\[+ A_x (0) G^e_{11; \kappa} (\vec{k}_1, \vec{k}_2, m)\]

\[- A_x (\vec{k}_1) G^e_{11; \kappa} (\vec{k}_1, \vec{k}_2, m)\]

\[+ \delta_{k_2, k_1} E_x (0) G^e_{11; \kappa} (\vec{k}_2, m-n)\]

\[- \delta_{k_2, k_1} E_x (\vec{k}_1) G^e_{11; \kappa} (\vec{k}_2, m-n), \alpha \neq \gamma,\]

where

\[(4.229) \quad B^e_{\kappa} (\vec{k}) = B^e_{\kappa} (\vec{k}, n) = \frac{S^e_{\kappa, q} (\vec{q}, n)}{m_{\kappa}} A_x (\vec{k}_2 + \vec{k}_2).\]

Eq. (4.228) can be written as

\[\begin{bmatrix}
- A_x (0) -1 \omega m G^e_{11; \kappa} (\vec{k}_1, \vec{k}_2, m) + A_x (\vec{k}_1) G^e_{11; \kappa} (\vec{k}_1, \vec{k}_2, m) \\
2 S^e_{11; \kappa} (\vec{q}, n) - \delta_{11} (N/2) G_{11} (\vec{k}_2, m-n) \\
+ E_x (0) G_{11} (\vec{k}_2, m-n) - E_x (\vec{k}_1) G_{21} (\vec{k}_2, m-n)
\end{bmatrix} = \delta_{k_2, k_1-q}\]
If \( \vec{k}_2 \neq (\vec{k}_1 - \vec{q}) \), Eq. (4.230) leads to homogeneous equations for the first order Green's functions, and these first order Green's functions vanish unless

\[
\Delta (\vec{k}_1, m) = (\omega_{k_1} - i \omega_m)(-\omega_{k_1} - i \omega_m) = 0
\]

with \( \omega_{k_1} = [A^2(0) - A^2(\vec{k}_1)]^{1/2} \),

which is impossible because both \( \omega_{k_1} \) and \( \omega_m \) are real. Thus one has

\[
(4.231) \quad G_{1;\vec{k}_1,\vec{k}_2, m}^\xi = \delta_{k_2, k_1 - q} G_{1;\vec{k}_1,\vec{k}_1 - \vec{q}, m}^\xi.
\]
After a long calculation, the solution of Eq. (4.230) is found to be

\[
G_{1;11}(\vec{k}_1, \vec{k}_1 - \vec{q}, m) = S_{1}(q, n) \sum_{\alpha} \frac{A_1(0) + \omega^\alpha_{k_1}}{\omega^\alpha_{k_1} (\omega^\alpha_{k_1} - 1 \omega^\alpha_m)}
\]

\[+ \frac{m_1}{2} \sum_{(\alpha\beta)} \frac{D_1^\alpha \left[ A_1(0) + \omega^\beta_{k_1 - q} \right] + D_2^\alpha A_2(\vec{k}_1 - \vec{q})}{\omega^\alpha_{k_1} \omega^\beta_{k_1 - q} (\omega^\alpha_{k_1} - 1 \omega^\beta_m) (\omega^\beta_{k_1 - q} - 1 \omega^\alpha_m)} \]

\[
G_{1;21}(\vec{k}_1, \vec{k}_1 - \vec{q}, m) = S_{1}(q, n) \sum_{\alpha} \frac{A_2(\vec{k}_1)}{\omega^\alpha_{k_1} (\omega^\alpha_{k_1} - 1 \omega^\alpha_m)}
\]

\[+ \frac{m_1}{2} \sum_{(\alpha\beta)} \frac{D_4^\alpha \left[ A_1(0) + \omega^\beta_{k_1 - q} \right] + D_3^\alpha A_2(\vec{k}_1 - \vec{q})}{\omega^\alpha_{k_1} \omega^\beta_{k_1 - q} (\omega^\alpha_{k_1} - 1 \omega^\beta_m) (\omega^\beta_{k_1 - q} - 1 \omega^\alpha_m)} \]

\[= \ (4.232) \]

\[
G_{1;12}(\vec{k}_1, \vec{k}_1 - \vec{q}, m) = S_{2}(q, n) \sum_{\alpha} \frac{A_1(\vec{k}_1)}{\omega^\alpha_{k_1} (\omega^\alpha_{k_1} - 1 \omega^\alpha_m)}
\]

\[+ \frac{m_2}{2} \sum_{(\alpha\beta)} \frac{D_2^\alpha \left[ A_2(0) + \omega^\beta_{k_1 - q} \right] + D_1^\alpha A_1(\vec{k}_1 - \vec{q})}{\omega^\alpha_{k_1} \omega^\beta_{k_1 - q} (\omega^\alpha_{k_1} - 1 \omega^\beta_m) (\omega^\beta_{k_1 - q} - 1 \omega^\alpha_m)} \]

\[
G_{1;22}(\vec{k}_1, \vec{k}_1 - \vec{q}, m) = S_{2}(q, n) \sum_{\alpha} \frac{A_2(0) + \omega^\alpha_{k_1}}{\omega^\alpha_{k_1} (\omega^\alpha_{k_1} - 1 \omega^\alpha_m)}
\]

\[+ \frac{m_2}{2} \sum_{(\alpha\beta)} \frac{D_3^\alpha \left[ A_2(0) + \omega^\beta_{k_1 - q} \right] + D_4^\alpha A_1(\vec{k}_1 - \vec{q})}{\omega^\alpha_{k_1} \omega^\beta_{k_1 - q} (\omega^\alpha_{k_1} - 1 \omega^\beta_m) (\omega^\beta_{k_1 - q} - 1 \omega^\alpha_m)} \]
with

\[(4.233)\]
\[
D_1^\alpha = D_1^\alpha (\vec{k}_1, \vec{q}, \xi)
\]
\[
\quad = [A_1(0) + \omega_{k_1}^\alpha] \left[ -(N/2) \delta_{15} + B_2(0) \right] - A_1(\vec{k}_1) B_2^\xi(\vec{k}_1),
\]
\[
D_2^\alpha = A_1(\vec{k}_1) \left[ -(N/2) \delta_{25} + B_1(0) \right] - \omega_{k_1}^\alpha B_1^\xi(\vec{k}_1) - A_1(0) B_2^\xi(\vec{k}_1),
\]
\[
D_3^\alpha = [A_2(0) + \omega_{k_1}^\alpha] \left[ -(N/2) \delta_{25} + B_1(0) \right] - A_2(\vec{k}_1) B_1^\xi(\vec{k}_1),
\]
\[
D_4^\alpha = A_2(\vec{k}_1) \left[ -(N/2) \delta_{15} + B_2(0) \right] - \omega_{k_1}^\alpha B_2^\xi(\vec{k}_1) - A_2(0) B_2^\xi(\vec{k}_1);
\]

where for simplicity the following notations are used

\[
\sum_\alpha f(\alpha) = f(1) + f(2),
\]
\[
\sum_{(\alpha \beta)} g(\alpha, \beta) = g(1,1) + g(1,2) + g(2,1) + g(2,2),
\]
\[(4.234)\]
\[
\omega_{k_1}^1 = \omega_{k_1},
\]
\[
\omega_{k_2}^2 = -\omega_{k_1}.
\]

The final quantity to be calculated is \(S_\alpha(\vec{q}, \eta)\). To do this one needs to have

\[(4.235)\]
\[
G_1^\xi; \alpha (\vec{k}_1, \vec{k}_1 - \vec{q}, \tau = 0^-)
\]
\[
= \frac{1}{\delta} \sum_m G_1^\xi; \alpha (\vec{k}_1, \vec{k}_1 - \vec{q}, \omega m, \xi = 0^+).
\]
After some manipulation, Eq. (4.235) leads to

\begin{equation}
G_{1;11}^\xi(\mathbf{k}_1,\mathbf{k}_1-\mathbf{q},0^-) = S_1^\xi(q,n) \left[ \frac{A_1(0)}{\omega_{\mathbf{k}_1}} \coth(\beta \omega_{\mathbf{k}_1}/2) - 1 \right]
+ \alpha_0^\xi(\mathbf{k}_1,q,n) + \alpha_1^\xi(\mathbf{k}_1,q,n) S_1^\xi(q,n) + \alpha_2(\mathbf{k}_1,q,n) S_2^\xi(q,n),
\end{equation}

\begin{equation}
G_{1;21}^\xi(\mathbf{k}_1,\mathbf{k}_1-\mathbf{q},0^-) = S_1^\xi(q,n) \frac{A_2(\mathbf{k}_1)}{\omega_{\mathbf{k}_1}} \coth(\beta \omega_{\mathbf{k}_1}/2)
+ \beta_0^\xi(\mathbf{k}_1,q,n) + \beta_1^\xi(\mathbf{k}_1,q,n) S_1^\xi(q,n) + \beta_2(\mathbf{k}_1,q,n) S_2^\xi(q,n),
\end{equation}

\begin{equation}
G_{1;12}^\xi(\mathbf{k}_1,\mathbf{k}_1-\mathbf{q},0^-) = S_2^\xi(q,n) \frac{A_1(\mathbf{k}_1^\ast)}{\omega_{\mathbf{k}_1}} \coth(\beta \omega_{\mathbf{k}_1}/2)
+ \gamma_0^\xi(\mathbf{k}_1,q,n) + \gamma_1^\xi(\mathbf{k}_1,q,n) S_1^\xi(q,n) + \gamma_2(\mathbf{k}_1,q,n) S_2^\xi(q,n),
\end{equation}

\begin{equation}
G_{1;22}^\xi(\mathbf{k}_1,\mathbf{k}_1-\mathbf{q},0^-) = S_2^\xi(q,n) \left[ \frac{A_2(0)}{\omega_{\mathbf{k}_1}} \coth(\beta \omega_{\mathbf{k}_1}/2) - 1 \right]
+ \delta_0^\xi(\mathbf{k}_1,q,n) + \delta_1^\xi(\mathbf{k}_1,q,n) S_1^\xi(q,n) + \delta_2(\mathbf{k}_1,q,n) S_2^\xi(q,n),
\end{equation}

where the following notations are used:

\begin{equation}
\alpha_0^\xi(\mathbf{k}_1,q,n) = (N/2) \frac{-m_1}{2\omega_{\mathbf{k}_1}\omega_{\mathbf{k}_1-\mathbf{q}}} \sum_{\mathbf{q}'} N_{\mathbf{q}'}(\mathbf{k}_1,\mathbf{q'},n)
\end{equation}

\begin{equation}
\times \left[ \frac{\delta_{1,5}[A_1(0) + \omega_{\mathbf{k}_1}]}{\omega_{\mathbf{k}_1}} \right] [A_1(0) + \omega_{\mathbf{k}_1-\mathbf{q}}]^\xi
+ \delta_{2,5}A_1(\mathbf{k}_1^\ast)A_2(\mathbf{k}_1-\mathbf{q})
\right],
\end{equation}
\[ \alpha_1 (\vec{k}_1, \vec{q}, n) = \frac{m_1}{2 \omega_{k_1} \omega_{k_1-q}} \left( \sum_{\kappa \phi} \right) N_{\kappa \phi} (\vec{k}_1, \vec{q}, n) \]

\[ \times \left[ A_1 (\vec{k}_1) A_2 (\vec{k}_1 - \vec{q}) A_1 (\vec{q}) / m_1 \right. \]

\[ \left. - \left[ A_1 (0) + \omega_{k_1} \right] A_2 (\vec{k}_1 - \vec{q}) A_1 (\vec{k}_1 - \vec{q}) / m_1 \right] \]

\[ \alpha_2 (\vec{k}_1, \vec{q}, n) = \frac{m_1}{2 \omega_{k_1} \omega_{k_1-q}} \left( \sum_{\kappa \phi} \right) N_{\kappa \phi} (\vec{k}_1, \vec{q}, n) \]

\[ \times \left[ \left[ A_1 (0) + \omega_{k_1} \right] A_1 (0) + \omega_{k_1-q} \right] A_2 (\vec{q}) / m_2 \]

\[ \left. - A_1 (\vec{k}_1) \left[ A_1 (0) + \omega_{k_1-q} \right] A_2 (\vec{k}_1 - \vec{q}) / m_2 \right] \]

\[ \beta_0^{\varphi} (\vec{k}_1, \vec{q}, n) = (N/2) \frac{-m_1}{2 \omega_{k_1} \omega_{k_1-q}} \left( \sum_{\kappa \phi} \right) N_{\kappa \phi} (\vec{k}_1, \vec{q}, n) \]

\[ \times \left[ \sum_{1^{\varphi}} A_2 (\vec{k}_1) \left[ A_1 (0) + \omega_{k_1-q} \right] \right. \]

\[ \left. + \sum_{2^{\varphi}} A_2 (0) + \omega_{k_1} \right] A_2 (\vec{k}_1 - \vec{q}) \] \]

\[ \beta_1 (\vec{k}_1, \vec{q}, n) = \frac{m_1}{2 \omega_{k_1} \omega_{k_1-q}} \left( \sum_{\kappa \phi} \right) N_{\kappa \phi} (\vec{k}_1, \vec{q}, n) \]

\[ \times \left[ \left[ A_2 (0) + \omega_{k_1} \right] A_2 (\vec{k} - \vec{q}) A_1 (\vec{q}) / m_1 \right. \]

\[ \left. - A_2 (\vec{k}_1) A_2 (\vec{k}_1 - \vec{q}) A_1 (\vec{k}_1 - \vec{q}) / m_1 \right] \]
\[ \beta_2(k_1,q,n) = \frac{m_1}{2\omega k_1 \omega k_1 - q} \sum_{\kappa \phi} N_{\kappa \phi}(k_1, q, n) \]

\[ \times \left[ A_2(k_1) [A_1(0) + \omega^\phi_{k_1 - q}] A_2(k_1 - q)/m_2 \right. \]
\[ - \left. [A_2(0) + \omega^\phi_{k_1}] A_1(0) + \omega^\phi_{k_1 - q}] A_2(k_1 - q)/m_2 \right] \]

\[ \gamma_0(k_1, q, n) = (N/2) \frac{-m_2}{2\omega k_1 \omega k_1 - q} \sum_{\kappa \phi} N_{\kappa \phi}(k_1, q, n) \]

\[ \times \left[ \delta_{15} [A_1(0) + \omega^\phi_{k_1}] A_1(k_1 - q) \right. \]
\[ + \left. \delta_{2r} A_1(k_1) [A_2(0) + \omega^\phi_{k_1 - q}] \right] \]

\[ \gamma_1(k_1, q, n) = \frac{m_2}{2\omega k_1 \omega k_1 - q} \sum_{\kappa \phi} N_{\kappa \phi}(k_1, q, n) \]

\[ \times \left[ A_1(k_1) [A_2(0) + \omega^\phi_{k_1 - q}] A_1(q)/m_1 \right. \]
\[ - \left. [A_1(0) + \omega^\phi_{k_1}] [A_2(0) + \omega^\phi_{k_1 - q}] A_1(k_1 - q)/m_1 \right] \]

\[ \gamma_2(k_1, q, n) = \frac{m_2}{2\omega k_1 \omega k_1 - q} \sum_{\kappa \phi} N_{\kappa \phi}(k_1, q, n) \]

\[ \times \left[ [A_1(0) + \omega^\phi_{k_1}] A_1(k_1 - q) A_2(q)/m_2 \right. \]
\[ - \left. A_1(k_1) A_1(k_1 - q) A_2(k_1 - q)/m_2 \right] \]
\[ \sum_0^{(k_1, \bar{q}, n)} = \left( \frac{N}{2} \right) \frac{m_2}{2 \omega_{k_1} \omega_{k_1-q}} \left( \sum_{k^\prime}^\Phi \right) N_{\alpha \beta}^{(k_1, \bar{q}, n)} \]

\[ \times \left[ \sum_{1}^{\sigma} A_2(k_1) A_1(k_1 - \bar{q}) \right. \]

\[ + \sum_{2}^{\tau} [A_2(0) + \omega_{k_1}^\alpha] [A_2(0) + \omega_{k_1-q}^\rho] \]

\[ S_{\alpha \beta}(k_1) A_2(0) + \omega_{k_1}^\rho \]

\[ \left. - A_2(k_1) [A_2(0) + \omega_{k_1-q}^\rho] A_1(k_1 - \bar{q})/m_1 \right] \]

\[ \sum_1^{(k_1, \bar{q}, n)} = \frac{m_2}{2 \omega_{k_1} \omega_{k_1-q}} \left( \sum_{k^\prime}^\Phi \right) N_{\alpha \beta}^{(k_1, \bar{q}, n)} \]

\[ \times \left[ A_2(0) + \omega_{k_1}^\alpha \right] [A_2(0) + \omega_{k_1-q}^\rho] A_1(k_1 - \bar{q})/m_1 \]

\[ \left. - A_2(k_1) [A_2(0) + \omega_{k_1-q}^\rho] A_1(k_1 - \bar{q})/m_1 \right] \]

\[ \sum_2^{(k_1, \bar{q}, n)} = \frac{m_2}{2 \omega_{k_1} \omega_{k_1-q}} \left( \sum_{k^\prime}^\Phi \right) N_{\alpha \beta}^{(k_1, \bar{q}, n)} \]

\[ \times \left[ A_2(k_1) A_1(k_1 - \bar{q}) A_2(k_1 - \bar{q})/m_2 \right. \]

\[ \left. - [A_2(0) + \omega_{k_1}^\alpha] A_1(k_1 - \bar{q}) A_2(k_1 - \bar{q})/m_2 \right] , \]
The self-consistency conditions for the Green's functions can be derived as follows. From Eqs. (4.219) and (4.220), one has

\begin{align*}
N_{11}(\vec{k}_1, \vec{q}, n) &= \frac{N(\omega_{k_1}) - N(\omega_{k_1-q})}{-\omega_{k_1} + \omega_{k_1-q} + i\omega_n}, \\
N_{12}(\vec{k}_1, \vec{q}, n) &= \frac{-N(\omega_{k_1}) - N(\omega_{k_1-q}) - 1}{-\omega_{k_1} - \omega_{k_1-q} + i\omega_n}, \\
N_{21}(\vec{k}_1, \vec{q}, n) &= \frac{N(\omega_{k_1}) + N(\omega_{k_1-q}) + 1}{\omega_{k_1} + \omega_{k_1-q} + i\omega_n}, \\
N_{22}(\vec{k}_1, \vec{q}, n) &= \frac{-N(\omega_{k_1}) + N(\omega_{k_1-q})}{\omega_{k_1} - \omega_{k_1-q} + i\omega_n}.
\end{align*}

(4.238)

\begin{align*}
N_{11}(\vec{k}_1, \vec{q}, n) &= \frac{N(\omega_{k_1}) - N(\omega_{k_1-q})}{-\omega_{k_1} + \omega_{k_1-q} + i\omega_n}, \\
N_{12}(\vec{k}_1, \vec{q}, n) &= \frac{-N(\omega_{k_1}) - N(\omega_{k_1-q}) - 1}{-\omega_{k_1} - \omega_{k_1-q} + i\omega_n}, \\
N_{21}(\vec{k}_1, \vec{q}, n) &= \frac{N(\omega_{k_1}) + N(\omega_{k_1-q}) + 1}{\omega_{k_1} + \omega_{k_1-q} + i\omega_n}, \\
N_{22}(\vec{k}_1, \vec{q}, n) &= \frac{-N(\omega_{k_1}) + N(\omega_{k_1-q})}{\omega_{k_1} - \omega_{k_1-q} + i\omega_n}.
\end{align*}

(4.240)

\begin{align*}
G^\xi_{\alpha_1, \alpha_1}(0^-) &= G_{\alpha_1, \alpha_1}(0^-) + \int G^\xi_{\alpha_1; \alpha_1, \alpha_1}(0^-) + O(\tau^2),
\end{align*}

(4.239)

\begin{align*}
\langle S^-_{\alpha_1} S^+_{\alpha_1} \rangle^\xi \big| \tau = 0^- \\
= 1/2 - \langle S^z_{\alpha_1} \rangle^\xi \big| \tau = 0^- \\
= 1/2 - m - f S^z_{\alpha_1}(n) - O(\tau^2).
\end{align*}

(4.240)
Hence one gets

\[(4.241) \quad S^e_{\alpha_1}(n) = G^e_{1;\alpha_1}(0^-),\]

and

\[(4.242) \quad S^e_{\alpha}(q,n) = \sum G^e_{1;\alpha_1}(0^-) \exp(-iq\cdot k_1).\]

By use of Eqs. (4.224) and (4.232), Eq. (4.242) becomes

\[(4.243) \quad S^e_{\alpha}(q,n) = (2/N) \sum G^e_{1;\alpha_1}(k_1, k_1 - q, 0^-).\]

This is the self-consistency condition. If this condition is written out in explicit form using Eq. (4.227), it follows that

\[(4.244) - S_1^e(q,n) = (2/N) \sum \left[ A_1(0) \coth(\omega_k/2)/\omega_k - 1 \right] S_1^e(q,n) + \alpha_0 + \alpha_1 S_1^e(q,n) + \alpha_2 S_2^e(q,n),\]

\[(4.244) - S_2^e(q,n) = (2/N) \sum \left[ A_2(0) \coth(\omega_k/2)/\omega_k - 1 \right] S_2^e(q,n) + \alpha_0 + \alpha_1 S_1^e(q,n) + \alpha_2 S_2^e(q,n).\]
where

\[ \alpha_0 = \frac{1}{2} \sum_k \alpha^2(k, q, n), \]

\[ \alpha_1 = \frac{1}{2} \sum_k \alpha_1(k, q, n), \text{ etc.} \]

Since \[ \langle S_{x_1} S_{x_1}^+ \rangle = 1/2 - m_\alpha \] for \( S = 1/2 \), one recognizes from Eq. (4.102) that

\[ (4.246) \quad \left( \frac{1}{2m_\alpha} \right) = \frac{1}{2} \sum_k \left[ \alpha^2(0) \coth(\varphi_k/2)/\omega_k \right]. \]

Thus, Eq. (4.244) leads to

\[ (1 + 2m_1 \alpha_1) S^x_1(q, n) + 2m_1 \alpha_2 S^x_2(q, n) = - 2m_1 \alpha_0, \]

\[ (4.247) \quad 2m_2 \bar{\alpha}_1 S^x_1(q, n) + (1 + 2m_2 \bar{\alpha}_2) S^x_2(q, n) = - 2m_2 \bar{\alpha}_0. \]

As \( m_1 = - m_2 = m \), the solution reads

\[ S^x_1(q, n) = - \frac{2m}{\Delta} \left[ \alpha_0^x - 2m(\alpha_0^x \alpha_2^x - \alpha_0^x \alpha_1^x) \right], \]

\[ (4.248) \quad S^x_2(q, n) = \frac{2m}{\Delta} \left[ \bar{\alpha}_0^x + 2m(\bar{\alpha}_0^x \alpha_1^x - \bar{\alpha}_0^x \alpha_2^x) \right], \]

with

\[ (4.249) \quad \Delta = 1 + 2m(\alpha_1^x - \alpha_2^x) - (2m)^2(\alpha_1^x \alpha_2^x - \alpha_2^x \alpha_1^x). \]
Putting these results into Eqs. (4.210) and (4.201), one finds the dynamical zz correlation functions of two spins (4.250)
\[
\langle S^z_{\alpha,-q}(t)S^z_{\beta,q}(0) \rangle
= \left\{ \frac{\alpha}{2\pi} \exp(-i\omega t) \frac{\alpha}{\exp(-i\omega t)} - 1 \right\} S^z_{q}(q,n) \bigg|_{n = -i\omega + \lambda}
\]
\[
= \left\{ \frac{\alpha}{2\pi} \exp(-i\omega t) \frac{\alpha}{\exp(-i\omega t)} - 1 \right\} S^z_{q}(q,n) \bigg|_{n = -i\omega - \lambda}
\]

Thus the task of calculating the dynamical zz correlation functions is accomplished.

In the following, some properties of the calculated zz correlation functions are discussed. To do this, the symmetry properties of \( S^z_{q}(q,n) \) and \( J_{\alpha,q}(q,\omega) \) are studied first. It can be shown (Appendix E) that

\[
\alpha^x_0(k,q,n) = -\delta^x_0 (k,\bar{q},-n),
\]
\[
\alpha^x_1(k,q,n) = -\delta^x_2 (k,\bar{q},-n),
\]
\[
\alpha^x_2(k,q,n) = -\delta^x_1 (k,\bar{q},-n),
\]

(4.251)
\[
\beta^x_0(k,q,n) = -\delta^x_0 (\bar{k},\bar{q},-n),
\]
\[
\beta^x_1(k,q,n) = -\gamma^x_2 (k,\bar{q},-n),
\]
\[
\beta^x_2(k,q,n) = -\gamma^x_1 (\bar{k},\bar{q},-n),
\]
where \( \Delta^{\pm 1} = \begin{cases} 2 & \text{if } \delta = 1 \\ 1 & \text{if } \delta = 2 \end{cases} \)

so it follows from Eq. (4.248) that

\[
(4.252) \quad S^\kappa_{\phi}(\vec{q},n) = S^{\kappa+1}_{\phi_{\pm 1}}(\vec{q},-n).
\]

The even property of \( A_\kappa(\vec{k}) \) with respect to \( \vec{k} \) guarantees that

\[
\alpha^\delta_0(\vec{q},n) = \alpha^\delta_0(-\vec{q},n),
\]

\[
(4.253) \quad \alpha^\delta_1(\vec{q},n) = \alpha^\delta_1(-\vec{q},n), \text{ etc.},
\]

for all twelve quantities in Eq. (4.237) (Appendix F). Using this one gets from Eq. (4.248) that

\[
(4.254) \quad S^\kappa_{\phi}(\vec{q},n) = S^\kappa_{\phi}(-\vec{q},n),
\]

which is exactly what one expects from the definition given by Eqs. (4.205) and (4.208) since \( S^\alpha_{\kappa,\phi} \) is even with respect to \( \vec{q} \). So Eq. (4.252) can be written alternatively as

\[
(4.255) \quad S^\kappa_{\phi}(\vec{q},n) = S^{\kappa+1}_{\phi_{\pm 1}}(-\vec{q},-n).
\]

As one can easily see from Eq. (4.210), the even property of \( S^\alpha_{\kappa}(\vec{q},n) \) with respect to \( \vec{q} \) and the symmetry property expressed by Eq. (4.252) are directly reflected in \( J^\alpha_{\kappa}(\vec{q},\omega) \). The even property of \( J^\alpha_{\kappa}(\vec{q},\omega) \) with respect to \( \vec{q} \) is simply obtained
from Eq. (4.210). This is exactly what one expects from the
definition of $J_{\alpha \beta}(\vec{q}, \omega)$ given in Eq. (4.201), since the two
operators in the left hand side of Eq. (4.201) are even with
respect to $\vec{q}$.

The symmetry property of $J_{\alpha \beta}(\vec{q}, \omega)$ with respect to the
sublattice indices can be derived from Eq. (4.252) or (4.255)
using the relation (4.210) as follows:

$$J_{\alpha \beta}(\vec{q}, n) = \frac{1}{\exp(-\varphi \omega) - 1} S^\alpha(\vec{q}, n) \bigg| \begin{array}{c} n = -i\omega + \varepsilon \\
= -i\omega - \varepsilon \end{array}$$

$$= \frac{1}{\exp(-\varphi \omega) - 1} S^\beta_{\varphi + 1}(-\vec{q}, -n) \bigg| \begin{array}{c} n = -i\omega + \varepsilon \\
= -i\omega - \varepsilon \end{array}$$

(4.256)

$$= \exp(\beta \omega) \frac{1}{\exp(\beta \omega) - 1} S^\alpha_{\varphi + 1}(-\vec{q}, n) \bigg| \begin{array}{c} n = i\omega + \varepsilon \\
= i\omega - \varepsilon \end{array}$$

$$= \exp(\beta \omega) J_{\alpha + 1, \varphi + 1}(-\vec{q}, -\omega).$$

For various combinations of $\alpha$ and $\beta$, Eq. (4.256) reads

$$J_{11}(\vec{q}, \omega) = \exp(\beta \omega) J_{22}(-\vec{q}, -\omega),$$

$$J_{12}(\vec{q}, \omega) = \exp(\beta \omega) J_{21}(-\vec{q}, -\omega),$$

(4.257)

$$J_{21}(\vec{q}, \omega) = \exp(\beta \omega) J_{12}(-\vec{q}, -\omega),$$

$$J_{22}(\vec{q}, \omega) = \exp(\beta \omega) J_{11}(-\vec{q}, -\omega).$$
From Eq. (3.21) and the definition (4.201), the following symmetry property of $J_{x'y'}(\vec{q}, \omega)$ is generally true:

(4.258) \hspace{1cm} J_{x'y'}(\vec{q}, \omega) = \exp(\beta \omega) J_{x'y'}(-\vec{q}, -\omega).

One immediately sees that the second and third equalities of Eq. (4.257) are equivalent to Eq. (4.258). If the relation (4.258) is applied to the first and last of Eq. (4.258), both of them reduce to

(4.259) \hspace{1cm} J_{11}(\vec{q}, \omega) = J_{22}(\vec{q}, \omega)

as is required by the symmetry of the problem.

To get the longitudinal correlation functions for the temperature range above the Néel point, one applies fictitious fields of the same magnitude along the preferred spin alignment directions in each sublattice and in the end takes the zero field limit. The zeroth order quantities are already discussed in Section G. For the first order quantities, the results are of the same forms as those that appear earlier in the present section except for the replacements

(4.260)

$A(0) \longrightarrow h + A(0)$,

$\omega_{k_1} = \left[ A^2(0) - A^2(\vec{E}_1) \right]^{1/2} \longrightarrow \omega_{k_1} = \left[ (h + A(0))^2 - A^2(\vec{E}_1) \right]^{1/2}$. 
These replacements appear in Eq. (4.218)-(4.255) and the symmetry properties of $J_{\alpha\phi}(\vec{q},\omega)$ still hold. The next step is to take the limit $h \to 0$. One introduces the order parameter $\chi$ and the quantity $a$ defined in Eqs. (4.172) and (4.174). The energy $\omega_{k_1}$ becomes very small and proportional to the applied fictitious field as given by Eq. (4.175). So in the limit $h \to 0$, the quantities defined in Eq. (4.238) reduces to

$$
(4.261) \quad N_{\alpha\phi}(\vec{k}_1,\vec{q},n) \to \frac{k_1^T}{\omega_{k_1} \omega_{k_1-q}} \delta_{n_0},
$$

which is independent of $\alpha$ or $\beta$. If one substitutes Eq. (4.261) into Eq. (4.237) and sums over $(\alpha\beta)$, all the terms with $\omega$'s cancel each other and the expressions simplify. So Eq. (4.237), after averaging over $\vec{k}_1$, leads to

$$
(4.262) \quad \bar{\alpha}_0^x(\vec{q},n) = \frac{2}{N} \sum_{\vec{k}_1} \bar{\alpha}_0^x(\vec{k}_1,\vec{q},n) = -\sum_{\vec{q}} \delta_{\vec{q}} \sum_{\vec{k}_1} \frac{2m}{2N} \lim_{h \to 0} \left[ \frac{\omega_{k_1-q}}{(\omega_{k_1} \omega_{k_1-q})^2} \right.
$$

$$
\times \left[ \sum_{\vec{k}_1} [h + \Delta(0)]^2 - \sum_{\vec{k}_1} A(\vec{k})A(\vec{k}-\vec{q}) \right].
$$
\( \tilde{\alpha}_1(\vec{q}, n) = -\tilde{\alpha}_2(\vec{q}, -n) \)

\[
= \lim_{h \to 0} \sum_{\text{no}} \frac{2}{(N/2) \sum_k \left( \omega_k \omega_{k-q} \right)^2} 
\times \left[ - A(k)A(k'q)A(q) + [h+A(0)]A(k-q)A(k-q) \right],
\]

\( \tilde{\alpha}_2(\vec{q}, n) = -\tilde{\alpha}_1(\vec{q}, -n) \)

\[
= \lim_{h \to 0} \sum_{\text{no}} \frac{2}{(N/2) \sum_k \left( \omega_k \omega_{k-q} \right)^2} 
\times \left[ [h+A(0)]^2A(q) - [h+A(0)]A(k)A(k-q) \right],
\]

and similar expressions for \( \bar{\chi} \)'s and \( \bar{\eta} \)'s which are omitted here. Putting Eq. (4.262) into Eq. (4.248), one can show (Appendix G) that

\[
S_1^1(\vec{q}, n) = S_2^2(-\vec{q}, -n)
= \frac{x(1 + ax)}{(1 + ax)^2 - (ax\gamma)^2} \sum_{\text{no}}.
\]

(4.263)

\[
S_2^1(\vec{q}, n) = S_1^2(-\vec{q}, -n)
= \frac{-ax^2\gamma}{(1 + ax)^2 - (ax\gamma)^2} \sum_{\text{no}}.
\]
using the notations in Eqs. (4.170)–(4.174). By Eqs. (4.205)–(4.208), using Eq. (4.263), one obtains

\[
\langle S_{\alpha,-q}^z S_{\phi,q}^z \rangle = \mathcal{G}_{-\phi}^z (q, \tau = 0^+) = (1/\phi) S_{\phi}^z (q, n=0); \tag{4.264}
\]

so that taking into account the even property of \( S_{\phi}^z (k, n) \) in \( k \), one sees that Eq. (4.263) is equivalent to

\[
\langle S_{1,-k}^z S_{1,k}^z \rangle = \langle S_{2,-k}^z S_{2,k}^z \rangle = (N/2\beta) \frac{x(1 + ax)}{(1 + ax)^2 - (ax\gamma)^2}, \tag{4.265}
\]

\[
\langle S_{1,-k}^z S_{2,k}^z \rangle = \langle S_{2,-k}^z S_{1,k}^z \rangle = (N/2\beta) \frac{-ax^2\gamma}{(1 + ax)^2 - (ax\gamma)^2}.
\]

These results together with Eq. (4.179) show that the xx, yy, and zz correlation functions are all equal. This is to be expected, because, when \( h \to 0 \) in the paramagnetic region, all spin directions in space must be equivalent.

There is sum rule for the static correlation functions of the spins, namely

\[
(2/N) \sum_k \langle S_{\alpha,-k}^z S_{\alpha,k}^z \rangle = (N/2) S(S+1). \tag{4.266}
\]
Above the Neél point, the left hand side is

\[
(3/\delta) \sum_k \frac{x(1 + ax)}{k (1 + ax)^2 - (ax')^2}
\]

which is equal to \((N/2)(3/4)\) if one uses the relation

\[
(1/2m) = \frac{h + A(0)}{2 \omega_k} \coth(\omega_k/2) \bigg|_{T > T_N}
\]

or

\[
(4.26?) \quad (1/4) = \frac{2/N}{1 + ax)^2 - (ax')^2}
\]

So the sum rule checks.

One expects the correlation functions to be continuous at the Neél temperature. From Eq. (4.265), by putting \(x \to \infty\) (which corresponds to \(T \to T_N^+\)), one observes that

\[
\langle S^Z_1, -k S^Z_1, k \rangle = \langle S^Z_2, -k S^Z_2, k \rangle
\]

\[
= (N/2) \frac{k T_N}{a(1 - \gamma^2)}
\]

(4.268)

\[
\langle S^Z_1, -k S^Z_2, k \rangle = \langle S^Z_2, -k S^Z_1, k \rangle
\]

\[
= (N/2) \frac{k T_N \gamma}{a(1 - \gamma^2)}
\]
By comparing these results with Eq. (4.183), one sees that the correlation functions are continuous at the Néel temperature. Thus the sum rule and rotational invariance of the correlation functions hold at and above the Néel temperature, and the correlation functions are continuous at the Néel temperature. One hopes that the sum rule checks below the Néel temperature, but there seems to be no easy way of checking it because of much complicated algebra. Perhaps one should not even expect to do so, because the expressions for the correlation functions are only approximate.

J. Parallel Susceptibility

The parallel susceptibility can be calculated from its definition as follows: A constant external field, which is parallel to the spin alignment direction, is applied to both sublattices simultaneously. It is to be noted that, in contrast with the previous discussions of the paramagnetic phase, the applied field here is a real physical field and of the same direction for both sublattices, so that the symmetry of two sublattices is broken. Then the susceptibility is given by the ratio of the total magnetization to the applied field.

For this purpose, the following Hamiltonian is used:

\[
H' = H - f \sum_{\alpha_1} S_{\alpha_1}^z \exp(\xi t)
\]

\[(4.269)\]

\[
= H - f \exp(\xi t)(S_{1,0}^z + S_{2,0}^z), \quad \xi = 0^+.
\]
Then the parallel susceptibility is given by

\[ \chi'' = (g \mu_B)^2 \sum_{\mathbf{k}} \langle S^z_{\mathbf{k},1} \rangle' \langle S^z_{\mathbf{k},2} \rangle' \exp(\xi t) \]

(4.270)

\[ = (g \mu_B)^2 (\langle S^z_{1,0} \rangle' + \langle S^z_{2,0} \rangle') \exp(\xi t). \]

In the imaginary time formalism, Eqs. (4.269) and (4.270) read

(4.271) \[ H' = H - f(S^z_{1,0} + S^z_{2,0}), \]

(4.272) \[ \chi'' = (g \mu_B)^2 (\langle S^z_{1,0} \rangle' + \langle S^z_{2,0} \rangle')/f. \]

All the notations retain their definitions given before. For example, \( m_\alpha \) means sublattice magnetization without field and \( \langle S^z_{\mathbf{k},1} \rangle' \) is that with field.

From Eqs. (3.51), (4.220), and (4.269), it follows that

\[ \langle S^z_{1,0} \rangle' = \langle S^z_{1,0} \rangle + f S^1_{1}(0,0) + f S^2_{1}(0,0) + O(f^2) \]

(4.273)

\[ = (N/2)m_1 + f S^1_{1}(0,0) + f S^2_{1}(0,0) + O(f^2), \]

\[ \langle S^z_{2,0} \rangle' = (N/2)m_2 + f S^1_{2}(0,0) + f S^2_{2}(0,0) + O(f^2), \]

where the quantities on the right hand sides are those already calculated in previous sections (with \( q = 0 \) and \( n = 0 \)).
Since \( m_1 = - m_2 = m \), by putting \((4.273)\) into \((4.272)\), one gets

\[
\chi_n = (g \mu_B)^2 [s_1^1(0,0) + s_2^0(0,0) + s_1^1(0,0) + s_2^0(0,0)]
\]

\[(4.274)\]

\[
= 2(g \mu_B)^2 \lim_{q \to 0} [s_1^1(q,0) + s_1^0(q,0)].
\]

The last step follows from the symmetry property of \( S_q^\phi(q,n) \) as given in Eq. \((4.255)\).

From the definition \((4.237)\), it follows that

\[
\alpha_0^\phi(k,\vec{q} = 0,n = 0)
\]

\[(4.275)\]

\[
= \lim_{q \to 0} \frac{m}{2 \omega_k \omega_{k-q}} \left( \sum_{\phi} \right) N_{\alpha\phi}(k,\vec{q},0)
\]

and there are similar expressions for all the other \( \alpha \)'s, \( \gamma \)'s, \( \varphi \)'s, and \( S \)'s. From the definitions \((4.237)\) and \((4.238)\), one finds

\[(4.276)\]

\[
\alpha_0^\phi(k,0,0) = - \delta_0^{\phi+1}(k,0,0)
\]
\[ \alpha_1(k,0,0) = -\varepsilon_2(k,0,0) = 0, \]
\[ \alpha_2(k,0,0) = -\varepsilon_1(k,0,0) \]

with

\[ (1,1) = \lim_{\rho \to 0} \left[ N_{11}(k,q,0) + N_{22}(k,q,0) \right] \]

(4.277) \[ = 2 \beta \exp(\beta \omega_k) / [\exp(\beta \omega_k) - 1]^2, \]

\[ (1,2) = \lim_{\rho \to 0} \left[ N_{12}(k,q,0) + N_{21}(k,q,0) \right]. \]

By substituting these expressions into Eq. (4.248), one gets \( S_q(0,0) \). The result can be shown (Appendix H) to be

(4.278) \[ \chi_n = (N/2)(g \mu_B)^2 2 \varepsilon(2m)^2 (2/N) \sum_k \frac{\exp(\beta \omega_k)}{[\exp(\beta \omega_k) - 1]^2} \]
One observes that

\[(4.279) \quad \chi_n \longrightarrow 0 \quad \text{as} \quad T \longrightarrow 0^+\]

since the quantity under summation signs vanishes as \( T \longrightarrow 0^+ \). At a temperature just below the Néel point, it is evident that

\[
\frac{\exp(\beta \omega_k)}{[\exp(\beta \omega_k) - 1]^2} \longrightarrow \frac{1}{(\beta \omega_k)^2} \quad \text{as} \quad T \longrightarrow T_N^-.
\]

So Eq. \((4.246)\) reduces to

\[
(1/2m) = (2/N) \sum_k \frac{2A(0)}{\beta (\omega_k)^2} \quad \text{as} \quad T \longrightarrow T_N^-.
\]

Hence, it follows that

\[
(\chi_n)_{T_N} = (N/2)(g \mu_B)^2 m/A(0) \bigg|_{T_N^-} \]

\[
(4.280)
\]

\[
= (N/2)(g \mu_B)^2/(2J_0) \bigg|_{T_N^-}
\]

\[
= (\chi_1)_{T_N}.
\]
The last step follows from Eq. (4.152). Thus the parallel susceptibility vanishes at absolute zero and becomes equal to the perpendicular susceptibility as the temperature approaches the Néel temperature.

If one uses the RPA method, Eq. (4.280) agrees with Lines' result (1964). It is to be noted that the second term of the denominator is absent in spin-wave theory and the spin-wave theory does not give factor \((2m)^2\) as one can see from Eq. (2.78). The extra term in the denominator vanishes at \(T = 0\) and is equal to unity at \(T = T_N\), while \((2m)^2\) varies from \((2m_0)^2\) to zero, so that the effects of these two terms compensate to some extent. At very low temperatures, \(m\) varies slightly with temperature and the extra term in the denominator is vanishingly small, so that one expects very good agreement with the spin-wave theory.

For \(S = 1/2\), numerical calculations of parallel and perpendicular susceptibilities have been carried out, and results are shown in Figs. 5 and 6.

K. Energy and Specific Heat

For the Heisenberg antiferromagnet with nearest neighbor interactions described by the Hamiltonian (4.1a) or (4.157), the internal energy is given by

\[
U = \langle H \rangle = -Nhm + (2zJ)(2/N) \sum_k \chi(k) \langle \vec{S}_{1,-k} \cdot \vec{S}_{2,k} \rangle
\]
Fig. 5. Susceptibilities for simple cubic structure ($S = 1/2$).
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SUSCEPTIBILITIES (ARBITRARY UNITS)

TEMPERATURE (T/Tn)

\( X_\perp \)

\( X_\parallel \)

\( X_P \)

MOLECULAR FIELD THEORY
Fig. 6. Susceptibilities for body centered cubic structure \((S = 1/2)\).
SUSCEPTIBILITIES (ARBITRARY UNITS)

TEMPERATURE \((T/T_N)\)

\(T_{\text{C1}}\)

\(T_{\text{C2}}\)

\(T_{\text{p}}\)
with \( \gamma(\tilde{r}) \) and \( S_\alpha, k \) defined in Eqs. (4.43) and (4.96). So the internal energy can be computed if the static correlation functions of the spins are known. Differentiating the internal energy with respect to temperature, one obtains the specific heat due to spin disorder. From this one can calculate the entropy of the system. In this manner, all the thermodynamic functions may be computed.

Although expressions for all the correlation functions have already been obtained, it is still hard to carry out this study at a general temperature because of the complex algebra involved. In this section, only the properties in the paramagnetic temperature region when \( h \to 0 \) will be studied. In this case, from Eqs. (4.179) and (4.281) it follows that

\[
U = - (2zJ) \frac{k_B T}{k} \gamma^2 \sum \frac{\alpha x^2}{(1 + ax)^2 - (ax\gamma)^2}
\]

(4.282)

\[
= - \frac{(3N/2)(2zJ)\gamma^2}{2} \frac{\alpha x^2}{(1 + ax)^2 - (ax\gamma)^2}
\]

with notations defined in Eqs. (4.170), (4.172), and (4.174).

Since \( x \to \infty \) as \( T \to T_N^+ \), one finds that

(4.283) \( U_N = - \frac{(3/2)Nk_B T(I_0 - 1)}{P_N} \)

with notations defined in Eqs. (4.111) and (4.112). From Eqs. (4.184) and (4.176), one finds that
\[(4.284) \quad a = 2zJ \left[ 1 + \frac{4ax^2}{9} - \frac{\gamma^2}{N} \sum_{k} \frac{1}{(1 + ax)^2 - (ax\gamma)^2} \right]. \]

\[(4.285) \quad \frac{1}{4x} = \left( \frac{1 + ax}{9} \right) \left[ \frac{2}{N} \sum_{k} \frac{1}{(1 + ax)^2 - (ax\gamma)^2} \right]. \]

and hence a relation between \(a\) and \(x\)

\[(4.286) \quad 1/4x = 1/9 + a^2/8zJ - a/2. \]

By use of Eq. (4.284), the internal energy can be written as

\[(4.287) \quad U = -(3/8)N(a - 2zJ). \]

So the specific heat is given by

\[(4.288) \quad C = (\frac{dU}{dT}) = -(3/8)N(\frac{da}{dT}). \]

Differentiating Eqs. (4.285) and (4.286) with respect to \(T\) and solving the result, one finds \(\frac{da}{dT}\). So the specific heat is given by

\[(4.289) \quad C = (3/8)N \left\{ \left[ \beta(1 + ax) + 4x \right] I_1 - 8x(1 + ax)^2 I_2 \right\} \]

\[\times \left\{ \beta ax^3 \left[ I_1 - 2(1 + ax)^2 I_2 \right] I_3 \right\}^{-1} \]

\[\times \left\{ - \frac{1}{(1/a)[(2 + ax)I_1 - 2(1 + ax)^2 I_2]} \right\}, \]
where

\[(4.290)\quad I_1 = (2/N) \sum_k \frac{1}{(1 + ax)^2 - (ax\gamma)^2},\]

\[(4.291)\quad I_2 = (2/N) \sum_k \frac{1}{[(1 + ax)^2 - (ax\gamma)^2]^2},\]

\[(4.292)\quad I_3 = (2/N) \sum_k \frac{\gamma^2}{(1 + ax)^2 - (ax\gamma)^2}.\]

Since \(x \to \infty\) as \(T \to T_N^+\), one finds

\[(4.293)\quad C_N = (3/8)N \frac{(a\beta + 4)I_o - 8I_4}{(8/a\beta)(I_o - 1)(I_o - 2I_4) - I_o},\]

where

\[(4.294)\quad I_4 = (2/N) \sum_k (1 - \gamma^2)^{-2},\]

\[(4.295)\quad I_o = (2/N) \sum_k (1 - \gamma^2)^{-1} > 1.\]

The latter constant was also defined in Eq. \((4.111)\). From Eqs. \((4.115)\), it follows that

\[(4.295)\quad (a\beta)_{T=T_N} = 4I_o.\]
so one gets

\[ C_n = (3/2)N \frac{I_0(I_0 + 1) - 2I_4}{2(1 - 1/I_0)(I_0 - 2I_4) - I_0} > 0. \]  

Using Eqs. (4.284) and (4.285), one can show that

\[ C = (3/8)N(zJ/T)^2(2/N)^2 \sum_k (\gamma^2 + O(T^{-3})) \text{ as } T \to \infty, \quad (k_B = 1). \]

One can also show this from Eq. (4.282) by expanding it in powers of \( T^{-1} \) and differentiating the result with respect to \( T \).
V. SUMMARY

The most important feature of the Green's function theory is that it has no restriction on the temperature range of its application, while the older theories suffer from the drawback that their applicability is limited to a certain range of temperatures. The present investigation reveals that the Green's function theory not only agrees with the limiting theories at both temperature limits but also shows improvements to the old theories in predicting more physical facts. In the following, the accomplishments of the present investigation are summarized and further work is suggested.

For arbitrary spin $S$, temperature $T$, and nearest neighbor interaction $J$, the energy spectrum ($\omega_k$), the sublattice magnetization per spin ($m$), and the transverse spin correlation functions ($\langle S^+_{\sigma,\mathbf{k}} S^-_{\sigma,\mathbf{j}} \rangle$ and $\langle S^+_{\sigma,\mathbf{k}} S^+_{\sigma,\mathbf{j}} \rangle$) are completely determined via a set of coupled equations: Eqs. (4.92), (4.94), (4.99), (4.101), and (4.105). At low temperatures, the results show very good agreement with the interacting spin-wave theory (Oguchi, 1960; Liu, 1966) in lowest order. The present theory also predicts the existence of Neél temperature and a second order phase transition there. For $S = 1/2$, the above-mentioned equations reduce to Eq. (4.106) and (4.107), and numerical work for Eq. (4.106) has been carried out and some results are shown in Figs. 1, 2, 3, and 4.
The perpendicular susceptibility for arbitrary spin value \( S \) is given by Eq. (4.152). It is found that the perpendicular susceptibility is slightly temperature-dependent, which is also predicted by the interacting spin-wave theory. The decrease of perpendicular susceptibility with rising temperature has been observed by Trapp and Stout (1963) for \( \text{MnF}_2 \). The temperature-independent term is the same as that of interacting spin-wave theory, while the \( T^2 \) term gives a deviation of order \( c/S \).

Analysis above the Néel temperature is presented in Section G and the continuity of a number of properties at the Néel temperature is shown. In Section H, the correlation length between two spins above the Néel point is derived in the long wavelength limit. The result is similar to Van Hove's result (1954) for ferromagnetism.

In Section I, the longitudinal correlation functions of two spins are calculated by extending Liu's work (1965) for ferromagnetism to antiferromagnetism. To do this, Callen's decoupling scheme for the three-spin Green's functions without perturbation has to be extended for Green's functions with perturbation. A proper extension was found and all the calculations in Sections I, J, and K are based on the extended scheme. The longitudinal correlation functions of two spins are given by Eqs. (4.248) and (4.250) with notations in Eqs. (4.237), (4.238) and (4.249). It is shown that the
correlation functions are rotationally invariant at and above the Neel temperature. Also the sum rule for spin operators is shown to hold over the same temperature range.

The parallel susceptibility is calculated in Section J and the result is given in Eq. (4.278). It vanishes at absolute zero and becomes equal to the perpendicular susceptibility as the temperature approaches the Neel temperature. At very low temperatures, the result is in very good agreement with the spin-wave theory. For $S = 1/2$, numerical calculations of parallel and perpendicular susceptibilities have been carried out, and the results are shown in Figs. 5 and 6. In Section K, the energy and specific heat above the Neel temperature are discussed.

The ground state energy of the antiferromagnetic spin system is an important physical quantity. As shown in Eq. (4.281), the internal energy is expressible in terms of dynamical correlation functions of two spins. The explicit calculation involves a great deal of labor and will be carried out in a separate investigation.
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VIII. APPENDICES

Appendix A. Values of Some Sums

\[(A.1) \quad c = (2/N) \sum_k \{1 - [1 - \gamma^2(k)]^{1/2}\} \approx \begin{cases} 0.097 & \text{for s.c.} \\ 0.073 & \text{for b.c.c.} \end{cases} \quad (1st \ zone)\]

\[(A.2) \quad c' = (2/N) \sum_k \{[1 - \gamma^2(k)]^{-1/2} - 1\} \approx \begin{cases} 0.156 & \text{for s.c.} \\ 0.150 & \text{for b.c.c.} \end{cases} \quad (1st \ zone)\]

\[(A.3) \quad \alpha = (2/N) \sum_k \{1 - \gamma^2(k)\}^{-1} \approx \begin{cases} 1.516 & \text{for s.c.} \\ 1.393 & \text{for b.c.c.} \end{cases} \quad (1st \ zone)\]

Appendix B. Derivation of Eqs. (4.50) and (4.51)

From the definition (4.43), it follows that

\[
\sum_{\mathbf{k'}} \gamma(\mathbf{k' - k}) \psi_\alpha(\mathbf{k'},0) = \sum_{\mathbf{k'}} \left[ (1/z) \sum_{\mathbf{s}} \exp(i\mathbf{k' \cdot s} - i\mathbf{k \cdot s}) \right] \psi(\mathbf{k'},0)
\]

\[
= (1/z) \sum_{\mathbf{s}} \exp(-i\mathbf{k \cdot s}) \left[ \sum_{\mathbf{k'}} \exp(i\mathbf{k' \cdot s}) \psi_\alpha(\mathbf{k'},0) \right].
\]

By symmetry, the sum over \( \mathbf{k'} \) is clearly independent of \( \mathbf{s} \), so that it can be replaced by

\[
(1/z) \sum_{\mathbf{s'}} \left[ \sum_{\mathbf{k'}} \exp(i\mathbf{k' \cdot s'}) \psi_\alpha(\mathbf{k'},0) \right].
\]
Hence Eq. (B.1) leads to

\[
\sum_{k'} \gamma(k' - k) \psi_n(k', 0)
\]

\[
= \frac{1}{z} \sum_{s} \exp(-ik\cdot s) \left[ \frac{1}{z} \sum_{k'} \exp(ik'\cdot s') \psi_n(k', 0) \right]
\]

\[
= \gamma(k) \sum_{k'} \gamma(k') \psi_n(k', 0),
\]

which is Eq. (4.50).

From the definitions of \( s_{11}^+ \) and \( s_{2j}^+ \), it follows that

\[
\langle s_{11}^- s_{2j}^+ \rangle = \langle s_{11}^- s_{11}^+ + s_{11}^- s_{2j}^- - \frac{1}{2}(s_{11}^- s_{2j}^- - s_{11}^+ s_{2j}^+) \rangle
\]

\[
= \langle s_{11}^- s_{2j}^- + s_{11}^+ s_{2j}^+ \rangle
\]

since \( \langle s_{11}^- s_{2j}^- \rangle = \langle s_{11}^- s_{2j}^+ \rangle \) by symmetry. Similarly one gets

\[
\langle s_{2j}^- s_{11}^+ \rangle = \langle s_{2j}^- s_{11}^- + s_{2j}^+ s_{11}^+ \rangle,
\]

so that one finds

\[
\langle s_{11}^- s_{2j}^+ \rangle = \langle s_{2j}^- s_{11}^+ \rangle.
\]

From Eq. (B.6), it follows that

\[
\gamma_{12}(k, 0) = \sum_{i-j} \langle s_{11}^- s_{2j}^+ \rangle \exp(ik\cdot i - ik\cdot 2j)
\]
\[ \sum_{i,j} \langle S^-_2 S^+_1 \rangle \exp(-i \bar{k} \cdot 2 \bar{j} + i \bar{k} \cdot \bar{i}) \]
\[ = \sum_{i,j} \langle S^-_2 S^+_1 \rangle \exp(i \bar{k} \cdot 2 \bar{j} - i \bar{k} \cdot \bar{i}) \]
\[ = \varphi_{21}(\bar{k}, 0), \]
which is Eq. (4.51).

Appendix C. Derivation of the Identity (4.59)

The identity is well-known and has been widely used. A simple derivation is shown below. As shown in Eq. (3.36), one has the transformation pair

\[ G(\tau) = \frac{1}{\beta} \sum_n G(n) \exp(-i \omega_n \tau), \quad \omega_n = (2\pi n/\beta), \]
(C.1)

\[ G(n) = \int_0^\beta d\tau \, G(\tau) \exp(i \omega_n \tau), \]
i.e., one has to solve for \( G(\tau) \) satisfying

\[ \frac{1}{\pm \omega_k - i \omega_n} G(n) = \int_0^\beta d\tau \, G(\tau) \exp(i \omega_n \tau) \]
(C.2)

to get the right hand side of the identity (4.59). If one puts

\[ G(\tau) = A \exp(\overline{\tau} \cdot \omega_k \tau), \]
(C.3)
the last equation gives

\[(C.4) \quad \frac{1}{\omega_k - i\omega_n} = G(n) = \frac{A [1 - \exp(\pm \omega_k)]}{\omega_k - i\omega_n}\]

so that

\[(C.5) \quad G(\tau) = \frac{\exp(\mp \omega_k \tau)}{1 - \exp(\pm \beta \omega_k)} ,\]

which is the right hand side of the identity (4.59).

Appendix D. Value of the Order Parameter \(x\) at the Neel Temperature

Above the Neel temperature, \(\phi\) is given by Eq. (4.177):

\[(D.1) \quad \phi \rightarrow (1/h) (2/N) \sum \frac{(1 + ax) k_B T}{k (1 + ax)^2 - (ax\gamma)^2} \]

so that \(\phi \rightarrow \infty\) as \(h \rightarrow 0\). Hence Callen's relation (4.94) for \(m\) reduces to

\[(D.2) \quad m \rightarrow S(S + 1)/3\phi ,\]

so it can be written as

\[(D.3) \quad \frac{S(S + 1)}{3x} = \frac{2k_B T}{N} \sum \frac{(1 + ax)}{k (1 + ax)^2 - (ax\gamma)^2} .\]
This is the equation for $x$. When $x \to \infty$, Eq. (D.3) reduces to

$$S(S + 1)/3 = \left( k_B T_\infty /a_\infty \right) (2/N) \sum \frac{1}{k (1 - \gamma^2)}$$

(D.4)  

$$= \left( k_B T_\infty /a_\infty \right) I_0.$$

On the other hand, from Eq. (4.176), $a_\infty$ is given by

$$a_\infty = 2zJ \left[ 1 + \frac{2a_\infty k_B T_\infty}{S^2 a_\infty^2 N} \sum \frac{\gamma^2}{k (1 - \gamma^2)} \right]$$

(D.5)  

$$= 2zJ \left[ 1 + k_B T_\infty (I_0 - 1)/a_\infty S^2 \right].$$

Putting (D.4) into (D.5), one obtains

(D.6)  

$$a_\infty = 2zJ \left[ 1 + (S + 1)(I_0 - 1)/3SI_0 \right].$$

Eqs. (D.4) and (D.6) give

(D.7)  

$$k_B T_\infty = \frac{2zJS(S + 1)}{3I_0} \left[ 1 + \frac{(S + 1)(I_0 - 1)}{3SI_0} \right].$$

From Eq. (4.117), one realizes that the right hand side of Eq. (D.7) is just $k_B T_N$. Thus the temperature at which $x$ diverges is the Néel temperature.
Appendix E. Derivation of Eq. (4.251)

From the definition (4.238), it is evident that

\[(E.1) \quad N_{\alpha\phi}(\vec{k}, \vec{q}, n) = N_{\alpha+1, \phi+1}(\vec{k}, \vec{q}, -n).\]

So, considering the fact that

\[\omega_k^\alpha = -\omega_k^{\alpha+1},\]

\[(E.2) \quad A_{\alpha}(\vec{k}) = -A_{\alpha+1}(\vec{k}),\]

\[m_\alpha = -m_{\alpha+1},\]

one obtains from Eq. (4.237) that

\[(E.3) \quad \chi^\xi(\vec{k}, \vec{q}, n) = \frac{-m_2(N/2)}{2\omega_k \omega_{k-q}} \sum_{\alpha, \phi} N_{\alpha\phi}(\vec{k}, \vec{q}, n)\]
\[\times \left[ \delta_{s1}[A_1(0) + \omega_k^\alpha] A_1(\vec{k} - \vec{q}) \right.\]
\[\ldots + \delta_{s2} A_1(\vec{k}) [A_2(0) + \omega_{k-q}^\phi]\]
\[= \frac{m_1(N/2)}{2\omega_k \omega_{k-q}} \sum_{\alpha, \phi} N_{\alpha+1, \phi+1}(\vec{k}, \vec{q}, -n)\]
\[\times \left[ \delta_{s1+2}[A_2(0) + \omega_k^{\alpha+1}] A_2(\vec{k} - \vec{q}) \right.\]
\[\ldots + \delta_{s1+2} A_2(\vec{k}) [A_1(0) + \omega_{k-q}^{\phi+1}]\]
where the running indices $\alpha$ and $\beta$ are relabeled by $(\alpha^\pm 1)$ and $(\beta^\pm 1)$. The last expression is just the definition of $\bar{\alpha}^0_{\bar{q},n}$. The other five identities can be derived similarly.

Appendix F. Derivation of Eq. (4.253)

From the definition (4.237), it follows that

$$\bar{\alpha}^0_{\bar{q},n} = \frac{2}{N} \sum_{k} \bar{\alpha}^0_{k,\bar{q},n}$$

$$= \sum_{k} \frac{-m_1}{2 \omega_{k,\bar{q},n}} \sum_{\alpha^\phi} N_{\alpha^\phi}(k,\bar{q},n)$$

(F.1)

$$\times \left[ \bar{\delta}_{\xi_1} [A_1(0) + \omega_{k}^\alpha] [A_1(0) + \omega_{k,q}^\beta] \right]$$

$$\quad + \bar{\delta}_{\xi_2} A_2(k) A_2(k-q)$$

Since $k$ is a running index over points inside the first Brillouin zone of $k$-space, it can be changed to $-k$ inside the summation sign. Then the replacements

(F.2) $\omega_{k} \rightarrow \omega_{-k} = \omega_{k}^\perp$, 
\[ \omega_{k-q} \rightarrow \omega_{-k-q} = \omega_{k+q}, \]
\[ A_{\alpha}(\mathbf{k}) \rightarrow A_{\alpha}(-\mathbf{k}) = A_{\alpha}(\mathbf{k}), \]
\[ A_{\alpha}(\mathbf{k} - \mathbf{q}) \rightarrow A_{\alpha}(-\mathbf{k} - \mathbf{q}) = A_{\alpha}(\mathbf{k} + \mathbf{q}) \]

are possible, and the equalities are guaranteed by the even character of \( A_{\alpha}(\mathbf{k}) \) and \( \omega_{k} \) with respect to \( \mathbf{k} \).

Appendix G. Derivation of Eq. (4.263)

For \( T \geq T_{N} \), Eq. (4.262) guarantees that \( \vec{\alpha}'s \) and \( \vec{\varepsilon}'s \) are even with respect to \( n \), so that taking into account their symmetry property on subscripts one gets

\[ (G.1) \quad \Delta = \lim_{h \to 0} \left[ 1 + 2m(\vec{\alpha}_1 + \vec{\alpha}_2) \right] \left[ 1 + 2m(\vec{\alpha}_1 - \vec{\alpha}_2) \right]. \]

One has, from Eq. (4.163), that

\[ (G.2) \quad G_{11}(\mathbf{k},m) = \int d\tau \exp(i\omega_{m}\tau) G_{11}(\mathbf{k},\tau) \]

\[ = m \left[ 1 + \frac{h + A(0)}{\omega_{k}} \right] \frac{1}{\omega_{k} - i\omega_{m}} \]

\[ - m \left[ 1 - \frac{h + A(0)}{\omega_{k}} \right] \frac{1}{\omega_{k} + i\omega_{m}}. \]

It is evident that

\[ (G.3) \quad \lim_{h \to 0} G_{11}(\mathbf{k},n) = \delta_{n0} \lim_{h \to 0} G_{11}(\mathbf{k},n = 0). \]
Now since

\[ G_{11}(\vec{k}, \tau = 0^-) = \frac{1}{\varphi} \sum_n G_{11}(\vec{k}, n) \exp(+i\omega_n \tau), \ \tau = 0^+ , \]

if

\[ G_{11}(\vec{k}, n) = \sum_{n=0} G_{11}(\vec{k}, n = 0), \]

one finds

\[ G_{11}(\vec{k}, \tau = 0^-) = \frac{1}{\varphi} G_{11}(\vec{k}, n = 0). \]

Hence, from the definition of \( G_{11}(\vec{k}, \tau) \) and Eqs. (G.2)-(G.4), one can derive the following identity:

\[ 1 = 2( \langle S^{-} S^{+} \rangle )_{T > T_{N}} \]

\[ = \lim_{h \to 0} (\sum_{n=0}^{\beta}) \frac{2}{N} \sum_{k} \frac{\mu_{m} h + A(0)}{(\omega_{k} \omega_{k-q})^2} \]

For brevity, the following notation will be adopted:

\[ [f(\vec{k})] = \lim_{h \to 0} (\sum_{n=0}^{\beta}) \frac{2}{N} \sum_{k} \frac{\mu_{m} h + A(0)}{(\omega_{k} \omega_{k-q})^2} f(\vec{k}). \]

Then, from Eqs. (4.262) and (G.5), it follows that

\[ \Delta = \lim_{h \to 0} [1 + 2m(\vec{\alpha}_{1} + \vec{\alpha}_{2})][1 + 2m(\vec{\alpha}_{1} - \vec{\alpha}_{2})] \]
\[
\begin{align*}
&= \left[ [h + A(0)] (\omega_{k-q})^2 - A(\vec{k})A(\vec{k}-\vec{q})A(\vec{q}) \\
&+ [h + A(0)]A(\vec{k}-\vec{q})A(\vec{k}-\vec{q}) + [h + A(0)]^2A(\vec{q}) \\
&- [h + A(0)]A(\vec{k})A(\vec{k}-\vec{q}) \right] \\
&\times \left[ [h + A(0)] (\omega_{k-q})^2 - A(\vec{k})A(\vec{k}-\vec{q})A(\vec{q}) \\
&+ [h + A(0)]A(\vec{k}-\vec{q})A(\vec{k}-\vec{q}) - [h + A(0)]^2A(\vec{q}) \\
&+ [h + A(0)]A(\vec{k})A(\vec{k}-\vec{q}) \right] \\
&= (\omega_q)^2 \left[ [h + A(0)]^2 - A(\vec{k})A(\vec{k}-\vec{q}) \right] \\
&\times \left[ [h + A(0)]^2 + A(\vec{k})A(\vec{k}-\vec{q}) \right].
\end{align*}
\]

Since Eq. (G.5) means
\[
(G.8) \quad 1 = \left[ [h + A(0)] (\omega_{k-q})^2 \right],
\]
it follows that
\[
(G.9) \quad \alpha_0^5 - 2m(\alpha_0^5 \bar{\delta}_2 - \bar{\delta}_0 \alpha_2)
\]
\[
= \alpha_0^5 \left[ [h + A(0)] (\omega_{k-q})^2 \right] - 2m(\alpha_0^5 \bar{\delta}_2 - \bar{\delta}_0 \alpha_2)
\]
\[
= - (N/4) \left[ \Sigma_{S1} [h + A(0)]^2 - \bar{\delta}_2 A(\vec{k})A(\vec{k}-\vec{q}) \right] \\
\times \left[ [h + A(0)]^3 - A(\vec{k})A(\vec{k}-\vec{q})A(\vec{q}) \right]
\]
\[ + \left( \frac{N}{4} \right) \left[ \sum_{s=1,2} \left[ h + A(0) \right]^2 - \sum_{s=1,2} A(\vec{k})A(\vec{k}-q) \right] \]
\[ \times \left[ \left[ h + A(0) \right]^2 - \left[ h + A(0) \right]A(\vec{k})A(\vec{k}-q) \right] \]
\[ = \left[ \left[ h + A(0) \right]^2 + A(\vec{k})A(\vec{k}-q) \right] \times \left[ \left[ h + A(0) \right]^2 - A(\vec{k})A(\vec{k}-q) \right] \]
\[ \times \left( \frac{N}{4} \right) \begin{cases} - \left[ h + A(0) \right] & \text{when } S = 1 \\
A(\vec{q}) & \text{when } S = 2. \end{cases} \]

If one substitutes (G.7) and (G.9) into Eq. (4.248), one gets Eq. (4.263).

Appendix H. Derivation of Eq. (4.278)

With Eq. (4.276), it follows from Eqs. (4.248) and (4.249) that

\[ \Delta = 1 - (2m \bar{x}_2)^2 \]
\[ = 1 - \left[ 4mA(0)\beta(2/N) \sum_{k} \frac{\exp(\beta \mu_k)}{\left[ \exp(\beta \mu_k) - 1 \right]^2} \right] \]
\[ S_1^1(0,0) + S_1^2(0,0) \]
\[ = \frac{-2m}{\Delta} (\bar{x}_0^1 + \bar{x}_0^2)(1 - 2m \bar{x}_2) \]
\[ = \frac{-2m(\bar{x}_0^1 + \bar{x}_0^2)}{1 + 2m \bar{x}_2} \]

Substituting (H.2) into Eq. (4.274), one gets Eq. (4.278).