UNIVERSITY OF SOUTHAMPTON

THE THEORY OF DYNAMIC CORRELATIONS IN CONDENSED MATTER SYSTEMS

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A thesis submitted for the Degree of Doctor of Philosophy

For my parents

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ABSTRACT

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THE THEORY OF DYNAMIC CORRELATIONS IN CONDENSED MATTER SYSTEMS

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This thesis is concerned mainly with spin waves in localised ferromagnetic systems. In the first four chapters we consider, for one-dimensional magnetic chains, the effect of two-spin-wave interactions on the single spin-wave lifetime and calculate the dispersion of two-spin-wave bound states and discuss how they affect the spectral weight, which can be measured by thermal neutron scattering. These calculations are done firstly for an easy-axis system and then for an easy-plane system. In the fifth chapter we use a linear spin-wave theory and discuss how it may be possible to determine the form of the Hamiltonian for some simple ferromagnetic systems using the experimental technique of neutron polarisation analysis. All of these calculations are done by using a Green function equation-of-motion method to calculate spin-spin correlation functions.

In the last chapter we consider a Fermi fluid system and attempt to calculate a density-density correlation function and obtain a self-energy, from which lifetime effects can be studied, for our particular choice of Hamiltonian. We use an equation-of-motion method similar to that used in the previous chapters. However, problems arise in the calculation that we are unable to solve.

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CHAPTER 1: INTRODUCTION TO ONE-DIMENSIONAL FERROMAGNETS

1.1 Physical Systems and Experiments

In this section we will give a very brief introduction to quasi-one-dimensional magnetic systems. Much work has been done on these systems in recent years (Steiner et al. 1976).

Truly one-dimensional magnets are obviously unobtainable in nature. However, there are some magnetic systems which behave as if they are one-dimensional above a critical temperature T_C. The reason for this is that the magnetic coupling, J, between nearest-neighbour atoms or ions along one direction in a three-dimensional crystal is much greater than the magnetic coupling, J′, between nearest-neighbour atoms or ions in the other two directions. This critical temperature, T_C, depends on the values of J and J′ and also on the nature of the interactions between the spins of the atoms or ions, for example T_C is less for a Heisenberg system than for an Ising system. Below T_C the interchain coupling leads to three-dimensional ordering. We will not be concerned with the evaluation of T_C, which is in fact proportional to J′, in this thesis.

Various measurements have been made on several materials with antiferromagnetic exchange coupling, $J<0$, and a few materials with ferromagnetic exchange coupling, $J>0$, that show the existence of one-dimensional behaviour. The static properties of these systems are studied by measuring the specific heat at constant magnetisation, the magnetic susceptibility, etc. Such measurements suggest that the correlations between spins are predominantly one-dimensional in some systems. Some of the dynamic properties can also be measured. For example, well-defined magnetic excitations can be studied using ferromagnetic or antiferromagnetic resonance and infra-red absorption, and diffuse dynamics studied using electron spin resonance and nuclear magnetic resonance. We will not be concerned with any of these experimental techniques in this thesis but will concentrate on thermal neutron scattering which can be used to measure the wave vector dependence of the magnetic excitations and also to show the existence of short-range order, a concept that will be discussed in Sec.1.4.

These quasi-one-dimensional systems usually consist of chains of magnetic atoms or ions with a large spacing and other, non-magnetic, atoms or ions between the chains.

We will be concerned with only localised magnets rather than itinerant ones in Chs.1 to 5.

1.2 Some Useful Definitions

In this section we will introduce some of the parameters and functions that we will need to use in solving the problems of the following chapters.

We will work throughout in the Heisenberg representation. A Heisenberg operator is time-dependent. At time t,

$$A(t) = e^{iHt} A e^{-iHt} \tag{1.2.1}$$

where H is the Hamiltonian, or energy operator, for the system being considered and A is the corresponding Schrodinger operator. We have set $\hbar=1$ here and everywhere else in this thesis. The wave functions are independent of time.

We will frequently take the thermal average of such an operator, defined by,

$$\begin{aligned} \langle A \rangle &= Z^{-1} \sum_{\lambda} \langle \lambda \mid e^{-H/T} A \mid \lambda \rangle \\ Z &= \sum_{\lambda} \langle \lambda \mid e^{-H/T} \mid \lambda \rangle \end{aligned} \tag{1.2.2}$$

where $|\lambda\rangle$ denotes a state of the system, T is the temperature and Z is the partition function. We have set Boltzmann's constant equal to one here and everywhere else in this thesis.

We define the commutator of two operators, A and B, by,

$$[\, A, B \,] = AB - BA \tag{1.2.3}$$

We will consider magnetic chains with N sites and work with spin operators denoted,

$$\underline{S}_l(t), \quad l = 1,2,\ldots N$$

or, in component form,

$$S_l^{\alpha}(t), \quad \alpha = x,\, y,\, z, \quad l = 1,2,\ldots N$$

for the spin at the site labelled by l. Because of translational invariance it will be more useful to work with the Fourier sum of these operators defined by,

$$S_k^{\alpha} = \sum_l e^{ikl}\, S_l^{\alpha} \qquad (1.2.4)$$

where we have chosen to work in units where the lattice spacing is equal to one, and k is a wave vector in the direction of the magnetic chain. In a three-dimensional system (kl) is replaced by ($\underline{k}.\underline{l}$) but in our magnetic chains the vector $\underline{l}$ lies along the chain direction so only the component of $\underline{k}$ in this direction is relevant. The inverse Fourier sum is,

$$S_l^{\alpha} = N^{-1} \sum_k e^{-ikl}\, S_k^{\alpha} \qquad (1.2.5)$$

where the sum is taken over the N allowed values of k in the first Brillouin zone, defined by,

$$-\pi \leqslant k \leqslant \pi$$

We will normally take N to be very large and replace this sum by an integral using,

$$\frac{1}{N}\sum_k \quad \rightarrow \quad \frac{1}{2\pi}\int_{-\pi}^{\pi} dk \qquad (1.2.6)$$

We will also find it useful to work with the linear combinations of the spin operators that form spin raising and lowering operators, defined by,

$$S_l^+ = S_l^x + i\, S_l^y$$
$$S_l^- = S_l^x - i\, S_l^y \qquad (1.2.7)$$

or,

$$S_k^+ = S_k^x + i\, S_k^y$$
$$S_k^- = S_{-k}^x - i\, S_{-k}^y \qquad (1.2.8)$$

where in Eqns.(1.2.7) and (1.2.8) the operators S^- are chosen to be the hermitian conjugates of the operators S^+.

The commutation relations for these spin operators will be discussed in Sec.1.5 when we will need to use them.

1.3 The Spectral Weight Functions

We will introduce the spectral weight functions by considering their role in magnetic neutron scattering (Marshall and Lovesey 1971). Neutrons are a weak probe of condensed matter systems and hence Fermi's Golden Rule, which is equivalent to linear response theory, can be used to describe the scattering of the neutrons. We record the result for the partial differential cross-section for purely magnetic scattering in the first Born approximation,

$$\frac{d^2\sigma}{d\Omega\, dE_f} = \left(\frac{\gamma\, e^2}{m_e\, c^2}\right)^2 \left|\, \frac{1}{2}\, g\, F(\underline{K}) \,\right|^2 \frac{k_f}{k_i}\; e^{-2W(\underline{K})} \sum_{\underline{k}} \delta_{\underline{K},\underline{k}+\underline{\tau}} \;\times$$
$$\times \sum_{\alpha,\beta} \left(\delta^{\alpha\beta} - K'^{\alpha} K'^{\beta} \right) S^{\alpha\beta}(k,\omega) \qquad (1.3.1)$$

$$\underline{K} = \underline{k}_i - \underline{k}_f$$

$$\omega = E_i - E_f$$

where $\underline{k}_i$ and $\underline{k}_f$ are the incident and scattered wave vectors of the neutrons, E_i and E_f are their incident and scattered energies, $F(\underline{K})$ is the form factor, $\exp\{-W(\underline{K})\}$ is the Debye–Waller factor, $\underline{\tau}$ is a reciprocal lattice vector and $\underline{K}'$ is a unit vector in the direction of $\underline{K}$ with components K'^a, a=x,y,z. The function $S^{ab}(k,\omega)$ is the spectral weight and the other parameters on the right–hand side of Eqn.(1.3.1) that we have not mentioned are constants. As explained in the previous section, we only consider the component of $\underline{k}$ parallel to the magnetic chain in our calculations. Then the spectral weight function is defined in terms of a spin operator correlation function by,

$$S^{\alpha\beta}(k,\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dt\ e^{i\omega t} < S^{\alpha}_{-k}(t)\ S^{\beta}_{k}(0) > \qquad (1.3.2)$$

$$\alpha,\ \beta = x,\ y,\ z$$

The spin operators in this equation are discussed and the angular brackets defined in Sec.1.2. The spectral weight function is the quantity that we aim to calculate in Chs.3 to 5. Eqn.(1.3.1) shows that it can be measured experimentally. It is purely real and positive and it contains information on the dynamics of the systems we study.

In Chs.3 and 4 we will be considering the transverse spectral weight function,

$$S(k,\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dt\ e^{i\omega t} < S^{-}_{k}(t)\ S^{+}_{k} > \qquad (1.3.3)$$

since it contains a lot of the useful information on the dynamics of the systems we study.

Finally in this section we mention briefly the dynamic susceptibility, $\chi(k,s)$, which describes the response of a system to an external perturbation and is related to the spectral weight function and the static susceptibility. It is usually defined by using linear response theory and we will not go into details here because it is rather involved (Lovesey 1980) and not necessary for our calculation.

1.4 Theoretical Models

We describe the one-dimensional magnetic systems in terms of the spins of the atoms or ions at sites, l, on the chain, denoted $\underline{S}_l$, and the interactions between the spins on different sites. We consider only localised magnets so the magnitude of each spin is a constant, denoted S. Depending on the nature of the interactions between the spins, various Hamiltonians can be constructed. Some of the most useful are the Heisenberg model,

$$H = - J \sum_{l,m} \underline{S}_l . \underline{S}_m + h \sum_{l} S_l^z \tag{1.4.1}$$

the Ising model,

$$H = - J \sum_{l,m} S_l^z \, S_m^z + h \sum_{l} S_l^z \tag{1.4.2}$$

and the XY model,

$$H = - J \sum_{l,m} (S_l^x \, S_m^x + S_l^y \, S_m^y) + h \sum_{m} S_l^x \tag{1.4.3}$$

where J is the ferromagnetic exchange coupling, J>0, h is an external magnetic field applied in the easy direction, h>0, and l and m are usually nearest-neighbour sites on the chain. For convenience we work in units where 4JS=1 here and in the following chapters.

All of these Hamiltonians possess translational symmetry since they are invariant under a translation of the lattice spacing along the chain direction. If we set the field, h, equal to zero they have different spin symmetries. The Heisenberg Hamiltonian, Eqn.(1.4.1), is invariant under any rotation of the spins, where each spin in the chain is rotated through the same angle about the same direction, i.e. it is a global symmetry. The XY Hamiltonian is invariant under rotations in the x,y-plane and the Ising Hamiltonian is only invariant under spin inversion. The application of a field, h≠0, breaks these symmetries. Such symmetries have important physical consequences. For example, there is no gap at zero wave vector in the spin-wave dispersion for systems with rotational spin symmetry but there is a gap when a field is applied, this will be shown in Sec.1.5.

We now give a short discussion on phase transitions in systems with these Hamiltonians (Steiner et al. 1976). In three dimensions all such systems have an ordered phase for low temperatures and a disordered phase for high temperatures. In two dimensions the existence of a phase transition from an ordered to a disordered phase at a finite temperature depends on the symmetry of the Hamiltonian. For the isotropic Heisenberg system there is no phase transition and the system is in an ordered phase only at zero temperature, but for the Ising system, which has uniaxial anisotropy, there is a phase transition at a finite temperature. The XY system also has a phase transition but it is unusual and will not be discussed here. In one dimension, the case of interest to us, there is no phase transition in any of these systems and they are disordered at any non-zero temperature. At zero temperature some of the systems are in an ordered, ferromagnetic, state and they lose their entropy in going from a disordered to an ordered phase as the temperature approaches zero by building up short-range order. Such systems have a wide critical region near zero temperature and critical properties can be studied over a large temperature range. We note that some systems do not have an ordered, ferromagnetic, phase even at zero temperature, for example the one we will study in Ch.4. Hence all these systems are in a paramagnetic phase at non-zero temperatures and spin-wave theory, which will be described in Sec.1.5, is therefore an approximation.

There are various reasons for studying the theory of magnetism in one dimension. One is that there are new features which do not appear in three dimensions, such as the occurrence of two-spin-wave bound states which are present for all wave vectors, these will be discussed in Sec.2.3. Another reason is that the theory simplifies in one dimension. For example, one-dimensional integrals occur instead of three-dimensional ones and in fact it is sometimes possible to obtain exact solutions.

Another advantage of working in one dimension is that it is often feasable to do detailed computer simulations and exact numerical calculations for finite chains of spins, that cannot be done in higher dimensions because of computer limitations. For example, Schneider and Stoll (1981) have made numerical calculations of the spectral weight for the Ising-Heisenberg chain in zero field, defined by the Hamiltonian,

$$H = -2J \sum_{l} \left(S_l^z S_{l+1}^z + g\, S_l^+ S_{l+1}^- \right) \qquad (1.4.4)$$

for spin S=1/2 and eight sites in the chain. This involves finding the eigenvalues and eigenvectors of a $2^N \times 2^N$ matrix. The Hamiltonian in Eqn.(1.4.4) is a special case of the Hamiltonian that we will study in Ch.3 and comparison can be made between these numerical results and our results.

1.5 Spin-wave Theory

Spin waves are small amplitude oscillations about the ground state of the spin system. They were introduced by Bloch (1930), who considered only non-interacting spin waves. Most of the subsequent work on spin waves has been concerned with the effects of interactions between them.

In this brief introduction to them we shall consider only the Heisenberg ferromagnet in the presence of a magnetic field, defined by the Hamiltonian in Eqn.(1.4.1). The simple Heisenberg Hamiltonian possesses full spin rotational symmetry and one of the effects of the magnetic field is to break this symmetry. We will consider other more complicated systems in Chs.3 and 4. The ferromagnetic ground state has all the spins aligned in the direction of the magnetic field and a single spin wave consists of one spin reversal spread coherently over these aligned spins. Spin-wave theory is an approximation in one dimension at finite temperature because, as explained in Sec.1.4, there is no ferromagnetism for non-zero temperature.

We now give a short discussion of spin-wave theory for the Heisenberg ferromagnet (Keffer 1966, Mattis 1965). The ground state energy is,

$$E_0 = -2NJS^2 - NhS \tag{1.5.1}$$

where N is the total number of spins in the chain. In a classical approach the spins precess about the z direction with angular velocity ω_k, and each sucessive spin differs in phase from the previous one by an angle of k. From the classical torque equations-of-motion for the spins, the dispersion relation for a single spin wave is found to be,

$$\omega_k = 1 - \cos(k) + h \tag{1.5.2}$$

This vanishes for h=0, k=0, in agreement with Goldstone's theorem which tells us that the symmetry of the Hamiltonian leads to bosons, in this case spin waves, with zero energy. For $h \neq 0$ the symmetry is broken and there is an energy gap.

Quantum mechanically, single spin-wave states are generated from the ground state by applying spin-raising operators S^+. Denoting the vacuum ground state by $|0>$, there are N such orthogonal states given by,

$$\Psi_l = (2S)^{-1/2} S_l^+ \mid 0 > \tag{1.5.3}$$

where l denotes sites on the chain, as in Sec.1.2.

Because of the translational symmetry of the Hamiltonian there are eigenfunctions of the translation operator, in this case the plane-wave states,

$$\psi_k = N^{-1/2} \sum_l e^{ikl} \Psi_l \tag{1.5.4}$$

that are eigenfunctions of the Hamiltonian. Hence these states diagonalise the Hamiltonian. The energy eigenvalues are,

$$E(k) = E_0 + \omega_k \tag{1.5.5}$$

as expected from the classical theory. Two-spin-wave states are more difficult to calculate because the plane-wave states are not automatically orthogonal to each other. Also they do not diagonalise the Hamiltonian and this gives rise to bound states. Physically these bound states occur because under certain conditions the interaction between spin waves is attractive.

The algebra of the spin operators is non-trivial because the commutator,

$$[\, S^+, S^- \,] = 2S^z \tag{1.5.6}$$

is not merely a complex number. There are many transformations, however, from spin operators to boson operators. The ones that we will consider treat spin waves as particles which are created and annihilated by the boson operators a^+ and a respectively.

One such transformation was introduced by Holstein and Primakoff (1940) and is given by,

$$\begin{aligned} S_l^- &= (2S)^{1/2} \left[1 - \frac{a_l^+ a_l}{2S} \right]^{1/2} a_l \\ S_l^+ &= (2S)^{1/2}\, a_l^+ \left[1 - \frac{a_l^+ a_l}{2S} \right]^{1/2} \\ S_l^z &= -S + a_l^+ a_l \end{aligned} \tag{1.5.7}$$

The boson operators satisfy the usual commutation relations,

$$\begin{aligned} [\, a_l, a_m \,] &= [\, a_l^+, a_m^+ \,] = 0 \\ [\, a_l, a_m^+ \,] &= \delta_{lm} \end{aligned} \tag{1.5.8}$$

and it is easy to show that the transformation given by Eqn.(1.5.7) then satisfies the correct spin commutation relations given by Eqn.(1.5.6) and,

$$[\, S_l^+, S_m^z \,] = -\, S^+ \,\delta_{lm} \tag{1.5.9}$$

$$[\, S_l^-, S_m^z \,] = S^- \, \delta_{lm}$$

It is usual to work with the Fourier sums of these boson operators, defined by,

$$a_k = N^{-1/2} \sum_l e^{-ikl} \, a_l$$
$$a_k^+ = N^{-1/2} \sum_l e^{ikl} \, a_l^+ \qquad (1.5.10)$$

which are also boson operators because they satisfy the correct commutation relations, similar to Eqn.(1.5.8). However, the Hamiltonian obtained from the spin Hamiltonian, Eqn.(1.4.1), by using the Holstein-Primakoff transformation is still difficult to use in calculations, partly because of complications due to the square roots which appear, and partly because the terms in it which are not quadratic in the boson operators are large compared to the quadratic terms so a perturbative treatment is not usually valid.

Another such transformation from a spin Hamiltonian to a boson Hamiltonian was proposed independently by Dyson (1956) and Maleev (1958). We will use this transformation in Ch.3. Its advantage over the Holstein-Primakoff transformation, apart from its being easier to use, is that the kinematical interaction between spin waves, which is due to the spin-wave states defined in the theory not being orthogonal to each other for states of two or more spin waves, is treated separately. Then the dynamical interaction between spin waves, due to the Hamiltonian not being diagonal in these states, has a non-quadratic part which is small compared to the part that is quadratic in the boson operators. The transformation can be written,

$$S_l^- = (2S)^{1/2} \, a_l$$
$$S_l^+ = (2S)^{1/2} \, a_l^+ \left(1 - \frac{a_l^+ \, a_l}{2S} \right) \qquad (1.5.11)$$
$$S_l^z = - S + a_l^+ \, a_l$$

and for the Heisenberg spin Hamiltonian it gives the boson Hamiltonian,

$$H = \sum_{k} \omega_k a_k^+ a_k + \frac{1}{2NS} \sum_{1,2,3,4} K(1,2,3,4)\, a_1^+ a_2^+ a_3 a_4$$

$$\omega_k = 1 - \cos(k) + h \tag{1.5.12}$$

$$K(1,2,3,4) = \delta_{1+2,3+4} \left[\cos(3) - \cos(1-3) \right]$$

where we have chosen to work in units with 4JS=1, as usual. The wave vectors in the quartic interaction are denoted by numbers here, for convenience. The boson Hamiltonian is not hermitian so it cannot be interpreted as a Hamiltonian for a real physical system and states like $a^+|0>$ cannot be real physical states. However this does not cause any problems in the calculation. We will not discuss the reasons why this transformation gives good results here.

Thermal averages, defined in Sec.1.2, of the boson operators are given by, with respect to the quadratic part of H,

$$< a_k a_p > = < a_k^+ a_p^+ > = 0$$

$$< a_k^+ a_p > = n_k \delta_{kp} \tag{1.5.13}$$

where the Bose factor is defined by,

$$n_k = [\exp(\omega_k/T) - 1]^{-1} \tag{1.5.14}$$

and is the average number of spin waves with wave vector k.

In our calculations we will always normal order the operators so that annihilation operators appear to the right of creation operators. This requires use of the commutation relations so that, for example,

$$a_k a_p^+ = a_p^+ a_k + \delta_{kp} \tag{1.5.15}$$

After normal ordering, a product of four operators, a^+a^+aa, is of higher order in the Bose factor than a product of two operators, a^+a, etc.

We conclude this section with a brief discussion of the, so-called, two-spin-wave continuum. For a state containing two spin waves of wave vectors k and p, the total energy, if we assume that they are non-interacting, is,

$$\omega_T = \omega_k + \omega_p$$

$$= 2 \left[1 + h - \cos(K/2) \cos(q/2) \right] \qquad (1.5.16)$$

$$K = k + p, \quad q = k - p, \quad -\pi \leqslant k,\ p \leqslant \pi$$

using Eqn.(1.5.12) for the single spin wave energy. The wave vector q can take any value in the range $-2\pi \leqslant q \leqslant 2\pi$ and so the total energy for the two spin waves which have total wave vector K lies in the range,

$$\omega_T \geqslant 2 \{ 1 + h - | \cos(K/2) | \}$$

$$\qquad (1.5.17)$$

$$\omega_T \leqslant 2 \{ 1 + h + | \cos(K/2) | \}$$

When we plot graphs of energy versus wave vector the area where Eqn.(1.5.17) is satisfied is the two-spin-wave continuum. The two-spin-wave bound states that we will study lie below this continuum of states.

CHAPTER 2: METHOD OF CALCULATION

2.1 Green Functions

Thermal Green functions are both useful and convenient for treating various complex problems, especially those in which it is necessary to do a non-perturbative calculation. However, there may be some subtle difficulties and the approximations used and results obtained should be dealt with carefully. We will consider two such problems, a simple one in Ch.3 and a more complicated one in Ch.4. These problems involve one-dimensional magnetic systems and require a non-perturbative treatment because of the two-spin-wave bound state which is present throughout the first Brillouin zone below the two-spin-wave continuum. This causes non-perturbative effects that no finite order of perturbation theory can give, for example, poles in the self-energy, which will be discussed in Sec.2.3.

Following Lovesey (1980), we define a causal thermal Green function for two Heisenberg operators, defined by Eqn.(1.2.1), A and B by,

$$\begin{aligned} G(t) &= -\, i\, \theta(t) < [\, A(t),\, B\,] > \\ &= \ll A(t);\, B \gg \end{aligned} \qquad (2.1.1)$$

where $\theta(t)$ is the unit step function, the angular brackets in the first equality denote a thermal average, defined by Eqn.(1.2.2), and the square brackets denote a commutator, defined in Eqn.(1.2.3). The operator A(t) satisfies the equation-of-motion,

$$\partial_t\, A(t) = -\, i\, [\, A(t),\, H\,] \qquad (2.1.2)$$

where H is the total Hamiltonian. For convenience, we define B=B(0). The second equality in Eqn.(2.1.1) defines a convenient notation.

The time Fourier transform of G(t) is,

$$G(\omega) = \int_{-\infty}^{\infty} dt\, e^{i\omega t}\, G(t)$$

To ensure that this is a convergent function we define our $G(\omega)$ to be,

$$G(\omega) = \int_{-\infty}^{\infty} dt\ e^{i(\omega+i\eta)t}\ G(t), \qquad \eta \to 0+ \tag{2.1.3}$$

$$= \langle\langle A; B \rangle\rangle_{\omega}$$

where the second equality defines a useful notation. The parameter η causes the integrand to tend to zero exponentially as time, t, tends to infinity. When we take real and imaginary parts of $G(\omega)$ we often have to let $\omega \to \omega + i\eta$ and then take the limit $\eta \to 0+$ explicitly.

It can be shown (Lovesey 1980) that the real and imaginary parts of $G(\omega)$ satisfy a Kramers-Kronig, or dispersion, relation, which, for our definitions, is,

$$\mathrm{Re}\ G(\omega) = -\frac{1}{\pi}\ P\int_{-\infty}^{\infty} \frac{du\ \mathrm{Im}\ G(u)}{\omega + u} \tag{2.1.4}$$

where P denotes the principal part of the integral. This relation is a direct result of $G(\omega)$ being a causal function and it is easily derived using the integral representation of the step function,

$$\theta(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{du\ e^{-iut}}{u + i\eta}, \qquad \eta \to 0+ \tag{2.1.5}$$

Another useful result that we will state here, but will not derive, is the relation between the spectral weight, $S(k,\omega)$, discussed in Sec.1.3, and the imaginary part of a Green function. This relation is,

$$\mathrm{Im} \langle\langle S_k^+; S_k^- \rangle\rangle_{\omega} = -\pi \left[1 - \exp(-\frac{\omega}{T}) \right] S(k,\omega) \tag{2.1.6}$$

It is, in fact, merely a statement of the well-known fluctuation--dissipation theorem (Kubo 1966). The spectral weight describes the spontaneous fluctuations of the system and the imaginary part of the Green function is simply related to the dissipative part of the dynamic susceptibility, mentioned in Sec.1.3, since,

$$G(\omega) \propto \chi(i\omega) \tag{2.1.7}$$

In Chs.3 and 4 we will write the Hamiltonians in terms of boson operators, as described in Sec.1.5, and will have to calculate a Green function,

$$G(k,\omega) = \langle\langle a_k ; a_k^+ \rangle\rangle_\omega \tag{2.1.8}$$

We will find that this Green function has the form,

$$G(k,\omega) = [\ \omega - \omega_k - \Sigma(k,\omega)\ ]^{-1} \tag{2.1.9}$$

where ω_k is the single spin-wave energy discussed in Sec.1.5. Eqn.(2.1.9) defines the self-energy, $\Sigma(k,\omega)$, which vanishes in the limit $T \to 0$ for the models of interest here. In this limit the Green function, $G(k,\omega)$, takes its non-interacting value, $G^{(0)}(k,\omega)$, which is,

$$G^{(0)}(k,\omega) = (\ \omega - \omega_k\ )^{-1} \tag{2.1.10}$$

and also,

$$\langle\langle S_k^- ; S_k^+ \rangle\rangle_\omega = 2S \langle\langle a_k ; a_k^+ \rangle\rangle_\omega \tag{2.1.11}$$

Hence to find the spectral weight we take the imaginary part of the Green function in Eqn.(2.1.10), letting $\omega \to \omega + i\eta$, $\eta \to 0+$, and using the identity,

$$\lim_{\eta \to 0} \int_{-\infty}^{\infty} \frac{du}{u + i\,\eta} = -\,i\,\pi\,\delta(u) + P \int_{-\infty}^{\infty} \frac{du}{u} \tag{2.1.12}$$

where $\delta(u)$ is the Dirac δ-function.
The result is,

$$S(k,\omega) = 2S\ \delta(\ \omega - \omega_k\ ) \tag{2.1.13}$$

so the spectral weight function has a resonance peak at the single spin-wave energy. For most three-dimensional systems at low temperature the lineshape of $S(k,\omega)$ is Lorentzian. The δ-function in Eqn.(2.1.13) can in fact be written as a Lorentzian in the limit that its width tends to zero,

$$\delta(\omega - \omega_k) = \frac{1}{\pi} \frac{\eta}{(\omega - \omega_k)^2 + \eta^2} , \quad \eta \to 0 \qquad (2.1.14)$$

where the parameter η is a measure of the width of the Lorentzian. The physical significance of our parameter η, introduced in Eqn.(2.1.3) is that it is a measure of the width of the resonance peak in the spectral weight.

We will find that for our one-dimensional systems in Chs.3 and 4 the self-energy, $\Sigma(k,\omega)$, has structure and is not merely a purely imaginary function of temperature. Hence the lineshape of $S(k,\omega)$ is not a Lorentzian, it is not symmetric about the single spin-wave energy in fact. From Eqn.(2.1.9) we see that the real part of the self-energy evaluated at the single spin-wave energy gives the energy shift in the resonance peak from the single spin-wave energy, to a first approximation. The imaginary part of the self-energy evaluated at the single spin-wave energy gives the width of the peak, which is a measure of the damping or inverse lifetime of the spin waves.

The self-energy arises because of processes involving interactions of spin waves. The nonlinear processes contain two-spin-wave bound states which arise because of the attractive interactions between spin waves. We will see that the self-energy has poles at the two-spin-wave bound states in Chs.3 and 4. These bound states can be found by investigating a Green function of the form,

$$<< a\, a\, ; a^+ a^+ >>_\omega \qquad (2.1.15)$$

which involves products of creation and annihilation operators, and this will be done as an example of the equation-of-motion method in Sec.2.3. This Green function does not appear directly in any of the equations which are used in the calculation of $G(k,\omega)$. However, the bound states do manifest themselves indirectly in the spectral weight which has a resonance peak at an energy close to the bound-state energy, for a given wave vector at low temperatures. This energy is given by,

$$\omega - \omega_k - \Sigma(k,\omega) = 0 \qquad (2.1.16)$$

where the left-hand side of this equation is the denominator of $G(k,\omega)$ in Eqn.(2.1.9). These resonances will be discussed in detail in Ch.3.

We conclude this section by recording a useful result involving the self-energy,

$$G(k,\omega) = G^{(0)}(k,\omega) + G^{(0)}(k,\omega)\ \Sigma(k,\omega)\ G(k,\omega) \qquad (2.1.17)$$

This is known as Dyson's equation.

The technique that we will use for calculating the Green functions is described in the next section.

2.2 The Equation-of-motion Method

We now turn to the calculation of the Green function $G(\omega)$, defined in Eqn.(2.1.3), from its equation-of-motion. Using the identity,

$$\partial_t\ \Theta(t) = \delta(t) \qquad (2.2.1)$$

and the equation-of-motion for the operator $A(t)$, Eqn.(2.1.2), we can write the equation-of-motion for $G(t)$, defined in Eqn.(2.1.1), as,

$$i\ \partial_t\ G(t) = \delta(t) < [\ A,\ B\ ] > + << [\ A(t),\ H\ ];\ B >> \qquad (2.2.2)$$

Then, differentiating both sides of Eqn.(2.1.3) with respect to time gives

$$\omega\ G(\omega) = < [\ A,\ B\ ] > + << [\ A,\ H\ ];\ B >>_{\omega} \qquad (2.2.3)$$

which is the equation-of-motion for $G(\omega)$. This equation provides a means of calculating the Green function $G(\omega)$. The last term in the equation is another Green function that is usually of higher order in the operators used, as we will see in the following chapters. Consequently, in most cases, it has to be approximated in some way and $G(\omega)$ cannot be calculated exactly. We will discuss the approximation to be used in Chs.3 and 4 in Sec.2.4.

2.3 Two-spin-wave Bound States

To obtain the two-spin-wave bound states explicitly we study the Green function, with p+q=p'+q',

$$G^{B.S.}(p,q;\omega) = \langle\langle a_p a_q ; a^+_{q'} a^+_{p'} \rangle\rangle_\omega \tag{2.3.1}$$

at zero temperature. The energy Fourier transform of this Green function involves the creation of two spin waves at zero time and their annihilation at time t. We will find that the calculation of $G^{BS}(p,q;\omega)$ involves an integral equation that can be solved because it has a separable kernel. If the kernel had not been separable then there would have been no two-spin-wave bound states in the system.

For simplicity, we will consider the boson Hamiltonian in Eqn.(1.5.12) here. The equation-of-motion for $G^{BS}(p,q;\omega)$ is, from Eqn.(2.2.3),

$$\begin{aligned}\omega\, G^{B.S.}(p,q;\omega) = &\langle [\, a_p a_q ,\, a^+_{q'} a^+_{p'} \,] \rangle + \\ &\langle\langle [\, a_p a_q ,\, H \,] ; a^+_{q'} a^+_{p'} \rangle\rangle_\omega\end{aligned} \tag{2.3.2}$$

Consider the second term on the right-hand side. The part of the commutator involving the non-interacting term in the Hamiltonian gives,

$$\Big[\, a_p a_q ,\, \sum_k \omega_k a^+_k a_k \,\Big] = (\, \omega_p + \omega_q \,)\, a_p a_q \tag{2.3.3}$$

where we have used the identity,

$$\begin{aligned}[\, AB, CD \,] = A\,[\, B, C \,]\,D + AC\,[\, B, D \,] + \\ [\, A, C \,]\,DB + C\,[\, A, D \,]\,B\end{aligned} \tag{2.3.4}$$

The rest of the commutator gives,

$$\Big[a_p\, a_q,\ \frac{1}{2NS} \sum_{1,2,3,4} K(1,2,3,4)\, a_1^+\, a_2^+\, a_3\, a_4 \Big] = \frac{1}{2NS} \sum_{1,2,3,4} K(1,2,3,4) \times$$

$$\{ \delta_{q2}\, a_1^+\, a_p\, a_3\, a_4 + \delta_{p2}\, a_1^+\, a_q\, a_3\, a_4 + \delta_{q1}\, a_2^+\, a_p\, a_3\, a_4 +$$

$$\delta_{p1}\, a_2^+\, a_q\, a_3\, a_4 + (\ \delta_{q1}\, \delta_{p2} + \delta_{p1}\, \delta_{q2}\ )\, a_3\, a_4\ \} \qquad (2.3.5)$$

Hence the equation-of-motion for $G^{BS}(p,q;\omega)$ contains six-particle Green functions of the form,

$$<< a_\alpha^+\, a_\beta\, a_\gamma\, a_\delta;\ a_{q'}^+,\ a_{p'}^+ >> \qquad (2.3.6)$$

We will now perform a Hartree-Fock approximation on the product of four operators,

$$a_\alpha^+\, a_\beta\, a_\gamma\, a_\delta \qquad (2.3.7)$$

which involves taking the sum of all possible terms in which the product of two operators is replaced by its thermal average. Using Eqn.(1.5.13), for the thermal averages of products of two boson operators, then gives, for Eqn.(2.3.7),

$$\delta_{\alpha\beta}\, n_\alpha\, a_\gamma\, a_\delta + \delta_{\alpha\gamma}\, n_\alpha\, a_\beta\, a_\delta + \delta_{\alpha\delta}\, n_\alpha\, a_\beta\, a_\gamma \qquad (2.3.8)$$

In the limit of zero temperature the Bose factor, and hence the expression in Eqn.(2.3.8), vanishes. In this limit all six-particle Green functions of the form in Eqn.(2.3.6) vanish. Hence, for T=0,

$$[\ a_p\, a_q,\ H\ ] = (\ \omega_p + \omega_q\ )\, a_p\, a_q + \frac{1}{2NS} \sum_{3,4} \{\ K(p,q,3,4) + K(q,p,3,4)\ \}\, a_3\, a_4 \qquad (2.3.9)$$

The first term on the right-hand side of Eqn.(2.3.2) is,

$$<[\ a_p\, a_q,\ a_{q'}^+\, a_{p'}^+\ ]> = \delta_{qq'} + \delta_{pq'} + \delta_{qq'}\, n_p + \delta_{pp'}\, n_q + \delta_{pq'}\, n_q + \delta_{qp'}\, n_p$$

which, in the limit T→0, is,

$$< [a_p a_q , a^+_{q'} a^+_{p'}] > = \delta_{qq'} + \delta_{pq'} \qquad (2.3.10)$$

Hence Eqn.(2.3.2) becomes,

$$(\omega - \omega_p - \omega_q) G^{B.S.}(p,q;\omega) = (\delta_{qq'} + \delta_{pq'}) + \frac{1}{2NS} \sum_{3,4} [K(p,q,3,4) + K(q,p,3,4)] G^{B.S.}(3,4;\omega) \qquad (2.3.11)$$

We note that K(1,2,3,4) in Eqn.(1.5.12) contains a δ-function. Using the change of variables,

$$p = K/2 + Q , \qquad q = K/2 - Q$$
$$3 = K/2 + X , \qquad 4 = K/2 - X \qquad (2.3.12)$$

and the expressions for the single spin-wave energy and the interaction in Eqn.(1.5.12) then give, for Eqn.(2.3.11),

$$[\omega - 2 (1 - \cos(K/2) \cos(Q) + h)] G^{B.S.}(K/2+Q,K/2-Q;\omega)$$
$$= (\delta_{K/2-Q,q'} + \delta_{K/2+Q,q'}) - \frac{1}{NS} \sum_{X} \cos(X) [\cos(K/2) - \cos(Q)] G^{B.S.}(K/2+X,K/2-X;\omega) \qquad (2.3.13)$$

where we have also used the fact that $G^{BS}(K/2+X,K/2-X;\omega)$ is an even function of X so that,

$$\sum_{X} \sin(K/2) \sin(X) G^{B.S.}(K/2+X,K/2-X;\omega) = 0 \qquad (2.3.14)$$

Eqn.(2.3.13) is an integral equation for $G^{BS}(K/2+Q,K/2-Q;\omega)$ which is easily solved. Writing it in the form,

$$G^{B.S.}(K/2+Q,K/2-Q;\omega) = \{ \omega - 2 [1 - \cos(K/2) \cos(Q) + h] \}^{-1} \times$$
$$(\delta_{K/2-Q,q'} + \delta_{K/2+Q,q'}) - \{ \omega - 2 [1 - \cos(K/2) \cos(Q) +$$

$$h \,] \, \}^{-1} \frac{1}{N\,S} \sum_{X} \cos(X) \, [\, \cos(K/2) - \cos(Q) \,] \times$$

$$G^{B.S.}(K/2+X, K/2-X; \omega)$$

multiplying by cos(Q) and taking the sum over wave vectors Q gives,

$$\sum_{X} \cos(X) \, G^{B.S.}(K/2+X, K/2-X; \omega) = [\, 1 - W(K) \,]^{-1} \times$$

$$\sum_{Q} (\, \delta_{K/2-Q,q'} + \delta_{K/2+Q,q'} \,) \cos(Q) \, \{ \, \omega - 2 \, [\, 1 -$$

$$\cos(K/2) \cos(Q) + h \,] \, \}^{-1} \qquad (2.3.16)$$

where

$$W(K) = \frac{1}{N\,S} \sum_{Q} \{ \, \omega - 2 \, [\, 1 - \cos(K/2) \cos(Q) + h \,] \, \}^{-1} \times$$

$$\cos(Q) \, [\, \cos(K/2) - \cos(Q) \,] \qquad (2.3.17)$$

Changing the sum into an integral,

$$\sum_{Q} \quad \rightarrow \quad \frac{N}{2\pi} \int_{-\pi}^{\pi} dQ \qquad (2.3.18)$$

and using the results,

$$\frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{dQ}{\cos(Q) - f} = - \operatorname{sign}(f) \, (\, f^2 - 1 \,)^{-1/2}, \quad |f| > 1$$

$$\frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{dQ}{\cos(Q) - f} = -i (\, 1 - f^2 \,)^{-1/2}, \quad |f| < 1 \qquad (2.3.19)$$

enables us to evaluate the function W(K).

If we define,

$$f = \frac{[\, 2 \, (\, 1 + h \,) - \omega \,]}{2 \cos(K/2)} \qquad (2.3.20)$$

then, for $|f|>1$,

$$\mathrm{Re}\, W(K) = \frac{[\, \cos(K/2) - f \,]}{2 \, S \cos(K/2)} \, [\, 1 - |f| \, (f^2 - 1 \,)^{-1/2} \,]$$

$$\mathrm{Im}\, W(K) = 0 \qquad (2.3.21)$$

and for $|f|<1$,

$$\mathrm{Re}\,W(K) = \frac{\cos(K/2) - f}{2\,S\,\cos(K/2)}$$

$$\mathrm{Im}\,W(K) = \frac{\cos(K/2) - f}{2\,S\,\cos(K/2)}\ (-f)\,(1 - f^2)^{-1/2} \qquad (2.3.22)$$

The region $|f|<1$ defines the two-spin-wave continuum, described in Sec.1.5.

The Green function $G^{BS}(K/2+Q,K/2-Q;\omega)$ contains a term with the factor $\{1-W(K)\}$ in its denominator. The two-spin-wave bound states are resonances of this Green function and they occur when,

$$\mathrm{Re}\,W(K) = 1$$

$$\mathrm{Im}\,W(K) = 0 \qquad (2.3.23)$$

The function $W(K)$ is also a function of energy, ω, and to obtain the dispersion of the bound states we look for a solution of Eqn.(2.3.23) below the two-spin-wave continuum, $f>1$, in the form $\omega=\omega(K)$. Eqn.(2.3.23) then gives,

$$\frac{[\cos(K/2) - f]}{2S\cos(K/2)}\ [\,1 - f\,(f^2 - 1)^{-1/2}\,] = 1 \qquad (2.3.24)$$

which can be written,

$$4S\cos(K/2)\,f^3 + [\,4S\,(S - 1)\cos^2(K/2) - 1\,]\,f^2 -$$

$$2\,(2S - 1)\cos(K/2)\,f - (2S - 1)\cos^2(K/2) = 0 \qquad (2.3.25)$$

This is a cubic equation in f. The analytic solution is very complicated but simplifies in two special cases. Firstly for $S=1/2$ it gives,

$$f = \frac{1 + \cos^2(K/2)}{2\cos(K/2)} \qquad (2.3.26)$$

or, using the definition of f, Eqn.(2.3.20),

$$\omega_B = \sin^2\left(\frac{K}{2}\right) + 2h \qquad (2.3.27)$$

secondly at the zone boundary, $K=\pi$, Eqn.(2.3.25) gives the result,

$$\omega_B = 2 - \frac{1}{2S} + 2h \qquad (2.3.28)$$

Apart from these two special cases we solve Eqn.(2.3.25) numerically.

We will discuss bound states and their effect on the spectral weight function further in Ch.3.

2.4 Approximation Method

When we use Eqn.(2.2.3) and a boson Hamiltonian with interaction terms, for example Eqn.(1.5.12), to write down an equation for $G(k,\omega)$, defined in Eqn.(2.1.8), we find that higher order Green functions are generated. Consider the Hamiltonian in Eqn.(1.5.12), to be specific. Then the exact equation-of-motion for $G(k,\omega)$ contains the temperature--independent term $G^{(0)}(k,\omega)$ added to a term which includes a four-particle Green function of the form,

$$G(p,q,q',k;\omega) = \langle\langle a_p^+ a_q a_{q'} ; a_k^+ \rangle\rangle_\omega \qquad (2.4.1)$$

which is temperature-dependent and vanishes in the limit that temperature, T, tends to zero. The exact equation-of-motion for this Green function includes terms with six-particle Green functions and so on. Hence we cannot calculate $G(k,\omega)$ exactly and we have to make some approximations.

For our Hamiltonian, n^{th} order perturbation theory corresponds to neglecting all terms in the Green functions which contain powers of the interaction that are greater than n. However, as we stated in Sec.2.1, perturbation theory is not adequate for describing these systems.

The approximation that we will use is valid for low temperatures but not necessarily small values of the interaction, and is as follows. The exact equation-of-motion for G(p,q,q',k;ω) contains a term which includes the same Green function and another term that is of the form,

$$<< [\, a_p^+ a_q a_{q'},\, a_1^+ a_2^+ a_3 a_4 \,];\, a_k^+ >>_\omega$$

$$= << a_p^+ [\, a_q a_{q'},\, a_1^+ a_2^+ \,] a_3 a_4;\, a_k^+ >>_\omega$$

$$+ << a_1^+ a_2^+ [\, a_p^+,\, a_3 a_4 \,] a_q a_{q'};\, a_k^+ >>_\omega \qquad (2.4.2)$$

The first term on the right-hand side of Eqn.(2.4.2) contains four-particle and six-particle Green functions and the second term contains only six-particle Green functions, after evaluating the commutators and normal ordering the operators, as described in Sec.1.5. Six particle Green functions are effectively higher order in temperature than four-particle Green functions since they are higher order in the Bose factor, defined in Eqn.(1.5.11). If we neglect all six-particle Green functions, the expression on the right-hand side of Eqn.(2.4.2) becomes,

$$(\, \delta_{q1} \delta_{q'2} + \delta_{q2} \delta_{q'1} \,) << a_p^+ a_3 a_4;\, a_k^+ >>_\omega \qquad (2.4.3)$$

which has the same form as our original four-particle Green function. Within this approximation the equation-of-motion for G(p,q,q',k;ω) is an integral equation which can be solved and hence we can calculate G(k,ω). Another way of stating our approximation, which brings out more of the physics of the system, is as follows. We approximate the first term on the right-hand side of Eqn.(2.4.2) by,

$$< [\, a_q a_{q'},\, a_1^+ a_2^+ \,] > << a_p^+ a_3 a_4;\, a_k^+ >>_\omega \qquad (2.4.4)$$

The thermal average of the commutator is merely the amplitude for the production of two-spin-wave bound states, as in Eqn.(2.3.2), and we evaluate it in the limit of zero temperature to obtain,

$$\delta_{q1} \delta_{q'2} + \delta_{q2} \delta_{q'1} \qquad (2.4.5)$$

Hence we obtain Eqn.(2.4.3). The second term on the right-hand side of Eqn.(2.4.2) arises from spin-wave collisions which result in energy shifts and damping in $G(p,q,q',k;\omega)$ and are neglected.

In summary, the approximation we use is basically to work to first order only in the Bose factors. In the language of diagrammatic perturbation theory it is called the one backward line approximation. This will be discussed in the next section.

2.5 Comparison With T-matrix Theory

We will now show that our approximation is equivalent to the standard T-matrix approximation as done by, for example, Pini et al. (1981) for similar systems to the ones that we consider. We will find, however, that the equation-of-motion method is particularly convenient in more complicated systems, with anisotropy for example.

For convenience we will use diagrams to describe the T-matrix approximation (Abrikosov et al. 1963, Fetter and Walecka 1971). In these diagrams the non-interacting Green function,

$$G^{(0)}(k,t) = \langle\langle a_k(t);\, a_k^+ \rangle\rangle^{(0)} \qquad (2.5.1)$$

is denoted by a straight line with an arrow pointing forward in time and the interaction, K(1,2,3,4) in Eqn.(1.5.12), by a wiggly line, as shown in Fig.2.1.

In perturbation theory the full Green function,

$$G(k,t) = \langle\langle a_k(t);\, a_k^+ \rangle\rangle \qquad (2.5.2)$$

is given by the expression,

$$\sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int dt_1..dt_n < \tau \,[\, H'(t_1)..H'(t_n)\; a_k(t)\; a_k^+(0) \,]\, >_c \qquad (2.5.3)$$

where τ denotes time-ordering, c denotes taking the sum over connected diagrams only, the perturbation, H', is the second term in the Hamiltonian of Eqn.(1.5.12) and n denotes the order of the perturbation theory. In our theory $t>0$ always. To lowest order, $n=0$, the expression in Eqn.(2.5.3) gives $G^{(0)}(k,t)$. To obtain the first order, $n=1$, connected diagrams we consider all possible pairings, or Wick contractions, of,

$$H'(t_1)\ a_k(t)\ a_k^+(0) =$$

$$a_1^+(t_1)\ a_2^+(t_1)\ a_3(t_1)\ a_4(t_1)\ a_k(t)\ a_k^+(0) \qquad (2.5.4)$$

For example consider,

$$a_1^+(t_1)\ a_2^+(t_1)\ a_3(t_1)\ a_4(t_1)\ a_k(t)\ a_k^+(0) \qquad (2.5.5)$$

which gives the diagram in Fig.2.2a. Other possible connected diagrams are given in Fig.2.2. Each of these gives a contribution to $G(k,t)$ of,

$$(-1) \int dt \sum_p K(p,k,p,k)\ G^{(0)}(p.0)\ G^{(0)}(k,t-t')\ G^{(0)}(k,t') \qquad (2.5.6)$$

All of these diagrams can be written in the abbreviated form of Fig.2.3. For $n=2$ there are approximately eighty possible pairings leading to connected diagrams and we will not go into the details.

In the T-matrix, or dilute gas, approximation we consider only the so-called "ladder" diagrams and neglect all others, i.e. we include only repeated pair interactions. The Green function $G(k,t)$ is then given by the expansion in Fig.2.4. To obtain $G(k,\omega)$ we take the time Fourier transform of this result and can write down the same diagrams as we used for $G(k,t)$ with energies as well as wave vectors labelling the lines and a slightly different prescription for calculating the contribution of each diagram to $G(k,\omega)$. The self-energy, defined by Eqn.(2.1.9) is then given by the expansion in Fig.2.5, where the T-matrix is defined by the diagrammatic equation in Fig.2.6. This equation is rewritten as an integral equation in Fig.2.7, which is similar to the integral equation for the four-particle Green function that will be solved in Chs.3 and 4, and is written algebraically as,

$$T(k,p,q,q') = K(k,p,q,q') + \sum_{u,v} \int K(k,p,3,4)\ G^{(0)}(3,u)\ \times$$

$$G^{(0)}(4,v)\ T(1,2,q,q')\ d3\ d4 \qquad (2.5.7)$$

The T-matrix approximation is valid for interactions which are short-ranged, but not necessarily small, so their effects are small. It is valid as a low temperature expansion for the systems we consider because it is considering the scattering of two particles which may, however, scatter from each other many times. Hence we only consider one particle, apart from our particle of wave vector k and energy ω, and so only need one power of the Bose factor, which is just the average number of particles with a given wave vector. We then, of course, integrate over all wave vectors to include all possible interactions of our particle, labelled by k and ω, with other particles in the system. For example diagrams like those in Fig.2.8 do not contribute because they contain factors $n_p n_q$. This demonstrates that our approximation is equivalent to the T-matrix approximation. A calculation of the self-energy evaluated at the single spin-wave energy for the easy-axis ferromagnet was done by Rastelli (1982) and it agrees with our result in Ch.3.

Figure 2.1: Non-interacting Green function and interaction

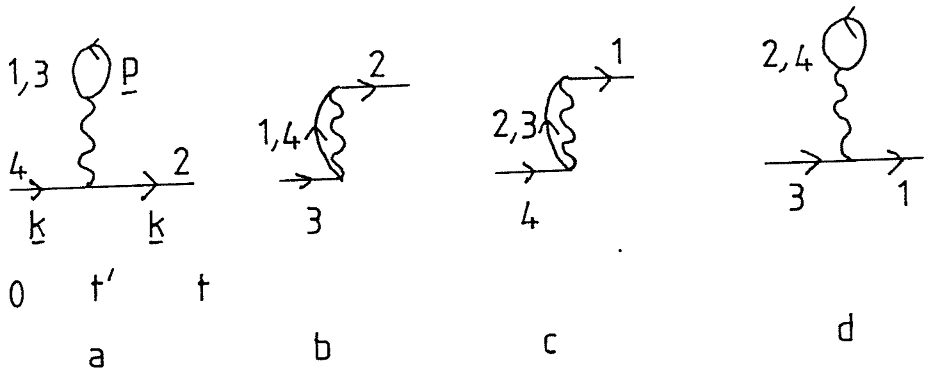

Figure 2.2: First order perturbation theory diagrams

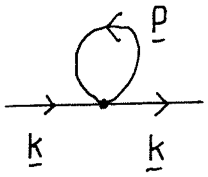

Figure 2.3: Abbreviated form of first order perturbation theory diagrams

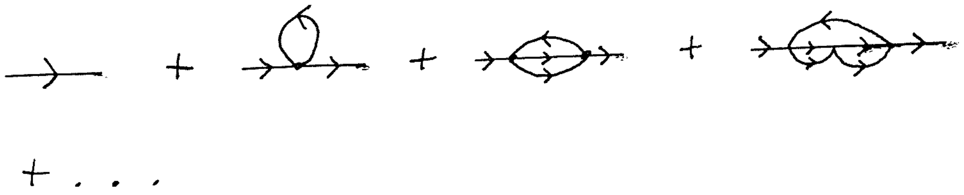

Figure 2.4: Expression for Green function

Figure 2.5: Expression for self-energy

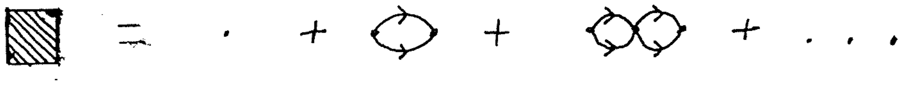

Figure 2.6: Definition of T-matrix

Figure 2.7: Equation for T-matrix

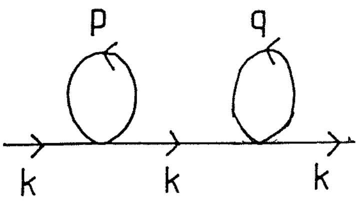

Figure 2.8: One diagram of higher order in temperature

CHAPTER 3: EASY-AXIS FERROMAGNET

3.1 Spin Hamiltonian

This chapter is concerned with the application of the previous results to an easy-axis ferromagnetic chain (Lovesey and Hood 1982). A more complicated system will be considered in Ch.4.

The Hamiltonian that we consider for the easy-axis ferromagnet is,

$$H = - J \sum_{l,m} (S_l^z S_m^z + g S_l^+ S_m^-) + \sum_l \{ h S_l^z - D (S_l^z)^2 \} \tag{3.1.1}$$

where J is the ferromagnetic exchange coupling and h is the applied magnetic field. The parameter g lies in the range between zero, the Ising limit, and one, the Heisenberg limit, and it is a measure of the exchange anisotropy. The parameter D is the single-site anisotropy. The spin operators are defined in Sec.1.2 and the first sum in Eqn.(3.1.1) is taken over all nearest-neighbour sites l and m. The parameter J is positive and the parameters h and D are either positive or zero. We note that for the special case S=1/2 the term involving D reduces to a constant and therefore has no effect on the dynamics of the system. This fact provides us with a useful check on our results. The parameter J causes the spins on the chain to tend to align parallel to each other. The parameters g, except for the Heisenberg limit g=1, and D cause them to align parallel or anti-parallel to the z-axis, which is the easy axis. The field h tends to align them in the negative z-direction. The ground state of the system has all the spins in the chain aligned along the negative z-direction. Spin waves are then small amplitude oscillations of the spins about this direction and we will discuss them in the following sections.

3.2 Boson Hamiltonian

We transform the spin Hamiltonian in Eqn.(3.1.1) to a boson Hamiltonian using the Dyson–Maleev transformation defined in Eqn.(1.5.11). This gives,

$$H = 2JS \sum_{l,m} [(a_l^+ a_l - g a_l^+ a_m) - \frac{1}{2S} (a_l^+ a_m^+ a_l a_m - g a_l^+ a_l^+ a_l a_m)] + \sum_l [\{ h + D (2S - 1) \} a_l^+ a_l - D a_l^+ a_l^+ a_l a_l] \qquad (3.2.1)$$

where we have used the commutation relations, Eqn.(1.5.8), to normal order the boson operators. We write these operators in terms of their Fourier sums, that is,

$$a_l = N^{-1/2} \sum_k e^{ikl} a_k$$
$$a_l^+ = N^{-1/2} \sum_k e^{-ikl} a_k^+ \qquad (3.2.2)$$

to obtain the boson Hamiltonian,

$$H = \sum_k \omega_k a_k^+ a_k + \frac{1}{2NS} \sum_{1,2,3,4} K(1,2,3,4)\, a_1^+ a_2^+ a_3 a_4$$
$$\omega_k = 1 + h + D (2S - 1) - g \cos(k) \qquad (3.2.3)$$
$$K(1,2,3,4) = \delta_{1+2,3+4} [g \cos(3) - \cos(1-3) - 2DS]$$

which is the same as the Hamiltonian in Eqn.(1.5.12) for the special case g=1, D=0, i.e. the Heisenberg ferromagnet, as required.

From the transformation, Eqn.(1.5.11), it is obvious that the Green function that we are aiming to calculate to obtain the transverse spectral weight function, Eqn.(1.3.3), is,

$$<< S_k^- ; S_k^+ >>_\omega = 2S << a_k ; a_k^+ >>_\omega -$$

$$\frac{1}{N} \sum_{1,2} << a_k ; a_1^+ a_2^+ a_{1+2-k} >>_\omega \qquad (3.2.4)$$

The calculation of this Green function is described in the next section.

3.3 Calculation

We now turn to the calculation of the two-particle Green function $G(k,\omega)$, defined in Eqn.(2.1.8). Its equation-of-motion is, from Eqn.(2.2.3),

$$\omega\, G(k,\omega) = < [\, a_k , a_k^+ \,] > + << [\, a_k , H \,] ; a_k^+ >>_\omega \qquad (3.3.1)$$

Using the commutation relations for the boson operators, Eqn.(1.5.8), and the boson Hamiltonian in Eqn.(3.2.3), we find,

$$[\, a_k , a_k^+ \,] = 1 \qquad (3.3.2)$$

and,

$$[\, a_k , H \,] = \omega_k\, a_k + \frac{1}{2NS} \sum_{2,3,4} \{ K(k,2,3,4) + K(2,k,3,4) \}\, a_2^+ a_3 a_4 \qquad (3.3.3)$$

so that Eqn.(3.3.1) becomes,

$$(\, \omega - \omega_k \,)\, G(k,\omega) = 1 + \frac{1}{2NS} \sum_{2,3,4} \{ K(k,2,3,4) + K(2,k,3,4) \} \times$$

$$<< a_2^+ a_3 a_4 ; a_k^+ >>_\omega \qquad (3.3.4)$$

This equation has a term which includes four-particle Green functions of the form $G(p,q,q',k;\omega)$ with $q+q'=p+k$ because of the Kronecker δ in the interaction $K(1,2,3,4)$, defined by Eqn.(2.4.1). Its equation-of-motion, from Eqn.(2.2.3), is,

$$\omega\, G(p,q,q',k;\omega) = < [\, a_p^+ a_q a_{q'},\, a_k^+ \,] > + \\ << [\, a_p^+ a_q a_{q'},\, H \,];\, a_k^+ >>_\omega \qquad (3.3.5)$$

The first term on the right-hand side of Eqn.(3.3.5) is,

$$< [\, a_p^+ a_q a_{q'},\, a_k^+ \,] > = (\, \delta_{qk} + \delta_{q'k} \,)\, n_p \qquad (3.3.6)$$

using the commutation relations, Eqn.(1.5.8), and the thermal averages of boson operators in Eqn.(1.5.13). The commutator in the second term is,

$$[\, a_p^+ a_q a_{q'},\, H \,] = (\, \omega_q + \omega_{q'} - \omega_p \,)\, a_p^+ a_q a_{q'} + \\ + \frac{1}{2NS} \sum_{1,2,3,4} K(1,2,3,4)\, [\, a_p^+ a_q a_{q'},\, a_1^+ a_2^+ a_3 a_4 \,] \qquad (3.3.7)$$

Hence the equation-of-motion, Eqn.(3.3.5), becomes,

$$(\, \omega + \omega_p - \omega_q - \omega_{q'} \,)\, G(p,q,q',k;\omega) = (\, \delta_{qk} + \delta_{q'k} \,)\, n_p + \\ \frac{1}{2NS} \sum_{1,2,3,4} K(1,2,3,4) << [\, a_p^+ a_q a_{q'},\, a_1^+ a_2^+ a_3 a_4 \,];\, a_k^+ >>_\omega \qquad (3.3.8)$$

We use the approximation method described in detail in Sec.2.4 to approximate the Green function in the last term on the right-hand side of Eqn.(3.3.8) by the expression in Eqn.(2.4.3). Hence Eqn.(3.3.8) becomes, in our approximation,

$$(\, \omega + \omega_p - \omega_q - \omega_{q'} \,)\, G(p,q,q',k;\omega) = (\, \delta_{qk} + \delta_{q'k} \,)\, n_p + \\ \frac{1}{2NS} \sum_{3,4} \{\, K(q,q',3,4) + K(q',q,3,4) \,\}\, G(p,3,4,k;\omega) \qquad (3.3.9)$$

We define the wave vector K by,

$$K = k + p = q + q' = 3 + 4 \qquad (3.3.10)$$

Then we change variables,

$$q = K/2 + Q\ , \qquad q' = K/2 - Q$$
$$3 = K/2 + Q'\ , \qquad 4 = K/2 - Q' \tag{3.3.11}$$

We treat k, p and ω as constants for the moment and define,

$$A(Q) = G(p,q,q',k;\omega) \tag{3.3.12}$$

Then Eqn.(3.3.9) can be written,

$$\{\ \omega - E(p,K/2+Q,K/2-Q)\ \}\ A(Q) = (\ \delta_{K/2+Q,k} + \delta_{K/2-Q,k}\ )\ n_p +$$
$$\frac{1}{2NS} \sum_{Q'} \{\ K(K/2+Q,K/2-Q,K/2+Q',K/2-Q') +$$
$$K(K/2-Q,K/2+Q,K/2+Q',K/2-Q')\ \}\ A(Q') \tag{3.3.13}$$

where,

$$E(p,K/2+Q,K/2-Q) = \omega_{K/2+Q} + \omega_{K/2-Q} - \omega_p$$
$$= 1 + h + D\ (2\ S - 1) + g\ \cos(p) - 2\ g\ \cos(K/2)\ \cos(Q) \tag{3.3.14}$$

Because the boson annihilation operators commute with each other, A(Q) is an even function of Q. Hence sums such as,

$$\sum_{Q} \sin(Q)\ A(Q)$$

vanish. Substituting the expression for the interaction K(1,2,3,4), in Eqn.(3.2.3), into Eqn.(3.3.13) then gives,

$$\{\ \omega - E(p,K/2+Q,K/2-Q)\ \}\ A(Q) = (\ \delta_{Q,k-K/2} + \delta_{Q,K/2-k}\ )\ n_p +$$
$$\frac{1}{N\ S}\ \{\ g\ \cos(K/2) - \cos(Q)\ \}\ F^{(1)} - \frac{1}{N\ S}\ \frac{D}{2\ J}\ F^{(2)} \tag{3.3.15}$$

where,

$$F^{(1)} = \sum_{Q'} \cos(Q')\ A(Q') \tag{3.3.16}$$

$$F^{(2)} = \sum_{Q'} A(Q')$$

Eqn.(3.3.15) is an integral equation for A(Q) which can be solved because it has a separable kernel. To solve it we divide both sides by,

$$\omega - E(p,K/2+Q,K/2-Q)$$

to obtain an expression for A(Q) which contains the numbers $F^{(1)}$ and $F^{(2)}$. Then taking the sum over all wave vectors Q in the first Brillouin zone gives an expression for $F^{(2)}$ in terms of $F^{(1)}$, $F^{(2)}$ and other numbers. Similarly multiplying by cos(Q) and then taking the sum gives an expression for $F^{(1)}$. Hence we obtain two equations for $F^{(1)}$ and $F^{(2)}$ of the form,

$$\begin{aligned} A_1\, F^{(1)} + A_2\, F^{(2)} &= B_1 \\ A_3\, F^{(1)} + A_4\, F^{(2)} &= B_2 \end{aligned} \qquad (3.3.17)$$

and we find,

$$\begin{aligned}
A_1 &= 1 - \frac{1}{N\,S} \sum_{Q} \frac{\cos(Q)\ \{\ g\cos(K/2) - \cos(Q)\ \}}{\omega - E(p,K/2+Q,K/2-Q)} \\
A_2 &= \frac{1}{N\,S}\,\frac{D}{2\,J} \sum_{Q} \frac{\cos(Q)}{\omega - E(p,K/2+Q,K/2-Q)} \\
A_3 &= -\frac{1}{N\,S} \sum_{Q} \frac{g\cos(K/2) - \cos(Q)}{\omega - E(p,K/2+Q,K/2-Q)} \\
A_4 &= 1 + \frac{1}{N\,S}\,\frac{D}{2\,J} \sum_{Q} \frac{1}{\omega - E(p,K/2+Q,K/2-Q)} \\
B_1 &= \sum_{Q} \frac{\cos(Q)}{\omega - E(p,K/2+Q,K/2-Q)}\; n_p\, (\ \delta_{Q,k-K/2} + \delta_{Q,K/2-k}\ ) \\
B_2 &= \sum_{Q} \frac{1}{\omega - E(p,K/2+Q,K/2-Q)}\; n_p\, (\ \delta_{Q,k-K/2} + \delta_{Q,K/2-k}\ )
\end{aligned} \qquad (3.3.18)$$

The solution of Eqn.(3.3.17) is,

$$F^{(1)} = \frac{A_4 B_1 - A_2 B_2}{1 - W}$$

$$F^{(2)} = \frac{A_1 B_2 - A_3 B_1}{1 - W} \qquad (3.3.19)$$

$$1 - W = A_1 A_4 - A_2 A_3$$

We will now perform the sums over wave vectors Q in Eqn.(3.3.18). For convenience we define the dimensionless parameter f by,

$$f = \frac{1 + h + D (2S - 1) + g \cos(p) - \omega}{2g \cos(K/2)} \qquad (3.3.20)$$

The two-spin-wave continuum discussed in Sec.1.5 is, for this system,

$$\omega_T \geqslant 2 \{ 1 + h + D (2S - 1) - g \mid \cos(K/2) \mid \}$$

$$(3.3.21)$$

$$\omega_T \leqslant 2 \{ 1 + h + D (2S - 1) + g \mid \cos(K/2) \mid \}$$

The region $|f| \leqslant 1$ is

$$\omega + \omega_p \geqslant 2 \{ 1 + h + D (2S - 1) - g \mid \cos(K/2) \mid \}$$

$$(3.3.22)$$

$$\omega + \omega_p \leqslant 2 \{ 1 + h + D (2S - 1) + g \mid \cos(K/2) \mid \}$$

In our low temperature approximation we work with p close to zero so ω_p is merely the energy gap in the single spin-wave dispersion. We will, in the rest of this chapter and in Ch.4, refer to the region $|f| \leqslant 1$ as the two-spin-wave continuum since we will be considering two-spin-wave states with total energy $(\omega + \omega_p)$.

Then, using Eqn.(3.3.14),

$$\omega - E(p,K/2+Q,K/2-Q) = 2g \cos(K/2) \{ \cos(Q) - f \} \qquad (3.3.23)$$

We also define a function Y(f) by,

$$Y(f) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{dQ}{\cos(Q) - f + i\eta} \quad , \quad \eta \to 0 \qquad (3.3.24)$$

The parameter η is included to make the integrand finite everywhere for $|f|<1$. The integral in Eqn.(3.3.24) can be calculated analytically and the result gives,

$$\begin{aligned} Y(f) &= - i \,(1 - f^2)^{-1/2} , \quad | f | < 1 \\ Y(f) &= - (f^2 - 1)^{-1/2} , \quad f > 1 \qquad (3.3.25) \\ Y(f) &= (f^2 - 1)^{-1/2} , \quad f < - 1 \end{aligned}$$

We note also that,

$$\begin{aligned} \frac{1}{2\pi}\int_{-\pi}^{\pi} \frac{\cos(Q)\, dQ}{\cos(Q) - f + i\eta} &= 1 + f\, Y(f) , \quad \eta \rightarrow 0 \\ & \qquad\qquad (3.3.26) \\ \frac{1}{2\pi}\int_{-\pi}^{\pi} \frac{\cos^2(Q)\, dQ}{\cos(Q) - f + i\eta} &= f + f^2\, Y(f) , \quad \eta \rightarrow 0 \end{aligned}$$

We then replace the sums in Eqn.(3.3.18) by integrals, using Eqn.(1.2.6), to obtain,

$$\begin{aligned} A_1 &= 1 - \frac{g\cos(K/2) - f}{2gS\cos(K/2)} \{ 1 + f\, Y(f) \} \\ A_2 &= \frac{D}{2J} \frac{1}{2gS\cos(K/2)} \{ 1 + f\, Y(f) \} \\ A_3 &= \frac{1}{2gS\cos(K/2)} \{ 1 + f\, Y(f) - g\cos(K/2)\, Y(f) \} \\ & \qquad\qquad (3.3.27) \\ A_4 &= 1 + \frac{D}{2J} \frac{1}{2gS\cos(K/2)} Y(f) \\ B_1 &= (\omega - \omega_k)^{-1} n_p \cos(\frac{k-p}{2}) \\ B_2 &= (\omega - \omega_k)^{-1} n_p \end{aligned}$$

where we have used the fact that,

$$E(p,p,k) = \omega_k \qquad (3.3.28)$$

to simplify the last two equations.

We now stop treating k, p and ω as constants and write Eqn.(3.3.15) as,

$$\{ \omega - E(p,K/2+Q,K/2-Q) \} \, G(p,K/2+Q,K/2-Q,k;\omega) =$$

$$(\delta_{2Q,k-p} + \delta_{2Q,p-k}) \, n_p + \frac{1}{N\,S} \{ g \cos(K/2) - \cos(Q) \} \times$$

$$\frac{A_4 B_1 - A_2 B_2}{1 - W} - \frac{1}{N\,S} \frac{D}{2\,J} \frac{A_1 B_2 - A_3 B_1}{1 - W} \qquad (3.3.29)$$

where K, k and p are not independent but are related by K=k+p and W is a function of two of these parameters and ω. We choose to write it as W(p,K;ω) and it is given by,

$$W(p,K;\omega) = \frac{1}{2\,S} \left[1 - \frac{f}{g \cos(K/2)} \right] \left[1 + f\,Y(f) \right] +$$

$$\frac{D}{2g^2 S^2 \cos^2(K/2)} \left[1 + f\,Y(f) - 2gS \cos(K/2)\, Y(f) \right] \qquad (3.3.30)$$

For the special case of the Heisenberg ferromagnet, g=1 and D=0, this expression has the same form as the expressions for W(K) in Eqns.(2.3.23) and (2.3.24). In fact the solution of the equation,

$$\mathrm{Re}\, W(0,k;\omega) = 1 \, , \quad f > 1 \qquad (3.3.31)$$

is,

$$\omega = \omega_B(K) - \omega_p \, , \quad p = 0 \qquad (3.3.32)$$

where $\omega_B(K)$ is the bound-state energy for wave vector K, i.e. the solution of Eqn.(3.3.31) is just the bound-state energy up to an additive number which is the gap in the single spin-wave energy at zero wave vector. Bound states will be discussed in detail for this system in Sec.3.6.

We substitute our expression for the four-particle Green function,

$$G(p,K/2+Q,K/2-Q;\omega)$$

given by Eqn.(3.3.29) into Eqn.(3.3.4) to obtain an expression for G(k,ω). There are three wave vectors to be summed over in the last term on the right-hand side of Eqn.(3.3.4). One of these is taken care of by the Kronecker δ in the interaction term. Another can be written in the form of the sums in Eqn.(3.3.16). Hence we find that Eqn.(3.3.4) becomes,

$$(\omega - \omega_k) G(k,\omega) = 1 + \frac{1}{N S} \sum_p \left[\left\{ g \cos\left(\frac{k+p}{2}\right) - \cos\left(\frac{k-p}{2}\right) \right\} \times F^{(1)} - \frac{D}{2 J} F^{(2)} \right] \qquad (3.3.33)$$

The functions $F^{(1)}$ and $F^{(2)}$ both contain the factor,

$$(\omega - \omega_k)^{-1}$$

and so we can write Eqn.(3.3.33) in the form,

$$(\omega - \omega_k) G(k,\omega) = 1 + \Sigma(k,\omega) (\omega - \omega_k)^{-1}$$

or, using Eqn.(2.1.10),

$$G(k,\omega) = G^{(0)}(k,\omega) + G^{(0)}(k,\omega) \Sigma(k,\omega) G^{(0)}(k,\omega) \qquad (3.3.34)$$

where

$$\Sigma(k,\omega) = \frac{1}{\pi S} \int_{-\pi}^{\pi-k} dp \, n_p \left(\left\{ g \cos\left(\frac{k+p}{2}\right) - \cos\left(\frac{k-p}{2}\right) \right\} \cos\left(\frac{k-p}{2}\right) + D \left[g \cos\left(\frac{k+p}{2}\right) \right]^{-1} \left[2 \cos\left(\frac{k-p}{2}\right) - 2gS \cos\left(\frac{k+p}{2}\right) - f - \left\{ \cos\left(\frac{k-p}{2}\right) - f \right\}^2 Y(f) \right] \right) \left[1 - W(p,k+p;\omega) \right]^{-1} \qquad (3.3.35)$$

We have changed the sum over wave vectors p to an integral, using Eqn.(1.2.6), in obtaining this equation. The upper limit of the integral is $(\pi-k)$, rather than π, to make the integrand finite everywhere as the parameter f diverges as $p \to \pi-k$. For low temperatures this is not important since the Bose factor ensures that the main contribution to the integral comes from small p. The integrand, apart from the Bose factor, is just a T-matrix, as discussed in Sec.2.5.

We note that Eqn.(3.3.34) is similar to Dyson's equation, Eqn.(2.1.17). To make it exactly the same we replace the last $G^{(0)}(k,\omega)$ in the second term on the right-hand side by $G(k,\omega)$, which enables us to identify $\Sigma(k,\omega)$ as the self-energy. Within our approximation of working to first order in the Bose factor this replacement does not affect our results because, if we expand the Green function in Eqn.(2.1.16), which satisfies Dyson's equation, in powers of the self-energy, we obtain,

$$G(k,\omega) = G^{(0)}(k,\omega) + G^{(0)}(k,\omega)\ \Sigma(k,\omega)\ G^{(0)}(k,\omega) + O\ [\ \Sigma(k,\omega)^2\ ] \tag{3.3.36}$$

where $G^{(0)}(k,\omega)$ is defined by Eqn.(2.1.10). The self-energy is of first order in the Bose factor. Neglecting terms of higher order in the self-energy causes Eqn.(3.3.36) to reduce to Eqn.(3.3.34). This replacement of the non-interacting Green function by the interacting one accounts for multiple scattering events instead of merely scattering from a single spin wave.

To obtain the spectral weight function we also need to calculate the four-particle Green function,

$$<< a_k ;\ a_t^+\ a_{t'}^+\ a_{t+t'-k} >>_\omega \tag{3.3.37}$$

which appears in Eqn.(3.2.4). This calculation is similar to the calculation of $G(k,\omega)$ and therefore we will omit some of the details. The equation-of-motion is,

$$\omega << a_k ;\ a_t^+\ a_{t'}^+\ a_{t+t'-k} >>_\omega = <\ [\ a_k ,\ a_t^+\ a_{t'}^+\ a_{t+t'-k}\ ]\ > + << [\ a_k ,\ H\ ] ;\ a_t^+\ a_{t'}^+\ a_{t+t'-k} >>_\omega \tag{3.3.38}$$

The commutator in the second term on the right-hand side of this equation is the same as in Eqn.(3.3.1) and in fact the only differences between the calculation of this Green function and $G(k,\omega)$ arise because of the different thermal averages. The thermal average in Eqn.(3.3.38) is,

$$< [a_{k}, a_{t}^{+} a_{t'}^{+} a_{t+t'-k}] > = \delta_{kt} n_{t'} + \delta_{kt'} n_{t} \qquad (3.3.39)$$

where we have used Eqns.(1.5.8) and (1.5.13), the definitions of commutators and thermal averages of the boson operators.

We obtain an integral equation for the Green function generated by the second term on the right-hand side of Eqn.(3.3.38),

$$A(Q) = << a_{p}^{+} a_{K/2+Q} a_{K/2-Q}; a_{t}^{+} a_{t'}^{+} a_{t+t'-k} >>_{\omega} \qquad (3.3.40)$$

which is the same as Eqn.(3.3.15) except that the first term on the right-hand side is, to lowest order in the Bose factors,

$$< [a_{p}^{+} a_{K/2+Q} a_{K/2-Q}, a_{t}^{+} a_{t'}^{+} a_{t+t'-k}] > =$$

$$(\delta_{K/2-Q,t} \delta_{K/2+Q,t'} + \delta_{K/2-Q,t'} \delta_{K/2+Q,t}) \delta_{p,t+t'-k} n_{p}$$

(3.3.41)

neglecting terms of the form $<a^{+}a^{+}aa>$ which are quadratic in the Bose factors. Hence if we change the parameters B_1 and B_2 in Eqn.(3.3.18) to,

$$B_{1} = \sum_{Q} \frac{\delta_{p,t+t'-k} (\delta_{K/2-Q,t} \delta_{K/2+Q,t'} + \delta_{K/2-Q,t'} \delta_{K/2+Q,t})}{\omega - E(p,K/2+Q,K/2-Q)} \times n_{p} \cos(Q)$$

$$= \frac{2}{\omega - E(p,t,t')} n_{p} \delta_{p,t+t'-k} \cos(\frac{t-t'}{2})$$

$$B_{2} = \sum_{Q} \frac{\delta_{p,t+t'-k} (\delta_{K/2-Q,t} \delta_{K/2+Q,t'} + \delta_{K/2-Q,t'} \delta_{K/2+Q,t}) n_{p}}{\omega - E(p,K/2+Q,K/2-Q)}$$

$$= \frac{2}{\omega - E(p,t,t')} n_{p} \delta_{p,t+t'-k} \qquad (3.3.42)$$

then we obtain,

$$(\omega - \omega_{k}) << a_{k}, a_{t}^{+} a_{t'}^{+} a_{t+t'-k} >>_{\omega} = \delta_{kt} n_{t'} + \delta_{kt'} n_{t} +$$

$$\frac{1}{N\,S} \sum_{p} \left\{ \left[g \cos\left(\frac{k+p}{2}\right) - \cos\left(\frac{k-p}{2}\right) \right] F^{(1)} - \frac{D}{2\,J} F^{(2)} \right\} \tag{3.3.43}$$

where $F^{(1)}$ and $F^{(2)}$ are given by Eqn.(3.3.19) and we use the new values of B_1 and B_2 in Eqn.(3.3.42).

We define a function $\Lambda(k,\omega)$ by,

$$\frac{1}{N} \sum_{t,t'} \langle\langle a_k ;\, a_t^+ \, a_{t'}^+ \, a_{t+t'-k} \rangle\rangle_\omega = G(k,\omega)\; 2S\; \Lambda(k,\omega) \tag{3.3.44}$$

so that,

$$\langle\langle S_k^- ;\, S_k^+ \rangle\rangle_\omega = 2S\; G(k,\omega) \left[1 - \Lambda(k,\omega) \right] \tag{3.3.45}$$

using Eqn.(3.2.4). The result for $\Lambda(k,\omega)$ is,

$$\begin{aligned} \Lambda(k,\omega) = {} & \frac{1}{2\pi S}\int_{-\pi}^{\pi} dp\, n_p + \frac{1}{4\pi^2 S^2} \int_{-\pi}^{\pi} dp\; n_p \int_{-\pi}^{\pi} \frac{dq}{\omega - E(p,q,k+p-q)} \times \\ & \frac{1}{1 - W(p,k+p;\omega)} \left\{ \left[g \cos\left(\frac{k+p}{2}\right) - \cos\left(\frac{k-p}{2}\right) \right] \cos\left(\frac{2q-k-p}{2}\right) + \right. \\ & \frac{D}{g \cos[(k+p)/2]} \left[\cos\left(\frac{k-p}{2}\right) + \cos\left(\frac{2q-k-p}{2}\right) - 2gS \cos\left(\frac{k+p}{2}\right) - \right. \\ & \left.\left. - f - \left\{ \cos\left(\frac{k-p}{2}\right) - f \right\} \left\{ \cos\left(\frac{2q-k-p}{2}\right) - f \right\} Y(f) \right] \right\} \end{aligned} \tag{3.3.46}$$

We note that the first term on the right-hand side of this equation can be written,

$$\begin{aligned} \frac{1}{2\pi S} \int_{-\pi}^{\pi} dp\; n_p &= \frac{1}{2\pi S} \int_{-\pi}^{\pi} dp \left(S + \langle S_p^z \rangle \right) \\ &= 1 + \frac{1}{S} \langle S^z \rangle \end{aligned} \tag{3.3.47}$$

We will now analyse the results obtained in this section.

3.4 Spin-wave Damping and Shift

In the limit of low temperatures, T<<J in our units, the Bose factor, defined by Eqn.(1.5.14), is small. Hence the self-energy and the function $\Lambda(k,\omega)$, which are first order in the Bose factor, are small.

The Green function that gives us the transverse spectral weight function can be written,

$$<< S_k^-;\, S_k^+ >>_\omega = \frac{2S\,[\,1 - \Lambda(k,\omega)\,]}{\omega - \omega_k - \mathrm{Re}\,\Sigma(k,\omega) - i\,\mathrm{Im}\,\Sigma(k,\omega)} \qquad (3.4.1)$$

using Eqns.(3.3.45) and (2.1.9). Since $\Sigma(k,\omega)$ and $\Lambda(k,\omega)$ are small, this Green function has a maximum, for a given k, at an energy close to the single spin-wave energy. This energy, the renormalised spin-wave energy, is approximately,

$$\begin{aligned} \Omega_k &= \omega_k + \mathrm{Re}\,\Sigma(k,\omega_k) \\ &= \omega_k - \Delta(k) \end{aligned} \qquad (3.4.2)$$

where $\Delta(k)$ is the spin-wave shift. We evaluate the self-energy at the single spin-wave energy, assuming that it does not vary much for energies close to the single spin-wave energy. The spin-wave damping, or inverse lifetime, is given by,

$$\Gamma(k) = -\,\mathrm{Im}\,\Sigma(k,\omega_k) \qquad (3.4.3)$$

and is a measure of the width of the spin-wave peak in the spectral weight function.

We will evaluate the self-energy, Eqn.(3.3.35), at the single spin-wave energy for low temperatures. The Bose factor, Eqn.(1.5.14), is largest for small wave vectors in this system. We will assume that the integrand in Eqn.(3.3.35) is dominated by small wave vectors p. We expand the integrand, except the Bose factor, in powers of p and retain only the lowest power. For convenience we define the integrals,

$$R_m(T) = \frac{1}{\pi}\int_0^\pi dp\; n_p\, \sin^m(p/2)\;, \quad m = 0,1,2,\ldots \qquad (3.4.4)$$

For $0<k<\pi$, the integrand is non-zero for p=0 and we obtain, after some simple algebra,

$$\Delta(k) = g\, R_0(T)\, \sin^2(k)\, \{ (1 - g) \cos^2(\tfrac{k}{2}) + D(2S - \tfrac{1}{g}) \} \times$$

$$\{ [\cos^2(\tfrac{k}{2}) - \tfrac{D}{g}] [2gS + 1 - g] + D (2S - 1) \} \frac{1}{F_k}$$

$$\Gamma(k) = 2g\, R_0(T) \cos^2(\tfrac{k}{2}) \sin(k)\, \{ (1 - g) \cos^2(\tfrac{k}{2}) + D (2S -$$

$$\tfrac{1}{g}) \} \{ (1 - g) [\cos^2(\tfrac{k}{2}) - \tfrac{D}{g}] + D (2S - 1) \} \frac{1}{F_k}$$

$$F_k = \{ [\cos^2(\tfrac{k}{2}) - \tfrac{D}{g}] (1 - g) + D (2S - 1) \}^2 + \sin^2(\tfrac{k}{2}) \times$$

$$4gS [\cos^2(\tfrac{k}{2}) - \tfrac{D}{g}] \{ [\cos^2(\tfrac{k}{2}) - \tfrac{D}{g}] (1 - g + gS) +$$

$$D (2S - 1) \} \geqslant 0 \qquad (3.4.5)$$

For the isotropic case, g=1 and D=0, the expressions for $\Delta(k)$ and $\Gamma(k)$ given in Eqn.(3.4.5) vanish and it is necessary to retain terms of higher order in p. In this case the shift and damping have been calculated by Lovesey (1981) and are given by,

$$\Delta(k) = \frac{[1 - \cos(k)] (S - 1) R(T)}{2 S^2}$$

$$\Gamma(k) = \frac{\sin(k) R(T)}{2 S^2} \qquad (3.4.6)$$

$$R(T) = 1.04\, T^{3/2}$$

For the anisotropic case and small wave vectors k, we note that the damping is linear in k and the shift is quadratic in k. At long wavelengths the damping is therefore the bigger effect and is likely to be more important experimentally.

At the first Brillouin zone boundary, $k=\pi$, we have to be careful when evaluating the shift and damping because the parameter f is singular for small p. At the single spin-wave energy f is given by, using Eqn.(3.3.20),

$$f = \frac{\cos(p) + \cos(k)}{2\cos[(k+p)/2]} \qquad (3.4.7)$$

Then for a given k, f has a singularity at $p=\pi-k$. For p slightly greater than $(\pi-k)$, f is large and positive. For p slightly less than $(\pi-k)$, f is large and negative. Hence for $k=\pi$, the singularity is at $p=0$ and $f>1$ for all $p>0$. The region given by $|f|<1$, which is the one that we are considering, is given by $-\pi<p<0$. To calculate the shift and damping we first set $k=\pi$ and then restrict the range of integration to $-\pi<p<0$. We then find, from Eqn.(3.3.35), that for $D\neq0$,

$$\Delta(\pi) = -2g(1+2gS)R_2(T)$$
$$\Gamma(\pi) = 2g(1+2gS)^2 R_3(T) \qquad (3.4.8)$$

and for $D=0$,

$$\Delta(\pi) = \frac{-2g(1+g)}{1+g-2gS} R_2(T)$$
$$\Gamma(\pi) = \frac{2g(1+g)^2}{(1+g-2gS)^2} R_3(T) \qquad (3.4.9)$$

Eqns.(3.4.8) and (3.4.9) give the same results for $S=1/2$, as expected. For the special case of $g=1$, $h=D=0$ and $S=1/2$, the damping is given by,

$$\Gamma(\pi) = \frac{\pi T^2}{3}, \quad T \to 0 \qquad (3.4.10)$$

from Eqn.(3.4.9).

3.5 Bound States

Two-spin-wave bound states for the Heisenberg ferromagnetic chain have been discussed in Sec.2.3 by studying a Green function of the form $\langle\langle aa;a^+a^+\rangle\rangle_\omega$. However, neutrons do not couple directly to such bound states and they cannot be observed. They do manifest themselves in the spectral weight as resonances caused by a spin wave, created by the scattering of a neutron, interacting with another spin wave in the system in such a way that they form a bound state. The energies of these resonance peaks in the spectral weight are usually less than the corresponding bound state energies.

The bound state is a solution of Eqn.(3.3.31), up to a constant additive term, Eqn.(3.3.32), that we will neglect. Using Eqns.(3.3.25) and (3.3.30), we find that Eqn.(3.3.31) becomes,

$$\frac{1}{2S}\left[1-\frac{f}{g\cos^2(k/2)}\right]\left[1-\frac{f}{(f^2-1)^{1/2}}\right]+$$

$$\frac{D}{2g^2S\cos^2(k/2)}\left[1+\frac{[\,2gS\cos(k/2)-f\,]}{(f^2-1)^{1/2}}\right]=1 \qquad (3.5.1)$$

which is difficult to solve analytically in most cases. We note that it reduces to Eqn.(2.3.24) for the case $g=1$ and $D=0$. At the zone boundary, $k=\pi$, the equation can be solved analytically and there are two solutions given by,

$$\begin{aligned}\omega_B &= 1+h+D(2S-1)+g-\frac{1}{2S}\\ \omega_B &= 1+h+D(2S-1)+g-2D\end{aligned} \qquad (3.5.2)$$

which are known as the exchange and single-site bound states respectively. These agree with the results of Silberglitt and Torrance (1970). From Eqn.(3.3.35), it can be seen that these are in fact poles of the self-energy, which contains a factor $\{1-W(p,k+p;\omega)\}$ in the denominator.

Below the two-spin-wave continuum, $f>1$, the imaginary parts of the self-energy and the function $\Lambda(k,\omega)$ are zero, because the integral $Y(f)$ is real, Eqn.(3.3.25). The spectral weight is obtained from the imaginary part of the Green function,

$$\langle\langle S_k^-;S_k^+\rangle\rangle_\omega=\frac{2S\,[\,1-\Lambda(k,\omega)\,]}{\omega-\omega_k-\Sigma(k,\omega)} \qquad (3.5.3)$$

using Eqns.(3.3.45) and (2.1.9), which can only be non-zero if the denominator,

$$L(k,\omega) = \omega - \omega_k - \Sigma(k,\omega) \tag{3.5.4}$$

vanishes. Let $\omega_0(k)$ be a resonance energy given by,

$$L(k,\omega_0) = 0 \tag{3.5.5}$$

Then for energies near this resonance energy,

$$\begin{aligned} L(k,\omega) &= L(k,\omega_0) + (\omega - \omega_0) L'(k,\omega_0) + \ldots \\ L'(k,\omega) &= \partial_\omega L(k,\omega) \end{aligned} \tag{3.5.6}$$

and we can write,

$$<< S_k^-; S_k^+ >>_\omega = \lim_{\eta \to 0} \frac{1}{L'(k,\omega_0)} \frac{2S [1 - \Lambda(k,\omega)]}{\omega - \omega_0 + i \eta} \tag{3.5.7}$$

Hence,

$$- \frac{1}{\pi} \operatorname{Im} << S_k^-; S_k^+ >>_\omega = \delta (\omega - \omega_k) \frac{2S [1 - \Lambda(k,\omega_0)]}{L'(k,\omega_0)} \tag{3.5.8}$$

The spectral weight function must be positive so only solutions which have a positive amplitude weighting the δ function, and hence a positive $L'(k,\omega_0)$, are physical.

We have not been able to obtain analytic expressions for the resonances and amplitudes, even in the low temperature limit, except at the zone boundary.

We follow the same procedure as in the previous section of expanding the integrand of the self-energy, Eqn.(3.3.35), in powers of p and retaining only the leading order term. We treat $\Lambda(k,\omega)$, Eqn.(3.3.46), in the same way. For $k=\pi$ we restrict the integration range to $-\pi<p<0$. The results are as follows.

For $k=\pi$ and $D=0$,

$$1 - W(0,k;\omega) = 1 - \frac{1}{4gSx} \tag{3.5.9}$$

where,

$$2gx = 1 + h + g - \omega \tag{3.5.10}$$

We then find,

$$L(k,\omega) = - 2gx + \frac{2 (1 + g) R_2(T)}{S [1 - 1/(4gSx)]} \tag{3.5.11}$$

and the solution of Eqn.(3.5.5) is,

$$x_0 = \frac{1}{4gS} [1 + 4 (1 + g) R_2(T)] \tag{3.5.12}$$

where the integrals $R_m(T)$ are defined in Eqn.(3.4.4). At this resonance energy,

$$\begin{aligned} L'(k,\omega_0) &= 1 + \frac{1}{4 (1 + g) R_2(T)} \\ \Lambda(k,\omega_0) &= \frac{R_0(T)}{S} - \frac{1}{4Sx_0} \end{aligned} \tag{3.5.13}$$

so the amplitude is,

$$\frac{2S - 2R_0(T) + 1/(2x_0)}{1 + 1/[4 (1 + g) R_2(T)]} \tag{3.5.14}$$

In Fig.3.1 we plot the bound state as a function of wave vector for g=0.9, S=1/2, h=0 and T=0.3. For these values the resonance at the zone boundary has energy 0.321 and the amplitude is 0.283.

For $k=\pi$ and $D\neq 0$, we simply set p=0 in the integrand of the self-energy and the function $\Lambda(k,\omega)$ and expand all functions in powers of cos(k/2). Then we set $k=\pi$ and obtain the results,

$$\begin{aligned} 1 - W(0,k;\omega) &= [1 - \frac{D}{gx}] [1 - \frac{1}{4gSx}] \\ L(k,\omega) &= - 2gx + 4D R_0(T) [1 - \frac{D}{gx}]^{-1} \end{aligned} \tag{3.5.15}$$

where now,

$$2gx = 1 + h + D\,(\,2S - 1\,) + g - \omega \tag{3.5.16}$$

The solution of Eqn.(3.5.5) is,

$$x_0 = \frac{D}{g}\,[\,1 + 2R_0(T)\,] \tag{3.5.17}$$

and at resonance,

$$\begin{aligned} L'(k,\omega_0) &= 1 + \frac{1}{2R_0(T)} \\ \Lambda(k,\omega_0) &= \frac{R_0}{S} + \frac{1}{2S} \end{aligned} \tag{3.5.18}$$

In Fig.3.2 we plot the resonance for the case g=1, D=0.1, S=1, h=0 and T=0.3. At the zone boundary the resonance energy is 1.750 and the amplitude is 0.106. This resonance exists only for a small range of wave vectors near the zone boundary and disappears into the two-spin-wave continuum at approximately $k= 0.9\pi$. It also has very little dispersion. The resonance due to the exchange bound state, that does not appear as a solution of Eqn.(3.5.5) with $L(k,\omega)$ given by Eqn.(3.5.15) because it involves higher powers of p in the integrand of the self-energy, has zero amplitude at the zone boundary. However, the amplitude increases as the wave vector decreases and it becomes a significant feature for small wave vectors. For example, for $k=\pi/3$ the resonance energy is 0.3 and the amplitude is 0.080.

We will discuss some of these results in the next section.

3.6 Discussion

Experimentally, the most important results of this calculation concern the spin-wave damping and the significant amplitude of the bound-state resonances.

From Eqn.(3.4.5) we see that the damping shows a pronounced wave vector dependence. For the isotropic case, g=1, D=0, h=0, and spin S=1, we see from Eqn.(3.4.9) that the damping diverges at the zone boundary. For the anisotropic case the damping increases significantly at the zone boundary but does not diverge. For other values of the spin, including S=1/2, the damping at the zone boundary is less than for S=1. For a classical system with this Hamiltonian, Eqn.(3.1.1), the damping at the zone boundary is zero. This suggests that S=1, rather than S=1/2, may exhibit the most pronounced quantum effects.

For the isotropic case, g=1 and D=h=0, we find, from Eqns.(3.4.6) and (3.4.9),

$$\begin{aligned} &\Gamma(k) \propto T^{3/2} \sin(k) \ , \quad T \to 0 \ , \quad k < \pi \\ &\Gamma(\pi) \propto T^{2} \ , \quad T \to 0 \end{aligned} \qquad (3.6.1)$$

and these results are consistent with the results obtained from a numerical study of quantum spin chains (Schneider and Stoll 1981). We will not go into the details of these numerical studies in this thesis. Agreement with numerical results is not as good for systems with any anisotropy.

We have shown in the previous section that for a temperature of 0.3, measured in units of 4JS as usual, the amplitude of the bound-state resonance is significant and the resonance would probably show up experimentally as a detectable peak in the spectral weight. Also the energies and amplitudes of these resonances depend strongly on the anisotropies, measured by g and D, and on the wave vector, k.

We conclude this section with a comparison of our results and the results of Cooke and Hahn (1970), who studied a similar system using the Holstein-Primakoff transformation, Eqn.(1.5.7). They obtained the result,

$$<< S_k^-; S_k^+ >>_\omega^{CH} = \frac{2S}{L^{CH}(k,\omega)} \qquad (3.6.2)$$

where,

$$L^{CH}(k,\omega) = (\omega - \omega_k) [1 + \Lambda(k,\omega)] - \Sigma(k,\omega) \qquad (3.6.3)$$

in our notation. These results were obtained after expanding the square roots in the transformation, normal ordering the operators and truncating the infinite series obtained. Within the approximation of working to first order in the Bose factors, this result coincides with our result, Eqns.(3.5.3) and (3.5.4), since,

$$[\ 1 + \Lambda(k,\omega)\ ]^{-1} = 1 - \Lambda(k,\omega) + O\ [\ \Lambda(k,\omega)^2\ ] \qquad (3.6.4)$$

and $[\Lambda(k,\omega)\Sigma(k,\omega)]$ is second order in the Bose factor, so is neglected.

However, there remains the question of what the form of the spectral weight is for higher temperatures, not working to first order only in the Bose factor. We will now consider how it may be possible to distinguish between the two forms of the spectral weight experimentally.

Firstly we note that the spin-wave damping and shift are the same since they depend only on the denominator of the spectral weight evaluated at the single spin-wave energy, and so depend only on $\Sigma(k,\omega_k)$ in both cases. However, the dispersion and amplitude of the bound states and resonances are different for the two forms of the spectral weight. We work at the zone boundary, $k=\pi$, for ease of comparison of results. We define,

$$x = [\ 1 + h + D\ (\ 2S - 1\ ) - \omega\ ]\ /\ 2 \qquad (3.6.5)$$

For D=0,

$$L^{CH}(k,\omega) = -\ 2gx\ [\ 1 + \frac{R_0(T)}{S}\ ] + \frac{(\ 1 + g\ )\ R_2(T)\ [\ 2 + 1/(2Sx)\ ]}{1 - W(0,k;\omega)} \qquad (3.6.6)$$

For S=1/2, g=0.9, h=0 and T=0.3, the resonance energy, which is a solution of,

$$L^{CH}(k,\omega_0) = 0 \qquad (3.6.7)$$

is 0.388 and the amplitude is 0.167. From Sec.3.5, our corresponding results are 0.321 and 0.283 respectively, so there is a difference.

For $D \neq 0$ and $g=1$,

$$L^{CH}(k,\omega) = -2x\left(1 + \frac{R_0}{S}\right) + \frac{2D\,R_0(T)\,(2S-1)}{S\,(1 - D/x)} \qquad (3.6.8)$$

For $D=0.1$, $h=0$, $S=1$ and $T=0.3$, the resonance energy, the solution of Eqn.(3.6.7), is 1.945 and the amplitude is 0.321. Our corresponding results are 1.750 and 0.106. Again the resonance energy obtained from the results of Cooke and Hahn (1970) is greater than ours and the amplitude is significantly larger. These differences may well be measurable experimentally.

Finally we note that working to higher order in the Bose factor should give the same results whichever transformation we use and should tell us the correct form of the spectral weight function. We have not, however, pursued such a calculation.

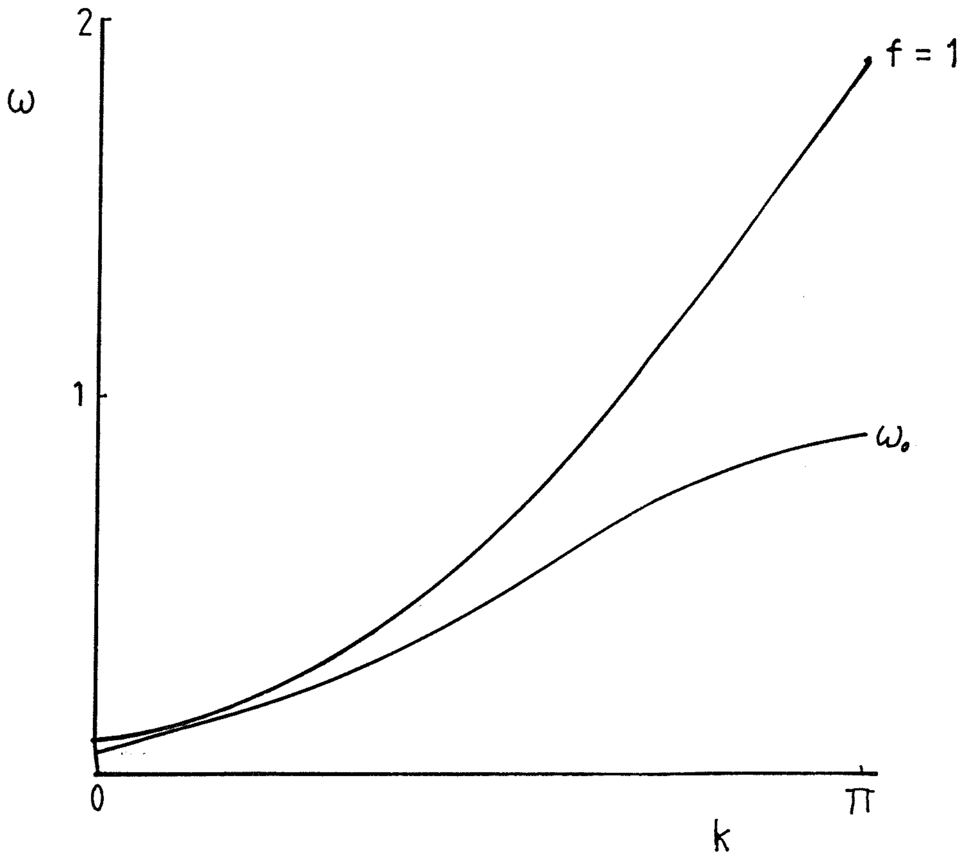

Figure 3.1: Dispersion of bound state for g=0.9, S=1/2, h=0 and T=0.3

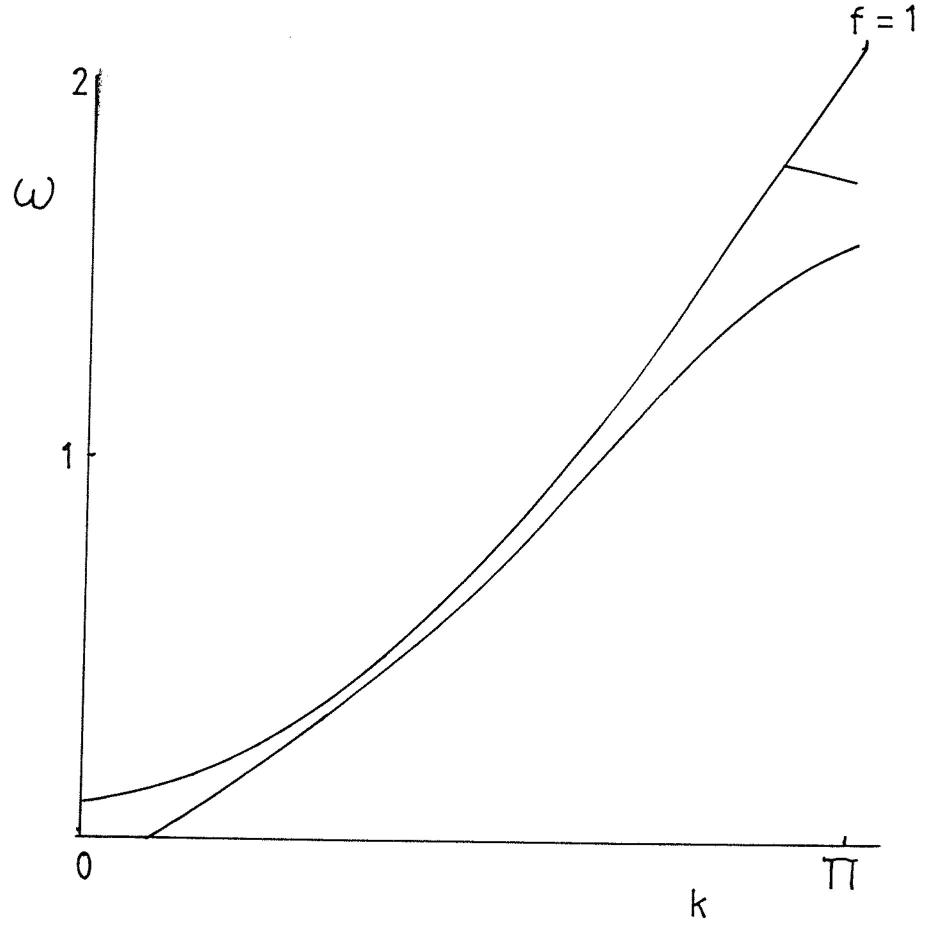

Figure 3.2: Dispersions of resonances for g=1, D=0.1, S=1, h=0 and T=0.3

CHAPTER 4: EASY-PLANE FERROMAGNET

4.1 Introduction to $CsNiF_3$

The compound $CsNiF_3$ has been studied extensively in recent years both experimentally and theoretically (Steiner 1981). It is quasi-one-dimensional above a temperature of approximately 2.66K. The exchange coupling is ferromagnetic and there is an easy-plane anisotropy that encourages the spins to lie in the plane perpendicular to the direction of the magnetic chain of Ni^{2+} ions. The Hamiltonian is assumed to be of the form,

$$H = - J \sum_{l,m} \underline{S}_l . \underline{S}_m + D \sum_{l} (S_l^x)^2 \qquad (4.1.1)$$

where l and m are nearest-neighbour sites, J is the exchange coupling and D is the single-site anisotropy. The magnetic chain lies along the x direction. For $CsNiF_3$ various measurements give J=11.8K and D=9.0K. The spin is S=1. We will describe one method of testing the form of the Hamiltonian for such a system in Ch.5 but will assume in this chapter that the Hamiltonian in Eqn.(4.1.1) describes $CsNiF_3$ well.

The specific heat, magnetic susceptibility, cross-sections for thermal neutron scattering and other quantities mentioned in Sec.1.1 have been measured for this compound. Again we will concentrate only on the neutron scattering results. It is found that the spectral weights contain peaks at $\omega=\pm\omega_k$, where ω_k is the linear spin-wave energy. The intensities of these peaks in $S^{yy}(k,\omega)$ and $S^{zz}(k,\omega)$, the "in-plane" components of the scattering, are greater than for the peaks in $S^{xx}(k,\omega)$, the "out-of-plane" components. For experiments done with a magnetic field applied in a direction which lies in the easy plane, there is also a central peak around $\omega=0$ which depends on the applied field. Unlike the spin-wave peaks, which broaden and decrease in height as the temperature is increased, this central peak increases in height as the temperature is increased. More experimental work on this compound, involving polarisation analysis, will be discussed in Ch.5.

Unlike the system discussed in Ch.3, there is no long-range order in the ground state of this system. Hence spin-wave theory may not be a good approximation. The Hamiltonian in Eqn.(4.1.1) is invariant under rotations in the y-z plane so there should not be a gap in the spin-wave dispersion, according to Goldstone's theorem. For the case of no applied field, Villain (1974) introduced a representation of the spin operators expected to be valid even in the absence of long-range order and made an expansion in the operators which correspond in the classical limit to the differences in angles in the y-z plane between nearest-neighbour sites. However, this approach is not easily generalized to the case where a magnetic field is applied in the easy plane because it is then necessary to make an expansion in operators which correspond to the angles themselves, rather than their variation from site to site, and these angles are not necessarily small.

In the calculation described in the following sections of this chapter (Hood 1984), we will use a transformation introduced by Lindgard and Kowalska (1976) that is easily generalized to non-zero field in the easy plane. This transformation is equivalent to the Holstein-Primakoff and Dyson-Maleev transformations within the framework of perturbation theory (Rastelli and Lindgard 1979) but has the advantage that it is easy to show that Goldstone's theorem is satisfied. It will be discussed further in Sec.4.2.

The Hamiltonian for the system with a magnetic field in the plane can be written,

$$H = - J \sum_{l,m} \underline{S}_l \cdot \underline{S}_m + D \sum_{l} (S_l^x)^2 + h \sum_{l} S_l^z \qquad (4.1.2)$$

We now briefly state some results obtained from the classical limit of Eqn.(4.1.2) involving solitons (Mikeska 1978). If we write the spins on the sites in the form,

$$S_l^x = S \sin(\theta_l)$$

$$S_l^y = S \cos(\theta_l) \sin(\phi_l) \qquad (4.1.3)$$

$$S_l^z = S\cos(\theta_l)\cos(\phi_l)$$

take the continuum limit,

$$\theta_l(t) \rightarrow \theta(x,t)$$

$$\phi_l(t) \rightarrow \phi(x,t) \qquad (4.1.4)$$

and linearise in the parameter θ, assuming that the spins deviate little from the y,z-plane, then the classical equations-of-motion give,

$$\partial_{tt}\phi - c_0^2\partial_{zz}\phi - \omega_0^2\sin(\phi) = 0 \qquad (4.1.5)$$

and,

$$\theta = \frac{1}{2DS}\,\partial_t\phi \qquad (4.1.6)$$

where,

$$c_0^2 = 4DJS^2$$

$$\omega_0^2 = 2DhS \qquad (4.1.7)$$

Eqn.(4.1.5) is the sine-Gordon equation which has three basic solutions, one corresponding to spin waves. Another solution corresponds to kink solitons where the parameter ϕ changes by 2π over a finite change in x. The other solution corresponds to breather solitons which are more complicated. We have mentioned solitons in this section because they are usually considered to be the cause of the central peak in the spectral weight function. However, this is a controversial topic and recent numerical work (Loveluck et al. 1980, Wysin et al. 1982) suggests that spin deviations out of the easy plane may be important.

The rest of this chapter concerns two-spin-wave processes and their effect on the spectral weight. The calculation is similar to that of Ch.3.

4.2 Boson Hamiltonian

In this section we transform the spin Hamiltonian of Eqn.(4.1.2) into a boson Hamiltonian using the transformation introduced by Lindgard and Kowalska (1976) that was mentioned in the previous section. Before doing this we give a very brief outline of how the transformation is obtained.

The aim is to express the spin operators as sums of products of boson creation and annihilation operators. For example,

$$S_1^z = c_0 + c_1 a_1 + c_2 a_1^+ + c_3 a_1^+ a_1 + c_4 a_1^2 + \ldots \qquad (4.2.1)$$

The coeffients, c_i, are determined by a method known as the Matching of Matrix Elements, that we will now describe. We denote the eigenstates of our Hamiltonian by $|\Psi_n\rangle$ with eigenvalues E_n, so that,

$$H \mid \Psi_n \rangle = E_n \mid \Psi_n \rangle \qquad (4.2.2)$$

and write the eigenstates in the form,

$$\mid \Psi_n \rangle = \sum_m b_m \mid S,m \rangle \qquad (4.2.3)$$

where,

$$\Big[\sum_l \underline{S}_l \Big]^2 \mid S,m \rangle = S (S + 1) \mid S,m \rangle$$

$$\sum_l S_l^z \mid S,m \rangle = m \mid S,m \rangle \qquad (4.2.4)$$

$$\sum_l S_l^{\pm} \mid S,m \rangle = [S (S + 1) - m (m \pm 1)]^{1/2} \mid S,m\pm1 \rangle$$

The states $|S,m\rangle$ are eigenstates of the Heisenberg Hamiltonian,

$$H_0 = -J \sum_{l,m} \underline{S}_l \cdot \underline{S}_m + h \sum_l S_l^z \tag{4.2.5}$$

It is possible to write the eigenstates in the form of Eqn.(4.2.3) since, for our Hamiltonian, the operator,

$$\left[\sum_l \underline{S}_l \right]^2$$

is a constant of the motion, i.e. it commutes with the Hamiltonian. We assume that for each state $|\Psi_n\rangle$ there is a state $|n\rangle$ containing n bosons and,

$$\begin{aligned} a^+ \mid n \rangle &= (n + 1)^{1/2} \mid n+1 \rangle \\ a \mid n \rangle &= n^{1/2} \mid n-1 \rangle \end{aligned} \tag{4.2.6}$$

We write,

$$\langle \psi_n \mid \sum_l S_l^z \mid \psi_n \rangle = \langle n \mid c_0 + c_1 a + c_2 a^+ + \ldots \mid n \rangle \tag{4.2.7}$$

and determine the coefficients, c_i, from this equation by setting n=0, then n=1, etc. For example n=0 gives the coefficient c_0.

We have not yet determined the eigenstates for our Hamiltonian. We do not calculate them exactly, but write,

$$H = H_0 + H_1 \tag{4.2.8}$$

so that,

$$H_1 = D \sum_l (S_l^x)^2 \tag{4.2.9}$$

and do first order perturbation theory, assuming that D<<J. Hence we are working to first order only in the parameter D. To this order we find,

$$S_1^z = -S + a_1^+ a_1 - \frac{DS}{2(4JS+h)}\left(1 - \frac{1}{2S}\right)^{1/2}\left[a_1^2 + (a_1^+)^2\right] + \frac{DS}{2(4JS+h)}\left(1 - \frac{1}{2S}\right)^{1/2}\left[1 - \left(1 - \frac{1}{S}\right)^{1/2}\right] \times \left[a_1^+ a_1^3 + (a_1^+)^3 a_1\right]$$

$$S_1^- = (2S)^{1/2}\left\{a_1 - \frac{DS}{2(4JS+h)}\left(1 - \frac{1}{2S}\right)a_1^+ - \left[1 - \left(1 - \frac{1}{2S}\right)^{1/2}\right]a_1^+ a_1^2 + \frac{DS}{2(4JS+h)}\left[1 - \frac{1}{2S} - \left(1 - \frac{1}{2S}\right)^{1/2}\left(1 - \frac{3}{2S}\right)\right](a_1^+)^2 a_1\right\}$$

$$(S_1^x)^2 = \frac{S}{2} + \left(S - \frac{1}{2}\right)a_1^+ a_1 + \frac{S}{2}\left(1 - \frac{1}{2S}\right)^{1/2}\left[a_1^2 + (a_1^+)^2\right] - \frac{1}{2}(a_1^+)^2 a_1^2 - \frac{S}{2}\left(1 - \frac{1}{2S}\right)^{1/2}\left[1 - \left(1 - \frac{1}{S}\right)^{1/2}\right] \times \left[a_1^+ a_1^3 + (a_1^+)^3 a_1\right] \qquad (4.2.10)$$

and S^+ is the hermitian conjugate of S^-. We have obtained the expansion for $(S^x)^2$ to zeroth order in D since it appears in the Hamiltonian multiplied by D. We have truncated these expressions so that only terms which contribute to quadratic and quartic terms in the boson Hamiltonian are included. In doing this calculation it was assumed that n is small and that each spin sits in the average field of the other spins. Derivations of these expansions are given in more detail by Lindgard and Kowalska (1976).

Since we have worked only to first order in the parameter D in obtaining these expansions we will work to first order in D throughout the calculation in this chapter.

The boson Hamiltonian obtained by substituting the transformation in Eqn.(4.2.10) into the Hamiltonian in Eqn.(4.1.2) is, after Fourier transforming to wave vector space,

$$H = \sum_k \left[E_1(k)\, a_k^+ a_k + B_1(k)\left(a_k a_{-k} + a_k^+ a_{-k}^+\right)\right] +$$

$$\frac{1}{N}\sum_{1,2,3,4} [\ \delta_{1+2,3+4}\ E_2(1,2,3,4)\ a_1^+ a_2^+ a_3 a_4 + \delta_{1,2+3+4} \times$$

$$B_2(1,2,3,4)\ (\ a_1^+ a_2 a_3 a_4 + a_2^+ a_3^+ a_4^+ a_1\ )\ ] \qquad (4.2.11)$$

where,

$$E_1(k) = 1 - \cos(k) + \frac{h}{4JS} + \frac{D}{4J}\ (\ 1 - \frac{1}{2S}\ )$$

$$B_1(k) = \frac{DS}{2\ (\ 4JS + h\ )}\ (\ 1 - \frac{1}{2S}\ )\ \cos(k)$$

$$E_2(1,2,3,4) = \frac{1}{2}\ [\ 1 - (\ 1 - \frac{1}{2S}\ )^{1/2}\ ]\ [\ \cos(1) + \cos(2) +$$

$$\cos(3) + \cos(4)\ ] - \frac{1}{2S}\cos(2-4) - \frac{D}{8JS}$$

$$B_2(1,2,3,4) = \frac{D}{2\ (\ 4JS + h\ )}\ (\ 1 - \frac{1}{2S}\ )^{1/2}\ \cos(2+3) - \frac{DS}{4JS + h} \times$$

$$[\ 1 - \frac{1}{2S} - (\ 1 - \frac{1}{2S}\ )^{1/2}\ (\ 1 - \frac{1}{S}\ )\ ]\ \cos(1)$$

$$(4.2.12)$$

This Hamiltonian is correct to first order in D and to fourth order in the boson operators. Unfortunately the quadratic term is not diagonal and the relations in Eqn.(1.5.13) do not hold in this case. This causes problems when we try to make power series expansions in the Bose factor as we did for the easy-axis system in Ch.3. We expect such problems to arise because the ground state of the system does not have all the spins aligned in the direction of the magnetic field so there are bosons, that are created and annihilated by the operators a^+ and a, present in the system even at zero temperature. In the next section we will make a transformation to new boson operators so that the quadratic part of the Hamiltonian obtained is diagonal.

4.3 Diagonalisation of the Hamiltonian

We wish to rewrite the Hamiltonian in Eqn.(4.2.11) in such a way that the quadratic part is diagonal. We write,

$$a_k = \cosh(\theta_k)\ \alpha_k - \sinh(\theta_k)\ \alpha^+_{-k} \tag{4.3.1}$$

The operators α and α^+ are also boson operators since they satisfy the correct commutation relations, Eqn.(1.5.8), for all values of θ_k. We note that θ_k is an even function of k. Substituting this expression for a_k, and its hermitian conjugate for a_k^+, into Eqn.(4.2.11) gives the quadratic terms,

$$\begin{aligned}
&\sum_k \{\ E_1(k)\ (\ c_k^2 + s_k^2\ ) - 4B_1(k)\ s_k\ c_k + \frac{1}{\bar{N}} \sum_p [\ 2E_2(k,p,p,k) \times \\
&(\ s_p^2\ c_k^2 + 2\ s_p\ c_p\ s_k\ c_k + s_p^2\ s_k^2\ ) + 2E_2(k,p,k,p)\ (\ s_p^2\ c_k^2 + \\
&s_p^2\ s_k^2\ ) - 2B_2(k,p,-p,k)\ (\ s_p\ c_p\ c_k^2 + s_p\ c_p\ s_k^2\ ) - 4B_2(k,k,p,-p) \\
&\times (s_p\ c_p\ c_k^2 + s_p\ c_p\ s_k^2\ ) - 4B_2(p,k,-k,p)\ s_p^2\ s_k\ c_k\ - \\
&8B_2(p,k,p,-k)\ s_p^2\ s_k\ c_k\ ]\ \}\ \alpha_k^+\ \alpha_k + \\
&\sum_k \{\ -E_1(k)\ c_k\ s_k + B_1(k)\ (\ c_k^2 + s_k^2\ ) + \frac{1}{\bar{N}} \sum_p [\ E_2(k,p,p,k) \times \\
&(\ -s_p\ c_p\ c_k^2 - s_p\ c_p\ s_k^2 - 2\ s_p^2\ c_k\ s_k\ ) - 2E_2(k,p,k,p)\ s_p^2\ s_k\ c_k + \\
&2B_2(k,p,-p,k)\ s_p\ c_p\ s_k\ c_k + 4B_2(k,k,p,-p)\ s_p\ c_p\ s_k\ c_k + \\
&B_2(p,k,-k,p)\ (\ s_p^2\ c_k^2 + s_p^2\ s_k^2\ ) + 2B_2(p,k,p,-k)\ (\ s_p^2\ c_k^2 + \\
&s_p^2\ s_k^2\ )\ ]\ \}\ (\ \alpha_k\ \alpha_{-k} + \alpha_k^+\ \alpha_{-k}^+\ )
\end{aligned} \tag{4.3.2}$$

where, for convenience,

$$s_k = \sinh(\theta_k)$$

$$c_k = \cosh(\theta_k)$$

This is diagonal if the coefficient of $(\alpha_k\alpha_{-k}+\alpha_k^+\alpha_{-k}^+)$ vanishes. Setting this coefficient equal to zero defines the variables $\cosh(\theta_k)$ and $\sinh(\theta_k)$. However, this condition gives an integral equation for $\cosh(\theta_k)$ or $\sinh(\theta_k)$ that we have been unable to solve. We have also not taken account of terms in the Hamiltonian that are of higher order in the operators a_k but still contribute to the quadratic terms in the operators α_k.

If the parameter D is equal to zero then the Hamiltonian is diagonal in the operators a_k and so,

$$\cosh(\theta_k) = 1 \ , \quad \sinh(\theta_k) = 0$$

For D≠0, $\sinh(\theta_k)$ is of order D, unless h=0 and k=0. Hence, to order D, Eqn.(4.3.2) becomes,

$$\sum_k \{ E_1(k)\, \alpha_k^+ \alpha_k + [\, B_1(k) - \sinh(\theta_k)\, E_1(k) - \frac{1}{N} \sum_p \sinh(\theta_p) \times$$

$$E_2(k,p,p,k)\,]\, (\, \alpha_k\, \alpha_{-k} + \alpha_k^+\, \alpha_{-k}^+ \,)\, \} \qquad (4.3.3)$$

so that the quadratic part is diagonal if,

$$\sinh(\theta_k) = \frac{B_1(k)}{E_1(k)} - \frac{1}{N}\frac{1}{E_1(k)} \sum_p \sinh(\theta_p)\, E_2(k,p,p,k) \qquad (4.3.4)$$

Replacing the sum by an integral, using Eqn.(1.2.6), this equation becomes an integral equation that can easily be solved. We find,

$$\sinh(\theta_k) = \frac{DS}{2\,(\,4JS + h\,)} (\, 1 - \frac{1}{2S}\,) \frac{1}{C - \cos(k)} \{ - C\, [\, 1 -$$

$$(\, 1 - \frac{1}{2S}\,)^{1/2}\,]\, [\, C\, (\, C^2 - 1\,)^{-1/2} - 1\,] + [\, (\, 1 - \frac{1}{2S}\,)^{1/2} +$$

$$[\, 1 - (\, 1 - \frac{1}{2S}\,)^{1/2}\,]\, C\, (\, C^2 - 1\,)^{-1/2} \cos(k)\, \}\, \{\, \frac{1}{2S}\, (\, 1 - C\,)$$

$$\times\, [\, C\, (\, C^2 - 1\,)^{-1/2} - 1\,] + 1\, \}^{-1} \qquad (4.3.5)$$

$$C = 1 + \frac{h}{4JS} + \frac{D}{4J} \left(1 - \frac{1}{2S} \right)$$

The method for solving Eqn.(4.3.4) is similar to the method for solving Eqn.(3.3.13).

The boson Hamiltonian is then,

$$\begin{aligned} H = & \sum_{k} \omega_k \alpha_k^{+} \alpha_k + \frac{1}{N} \sum_{1,2,3,4} \{ \delta_{1+2,3+4} E(1,2,3,4) \alpha_1^{+} \alpha_2^{+} \alpha_3 \alpha_4 + \\ & \delta_{1,2+3+4} B(1,2,3,4) (\alpha_1^{+} \alpha_2 \alpha_3 \alpha_4 + \alpha_2^{+} \alpha_3^{+} \alpha_4^{+} \alpha_1) \} \qquad (4.3.6) \end{aligned}$$

where,

$$\omega_k = 1 - \cos(k) + \frac{h}{4JS} + \frac{D}{4J} \left(1 - \frac{1}{2S} \right)$$

$$\begin{aligned} E(1,2,3,4) = & \frac{1}{2} \left[1 - \left(1 - \frac{1}{2S} \right)^{1/2} \right] [\cos(1) + \cos(2) + \\ & \cos(3) + \cos(4)] - \frac{1}{2S} \cos(2-4) - \frac{D}{8JS} \end{aligned}$$

$$\begin{aligned} B(1,2,3,4) = & - \sinh(\theta_2) \left\{ \left[1 - \left(1 - \frac{1}{2S} \right)^{1/2} \right] [\cos(1) + \right. \\ & \left. \cos(2) + \cos(3) + \cos(4)] - \frac{1}{2S} [\cos(1-4) + \cos(2+4)] \right\} + \\ & \frac{D}{2 (4JS + h)} \left(1 - \frac{1}{2S} \right)^{1/2} \cos(2+3) - \frac{DS}{4JS + h} \left[1 - \frac{1}{2S} - \right. \\ & \left. \left(1 - \frac{1}{2S} \right)^{1/2} \left(1 - \frac{1}{S} \right) \right] \cos(4) - \frac{1}{N} \sum_{t} \sinh(\theta_t) \times \\ & \left\{ - \left[1 - \left(1 - \frac{1}{2S} \right)^{1/2} \right]^2 [\cos(2) + 2 \cos(3+4-t)] - \right. \\ & \frac{1}{2} \left[1 - 2 \left(1 - \frac{1}{2S} \right)^{1/2} + \left(1 - \frac{1}{S} \right)^{1/2} \right] [\cos(1) + \\ & \left. 3 \cos(2) + 2 \cos(t)] \right\} \qquad (4.3.7) \end{aligned}$$

The term involving $\sinh(\theta_t)$ in B(1,2,3,4) comes from a term of the form,

$$a_1^+ a_2^+ a_3^+ a_4 a_5 a_6$$

that we have previously omitted. However, the terms involving B(1,2,3,4) will not enter our calculation so we will not derive the expression for B(1,2,3,4) here. All other higher order terms in the operators a_k do not contribute to quadratic and quartic terms in the operators α_k to first order in D.

Eqn.(4.3.3) is not valid for the special case h=0 and k=0 because then $E_1(k)$ is of order D and we cannot assume that $\sinh(\theta_k)$ is of order D. Also the spin-wave energy, ω_k, in Eqn.(4.3.7) does not vanish for h=0 and k=0, violating Goldstone's theorem. Small wave vectors will be important in our low temperature calculation since they correspond to low energies. Hence we conclude that our calculation is not valid in the case of zero applied field, and indeed it may only be valid when the applied field h is equal to or greater than DS.

This problem with the diagonalisation could apparently be avoided by working with the operators a_k instead of the operators α_k. However, we would find that, for example, six-particle Green functions are not of higher order in the Bose factor than four-particle Green functions, and in fact we would need to take Green functions of all orders in the operators a_k into account in the calculation, at least for h=0 and small wave vectors. The difficulty is basically the same as the one that we encounter in the diagonalisation.

We describe the calculation in the next section.

4.4 Calculation

As in Ch.3, the spin-wave damping and two-spin-wave bound states and resonances are obtained from the self-energy. We obtain the self-energy by calculating the two-particle Green function,

$$\begin{aligned} \langle\langle \alpha_k ; \alpha_k^+ \rangle\rangle_\omega &= \{ \omega - \omega_k - \Sigma(k,\omega) \}^{-1} \\ &= G(k,\omega) \end{aligned} \qquad (4.4.1)$$

where the second equality defines a useful notation.

There are other two-particle Green functions that contribute to $\langle\langle S_k^-;S_k^+\rangle\rangle_\omega$, for example $\langle\langle \alpha_k;\alpha_{-k}\rangle\rangle_\omega$, but they all give terms that are of order D^2 and so we neglect them. The operators α_k satisfy,

$$\begin{aligned} &< \alpha_k^+ \alpha_p > = \delta_{kp}\, n_k \\ &< \alpha_k \alpha_p > = < \alpha_k^+ \alpha_p^+ > = 0 \end{aligned} \qquad (4.4.2)$$

and we use the same, T-matrix, approximation that we used in Ch.3. The calculation is very similar to the calculation in Sec.3.3 and we will not go into much detail here. In the equation-of-motion for $G(k,\omega)$ the Green functions generated by the terms in the Hamiltonian with the coefficient $B(1,2,3,4)$ have the forms,

$$\langle\langle \alpha_p \alpha_q \alpha_r ; \alpha_k^+ \rangle\rangle_\omega \quad , \qquad \langle\langle \alpha_p^+ \alpha_q^+ \alpha_r ; \alpha_k^+ \rangle\rangle_\omega \qquad (4.4.3)$$

or are higher order in α_k. Both of the Green functions in Eqn.(4.4.3) are of order D and, since they are multiplied by a factor that is also of order D, contribute terms of order D^2 to $G(k,\omega)$. Hence we neglect them.

We find that the self-energy is,

$$\Sigma(k,\omega) = \frac{1}{\pi S} \int_{-\pi}^{\pi-k} dp\; n_p \; \frac{F(k,p)}{1 - W(p,k+p;\omega)} \qquad (4.4.4)$$

where,

$$1 - W(p,2K;\omega) = 1 - \frac{1}{2S} \left[1 - \frac{f}{\cos(K)} \right] \left[1 + f\, Y(f) \right] - \frac{D}{4JS} \times$$

$$\left[\cos(K) \right]^{-2} \left\{ \frac{1}{4S} \left[1 + f\, Y(f) \right] - \frac{1}{2} \cos(K)\, Y(f) \right\}$$

$$F(k,p) = \left\{ 2S \left[1 - \left(1 - \frac{1}{2S} \right)^{1/2} \right] \cos(K) \cos(Q) - \frac{D}{4J} \right\} \times$$

$$\left\{ \left[\left(1 - \frac{1}{2S} \right)^{1/2} + \frac{1}{2S} \frac{f}{\cos(K)} - \frac{1}{2S} \frac{\cos(Q)}{\cos(K)} \right] \left[1 + f\, Y(f) \right] + \right.$$

$$\left. \left[\cos(Q) - \left(1 - \frac{1}{2S} \right)^{1/2} \cos(Q) - f \right] Y(f) \right\} + \left\{ - \cos(Q) + \right.$$

$$\left. 2S \left[1 - \left(1 - \frac{1}{2S} \right)^{1/2} \right] \cos(K) \right\} \left\{ \left[\left(1 - \frac{1}{2S} \right)^{1/2} \cos(Q) - \right. \right.$$

$$\frac{D}{8JS}\,\frac{1}{\cos(K)} + f - \left(1 - \frac{1}{2S} \right)^{1/2} f \;]\; [\; 1 + f\, Y(f) \;] - [\; \cos(Q) +$$

$$\frac{D}{8JS}\,\frac{\cos(Q)}{\cos(K)} \;]\; f\, Y(f) \;\} \qquad (4.4.5)$$

$$f = \frac{1}{2\cos(K)} \left[\, 1 + \frac{h}{4JS} + \frac{D}{4J} \left(1 - \frac{1}{2S} \right) + \cos(K) - \omega \,\right\}$$

$$K = \frac{k + p}{2}, \qquad Q = \frac{k - p}{2}$$

and Y(f) is defined in Eqn.(3.3.24) and evaluated in Eqn.(3.3.25).

We will analyze this result in the next section.

4.5 Spin-wave Damping

The spin-wave damping is given by Eqn.(3.4.3). For $\omega=\omega_k$, given by Eqn.(4.3.7), we find that f, defined in Eqn.(4.4.5), is,

$$f = \cos\left(\frac{k - p}{2} \right) \qquad (4.5.1)$$

Then, taking the imaginary part of the self-energy for this value of f, we find, for $k<\pi$,

$$\Gamma_k = \frac{1}{\pi} \int_{-\pi}^{\pi-k} dp\; n_p \left\{ \frac{2\cos(K)\sin(Q)\, X^2}{X^2 + Y^2} - \frac{D}{2JS} \left(1 - \frac{1}{2S} \right) \times \right.$$

$$\left. \frac{[\,\cos(K)\,]^2\, X\, Y}{[\, X^2 + Y^2 \,]^2} \right\} \qquad (4.5.2)$$

where,

$$X = \cot(Q)\, [\, \cos(K) - \cos(Q) \,]$$

$$(4.5.3)$$

$$Y = (\, 2S - 1 \,)\cos(K) + \cos(Q)$$

and at the zone boundary,

$$\Gamma_\pi = \frac{1}{\pi}\int_0^\pi dp\ n_p\ \{\ \frac{2\ [\ \sin(p/2)\ ]^3\ \cos(p/2)}{(\ S\ -\ 1\ )^2\ [\ \cos(p/2)\ ]^2\ +\ [\ \sin(p/2)\ ]^2}\ +$$

$$\frac{D}{4J}\ (2S\ -\ 1)\ (S\ -\ 1)\ \frac{\sin(p/2)\ [\ \cos(p/2)\ ]^3}{(\ [S\ -\ 1]^2\ [\ \cos(p/2)\ ]^2\ +\ [\ \sin(p/2)\ ]^2\ )^2}\}$$

(4.5.4)

For the special case of S=1,

$$\Gamma_\pi = \frac{1}{\pi}\int_0^\pi dp\ n_p\ \sin(p) \qquad (4.5.5)$$

which is very large compared to the results for $S \neq 1$ or $k \neq \pi$. This behaviour was also found for the easy-axis system of Ch.3 and was discussed in Sec.3.6.

We have calculated the damping numerically for J=11.8K, D=9.0K, h=1.0K and S=1 with T=4.0K and T=12.0K and the results are shown in Fig.4.1. There are problems for small wave vectors because the second term in Eqn.(4.5.2) dominates the first one and the result is negative. This suggests that in this region it is not sufficient to work to order D only.

We have not calculated the spin-wave energy shift for this system as it is not so important from an experimental point of view.

4.6 Bound States

As in the easy-axis system, the two-spin-wave bound states are solutions of Eqn.(3.3.31) and the resonances are solutions of Eqn.(3.5.5). Their contribution to the spectral weight is,

$$\delta(\omega\ -\ \omega_0)\ \frac{2S}{1\ -\ \exp(\ -\omega_0/T)}\ \left(\ \frac{\partial L(k,\omega)}{\partial\omega}\ \Big|_{\omega=\omega_0}\ \right)^{-1} \qquad (4.6.1)$$

where ω_0 is a solution of Eqn.(3.5.5). We have neglected the contribution to the spectral weight from higher order Green functions for this system.

Below the two-spin-wave continuum, $f<-1$, the self-energy is,

$$\begin{aligned}\Sigma(k,\omega) = \frac{1}{\pi}\int_{-\pi}^{\pi-k} dp\, \frac{n_p}{1 - W(p,k+p;\omega)} \Big\{ \Big[4\Big(1 - \frac{1}{2S} \Big)^{1/2} - 4 + \frac{1}{S} + \\ \frac{D}{8JS^2}\,\frac{1}{\{ \cos(K) \}^2} \Big] \cos(K) \,[\cos(Q) - f]\, [1 + \{ \cos(Q) - \\ f \}\, \{ f^2 - 1 \}^{-1/2}] + \frac{1}{S} \cos(Q)\, [\cos(K) - \cos(Q)] - \\ \frac{D}{4JS} \Big[1 - \frac{1}{2S}\,\frac{\cos(Q)}{\cos(K)} \Big] \Big\} \qquad (4.6.2)\end{aligned}$$

where K, Q and f are defined in Eqn.(4.4.5) and,

$$\begin{aligned}1 - W(p,k+p;\omega) = 1 - \frac{1}{2S} \Big\{ 1 - \frac{f}{\cos(K)} + \frac{D}{8JS}\,\frac{1}{[\cos(K)]^2} \Big\} \times \\ \{ 1 - f\, (f^2 - 1)^{-1/2} \} - \frac{D}{8JS}\,\frac{1}{\cos(K)}\, (f^2 - 1)^{-1/2} \qquad (4.6.3)\end{aligned}$$

For this $W(p,k+p;\omega)$ we find that Eqn.(3.3.31) has one solution for small wave vectors and two solutions near the zone boundary. At the zone boundary it can be solved easily and the solutions are,

$$\begin{aligned}\omega_1 &= \omega_\pi - \frac{1}{2S} \\ \omega_2 &= \omega_\pi - \frac{D}{4JS}\end{aligned} \qquad (4.6.4)$$

which correspond to the exchange and single-site bound states respectively. We have solved Eqn.(3.3.31) numerically and the results are shown in Fig.4.2 for J=11.8K, D=9.0K, h=1.0K and S=1.

In studying the resonances, we use the same approximation as we used in Secs.3.4 and 3.5 of retaining only the leading order terms in p in the integral of Eqn.(4.6.2). Hence we use,

$$\begin{aligned}\Sigma(k,\omega) = \frac{R(T)}{1 - W(0,k;\omega)} \Big\{ \Big[4\Big(1 - \frac{1}{2S} \Big)^{1/2} - 4 + \frac{1}{S} + \frac{D}{8JS^2} \times \\ \frac{1}{[\cos(k/2)]^2} \Big] \cos\Big(\frac{k}{2}\Big) \Big[\cos\Big(\frac{k}{2}\Big) - f \Big] \Big(1 + \Big[\cos\Big(\frac{k}{2}\Big) - f \Big] \times \\ [f^2 - 1]^{-1/2} \Big) - \frac{D}{4JS} \Big(1 - \frac{1}{2S} \Big) \Big\} \qquad (4.6.5)\end{aligned}$$

$$R(T) = \frac{1}{\pi}\int_{-\pi}^{\pi-k} dp\, n_p$$

We solved Eqn.(3.5.5), to find the resonance energies, numerically for the values of J, D, h and S used in Fig.4.2 and temperatures of T=4K and T=12K. The energies were very slightly lower that the bound-state energies and almost indistinguishable from them on the scale of Fig.4.2. The amplitude corresponding to the exchange bound state is largest for small wave vectors whereas the amplitude corresponding to the single-site bound state is largest at the zone boundary. These results are similar to those found for the easy-axis system in Ch.3.

4.7 Discussion

The case S=1 seems to be special, as it was for the easy-axis system in Ch.3. There is again an increase in the spin-wave damping at the zone boundary, Eqn.(4.5.5). There has not yet, to our knowledge, been any experimental test of this result, however.

As we noted in the previous section, the results concerning the two-spin-wave resonances and their contribution to the spectral weight are also similar to those for the easy-axis system.

We note that a similar calculation to order D^2 would be very much more difficult. Firstly the transformation to boson operators would be more complicated and the boson Hamiltonian would be more difficult to diagonalise since it would contain terms not present in Eqn.(4.2.11). Then it would be necessary to keep terms in $\sinh^2(\theta_p)$, $\sinh^2(\theta_k)$ and $[\sinh(\theta_p)\sinh(\theta_k)]$ in the equation corresponding to Eqn.(4.3.2) in our calculation. Also it would be necessary to take account of higher order than quartic terms in the operators a_k to obtain the diagonalised boson Hamiltonian, corresponding to the Hamiltonian in Eqn.(4.3.6) in our calculation. In calculating the two-particle Green function $G(k,\omega)$, Green functions such as those in Eqn.(4.4.3) could no longer be neglected. Also other two-particle Green functions, for example $\langle\langle\alpha_k;\alpha_{-k}\rangle\rangle_\omega$, would contribute to the transverse spectral weight. There may be many other complications not mentioned here.

Finally we note that for the Hamiltonian in Eqn.(4.2.11) the variables $E_1(k)$ and $B_1(k)$ are of zeroth order in (1/S), and $E_2(1,2,3,4)$ and $B_2(1,2,3,4)$ are of order (1/S). Also the terms involving products of six boson operators are of order $(1/S^2)$, etc. Another approach to this problem is to do the calculation to various orders in the parameter (1/S). This gives results for the spin-wave damping but does not give any result concerning two-spin-wave bound states, since it is a perturbative calculation.

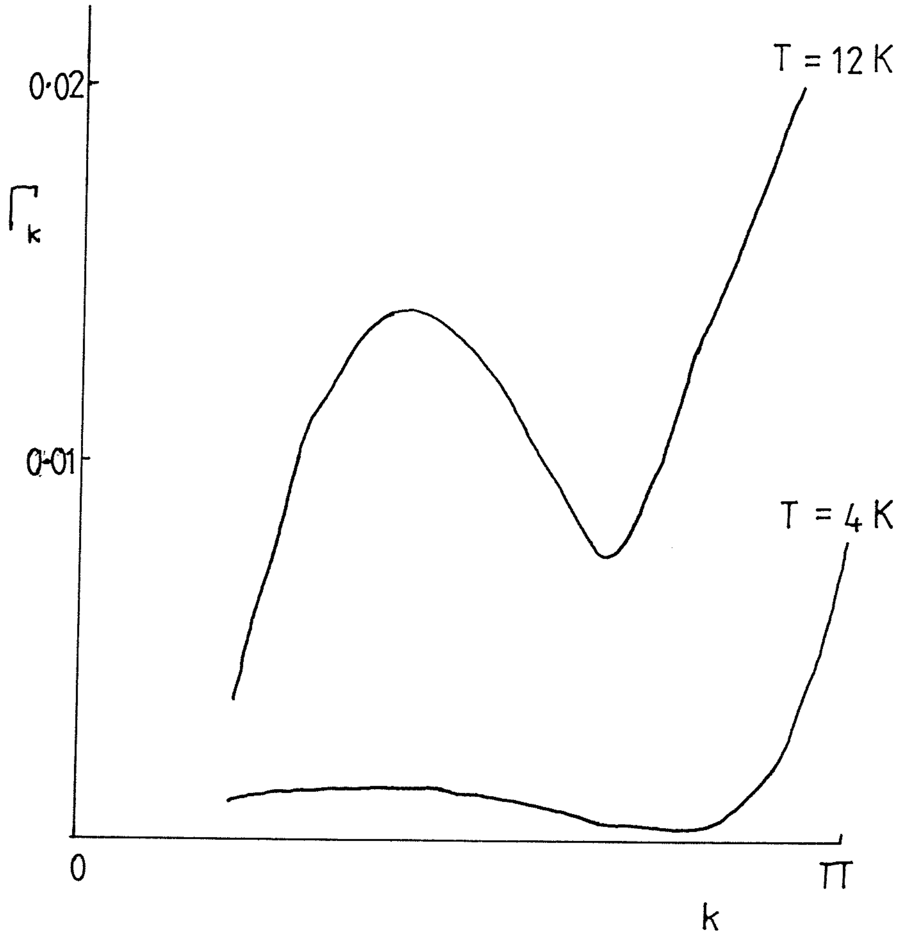

Figure 4.1: Spin-wave damping for J=11.8K, D=9.0K, h=1.0K and S=1 with T=4.0K and T=12.0K

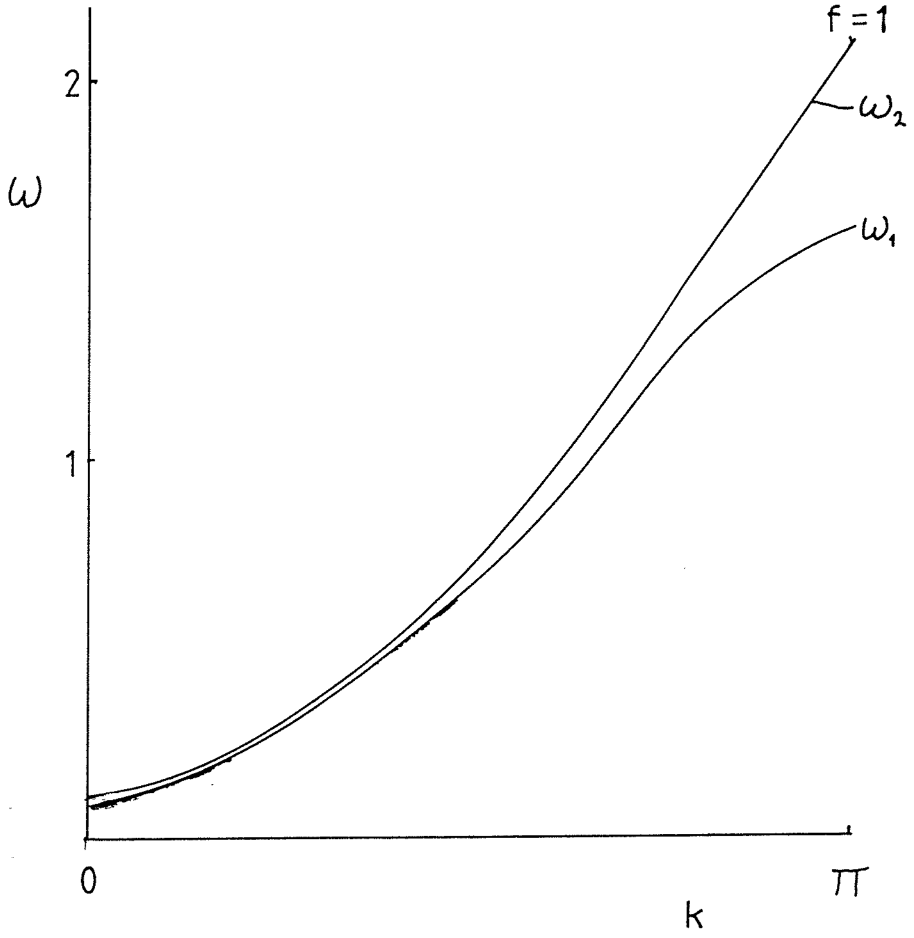

Figure 4.2: Dispersions of bound states for J=11.8K, D=9.0K, h=1.0K and S=1

CHAPTER 5: DETERMINATION OF SIMPLE FERROMAGNETIC HAMILTONIANS BY NEUTRON POLARISATION ANALYSIS

5.1 Introduction

Neutrons are particles with S=1/2 so if we measure the spin of a neutron along any axis of quantisation there are two possible results. For a beam of neutrons we define the polarisation, $\underline{P}$, to be twice the average spin of the neutrons in the beam. Hence $|\underline{P}|\leqslant 1$. In the previous chapters we have considered only scattering of unpolarised neutrons, i.e. $|\underline{P}|=0$, as Eqn.(1.3.1) is not valid for polarised neutrons.

Experimentally it is possible to polarise the incident neutron beam and measure the polarisation of the scattered beam but both of these processes involve large reductions in neutron intensity and polarisation analysis has not been used much in the past. However, there have been recent improvements in the production and analysis of polarised neutron beams and there is at least one high intensity pulsed neutron source being built so there may be greater use of polarisation analysis in the future (Fender et al. 1980).

It has long been known that polarisation analysis can provide information on systems that is not obtained in other ways (Halpern and Johnson 1939, Moon et al. 1969, Marshall and Lovesey 1971). For example, it can be used for separating magnetic from nuclear scattering, and paramagnetic scattering from the total cross-section. It is a useful technique for identifying spin-dependent processes.

In this chapter we will be concerned with using polarisation analysis in inelastic magnetic scattering to determine the forms of the Hamiltonians for some simple ferromagnetic systems (Hood 1983).

5.2 Polarisation of the Scattered Beam

For convenience we define a spin operator $\underline{S}^{(1)}$ by,

$$\underline{S}^{(\perp)} = \underline{K}' \times (\underline{S} \times \underline{K}') \qquad (5.2.1)$$

where $\underline{K}'$ is defined in Sec.1.3. In terms of this operator the inelastic neutron scattering cross-section is proportional to (Marshall and Lovesey 1971),

$$F(\underline{k},\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dt\, e^{i\omega t} \{ < \underline{S}^{(\perp)}_{-\underline{k}}(t) \,.\, \underline{S}^{(\perp)}_{\underline{k}} > +$$

$$i\, \underline{P}. < \underline{S}^{(\perp)}_{-\underline{k}}(t) \times \underline{S}^{(\perp)}_{\underline{k}} > \} \qquad (5.2.2)$$

where $\underline{P}$ denotes the polarisation of the incident beam and ω is defined in Eqn.(1.3.1). The polarisation of the scattered beam is,

$$\underline{P}' = \frac{G(k,\omega)}{F(\underline{k},\omega)} \qquad (5.2.3)$$

where,

$$\underline{G}(\underline{k},\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dt\, e^{i\omega t} \{ < \underline{S}^{(\perp)}_{-\underline{k}}(t) [\underline{P} \,.\, \underline{S}^{(\perp)}_{\underline{k}}] > +$$

$$< [\underline{P} \,.\, \underline{S}^{(\perp)}_{-\underline{k}}(t)] \underline{S}^{(\perp)}_{\underline{k}} > - \underline{P} < \underline{S}^{(\perp)}_{-\underline{k}}(t) \,.\, \underline{S}^{(\perp)}_{\underline{k}} > -$$

$$i < \underline{S}^{(\perp)}_{-\underline{k}}(t) \times \underline{S}^{(\perp)}_{\underline{k}} > \} \qquad (5.2.4)$$

As in Sec.1.3, the scattering occurs at wave vectors $\underline{K}=\underline{k}+\underline{\tau}$ where $\underline{\tau}$ is a reciprocal lattice vector.

Experimentally the polarisation of the incident neutron beam entering the sample must be in the same direction as the applied magnetic field and only the component of the polarisation parallel to this field can be measured (Moon et al. 1969). This is because the neutron spin precesses about any field that it is not parallel to. Also it is necessary to apply a finite magnetic field to avoid depolarisation effects. We choose the z-axis to be the field direction, set $P_x=P_y=0$, $P_z=P$ and measure only P_z'.

We will be working with a linear spin-wave theory in which the only non-zero spectral weight functions are,

$$S^{xx}(\underline{k},\omega) \;,\; S^{yy}(\underline{k},\omega) \;,\; S^{xy}(\underline{k},\omega) \;,\; S^{yx}(\underline{k},\omega) = - S^{xy}(\underline{k},\omega)$$

since the other ones involve two-spin-wave processes. With these simplifications Eqns.(5.2.2) and (5.2.4) reduce to,

$$F(\underline{k},\omega) = (1 - K'^{2}_{x}) S^{xx}(\underline{k},\omega) + (1 - K'^{2}_{y}) S^{yy}(\underline{k},\omega) + 2 i P K'^{2}_{z} S^{xy}(\underline{k},\omega) \qquad (5.2.5)$$

and,

$$G_{z}(\underline{k},\omega) = P (2 K'^{2}_{x} K'^{2}_{z} + K'^{2}_{x} - 1) S^{xx}(\underline{k},\omega) + P (2 K'^{2}_{y} K'^{2}_{z} + K'^{2}_{y} - 1) S^{yy}(\underline{k},\omega) - 2 i K'^{2}_{z} S^{xy}(\underline{k},\omega) \qquad (5.2.6)$$

where we have used the definitions for the spectral weights, Eqn.(1.3.2), in deriving these equations.

In the next section we will discuss the Hamiltonians used, before going on to calculate the spectral weights for them in the following section.

5.3 Spin Hamiltonians

The Hamiltonians that we will consider are all special cases of the Hamiltonian,

$$H = - \sum_{l,m} (J^{x} S^{x}_{l} S^{x}_{m} + J^{y} S^{y}_{l} S^{y}_{m} + J^{z} S^{z}_{l} S^{z}_{m}) - D^{z} \sum_{l} (S^{z}_{l})^{2} + D^{x} \sum_{l} (S^{x}_{l})^{2} + h \sum_{l} S^{z}_{l} \qquad (5.3.1)$$

where the parameters J^{x}, J^{y}, J^{z}, D^{x}, D^{z} and h are all either positive or zero, and l and m label nearest-neighbour sites.

We define five special cases of interest:

(A) $J^x=J^y=J^z=J$, $D^x=D^z=0$;

(B) $J^x=J^y=J$, $J^z=J(1+\eta)$, $D^x=0$, $D^z=D$, with $\eta>0$;

(C) $J^x=J^y=J^z=J$, $D^z=0$, $D^x=D$;

(D) $J^y=J^z=J$, $J^x=J(1-\eta)$, $D^x=D^z=0$, with $\eta>0$;

(E) $D^x=D^z=0$.

Model (A) is the Heisenberg model and model (B) is an easy-axis system, the same as the one considered in Ch.3. For these two models the total z component of spin commutes with the Hamiltonian and so is a constant of the motion. Hence correlation functions of the form $<S^+S^+>$ and $<S^-S^->$ vanish and the expressions that we obtain for the cross-section and polarisation are simpler than for the other models. Model (C) is an easy-plane system with single-site anisotropy and model (D) is an easy-plane system with exchange anisotropy. In both cases the easy plane is perpendicular to the x-axis. Model (C) was studied in Ch.4. Finally model (E) has a different exchange interaction for each component of the spin. In this model, if we set $J^x=0$ and $J^y=J^z=J$ we obtain the familiar XY model, whereas $J^x=J^y=0$ gives the Ising model.

For models (A) and (B) the ground states are known. However, for most of the other models in one dimension there are zero-point quantum fluctuations since the correlation functions $<S^+S^+>$ and $<S^-S^->$ do not vanish. As we mentioned in Ch.1, spin-wave theory is not as good an approximation in systems of low spatial dimensionality as it is in higher dimensions, because of the lack of long-range order. The theory used in this chapter is expected to work best for models (A) and (B) which have long-range order at zero temperature, and for small anisotropies in the other models, when we are considering magnetic chains.

5.4 Calculation

As mentioned in Sec.5.2, we use a linear spin-wave theory to calculate the spectral weights. Such a theory is only valid at low temperatures and is probably the simplest one possible. Within this theory the Holstein-Primakoff transformation reduces to,

$$\begin{aligned} S_l^- &= (2S)^{1/2} a_l \\ S_l^+ &= (2S)^{1/2} a_l^+ \\ S_l^z &= - S + a_l^+ a_l \end{aligned} \qquad (5.4.1)$$

Substituting this into our Hamiltonian, Eqn.(5.3.1), gives the quadratic boson Hamiltonian,

$$H = \sum_{\underline{k}} \{ E(\underline{k}) a_{\underline{k}}^+ a_{\underline{k}} + B(\underline{k}) (a_{\underline{k}} a_{-\underline{k}} + a_{\underline{k}}^+ a_{-\underline{k}}^+) \} \qquad (5.4.2)$$

after taking the Fourier transform to wave vector space, where,

$$\begin{aligned} E(\underline{k}) &= 2rJ^zS - r(J^x + J^y)S\gamma(\underline{k}) - D^z(1 - 2S) + D^x(S - \tfrac{1}{2}) + h \\ B(\underline{k}) &= \tfrac{1}{2} (J^y - J^x)S\gamma(\underline{k}) + \tfrac{1}{2} D^x S(1 - \tfrac{1}{2S})^{1/2} \end{aligned} \qquad (5.4.3)$$

r is the number of nearest neighbours per site and we have defined,

$$\gamma(\underline{k}) = \frac{1}{r} \sum_{\underline{\delta}} \cos(\underline{k}.\underline{\delta}) \qquad (5.4.4)$$

where $\underline{\delta}$ is a vector from one site to a nearest-neighbour site. If we try to diagonalise the Hamiltonian, using Eqn.(4.3.1) and ignoring the diagonalisation problems that we encountered in Sec.4.3, we obtain,

$$H = \sum_{\underline{k}} \{ [E(\underline{k}) \cosh(2\theta_{\underline{k}}) - 2 B(\underline{k}) \sinh(2\theta_{\underline{k}})] \alpha_{\underline{k}}^+ \alpha_{\underline{k}} +$$

$$[\ B(\underline{k})\ \cosh(2\theta_{\underline{k}}) - \frac{1}{2}\ E(\underline{k})\ \sinh(2\theta_{\underline{k}})\ ]\ [\ \alpha_{\underline{k}}\ \alpha_{-\underline{k}} +$$

$$\alpha^{+}_{\underline{k}}\ \alpha^{+}_{-\underline{k}}\ ]\ \} \qquad (5.4.5)$$

so the Hamiltonian is diagonal if,

$$\tanh(2\theta_{\underline{k}}) = \frac{2\ B(\underline{k})}{E(\underline{k})} \qquad (5.4.6)$$

Hence we have,

$$H = \sum_{\underline{k}} \omega(\underline{k})\ \alpha_{\underline{k}}\ \alpha_{\underline{k}} \qquad (5.4.7)$$

with the spin-wave dispersion,

$$\omega(\underline{k}) = \{\ [\ E(\underline{k})\ ]^{2} - 4\ [\ B(\underline{k})\ ]^{2}\ \}^{1/2} \qquad (5.4.8)$$

It is very easy to calculate the two-particle Green functions using the equation-of-motion method described in Sec.2.2 and we find,

$$\begin{aligned} &<< \alpha_{\underline{k}};\ \alpha^{+}_{\underline{k}} >>_{\omega} = \frac{1}{\omega - \omega(\underline{k})} \\ &<< \alpha^{+}_{\underline{k}};\ \alpha_{\underline{k}} >>_{\omega} = -\ \frac{1}{\omega + \omega(\underline{k})} \qquad (5.4.9) \\ &<< \alpha_{\underline{k}};\ \alpha_{-\underline{k}} >>_{\omega} = << \alpha^{+}_{\underline{k}};\ \alpha^{+}_{-\underline{k}} >>_{\omega} = 0 \end{aligned}$$

From Eqn.(1.2.8) we have,

$$\begin{aligned} &S^{x}_{\underline{k}} = \frac{1}{2}\ (\ S^{+}_{\underline{k}} + S^{-}_{-\underline{k}}\ ) \\ & \qquad\qquad\qquad\qquad (5.4.10) \\ &S^{y}_{\underline{k}} = \frac{1}{2i}\ (\ S^{+}_{\underline{k}} - S^{-}_{-\underline{k}}\ ) \end{aligned}$$

Hence we can write down expressions for the Green functions,

$$<< S^{x}_{-\underline{k}};\ S^{x}_{\underline{k}} >>_{\omega}\ ,\ << S^{y}_{-\underline{k}};\ S^{y}_{\underline{k}} >>_{\omega} \text{ and } << S^{x}_{-\underline{k}};\ S^{y}_{\underline{k}} >>_{\omega}$$

and use Eqn.(2.1.6) to calculate the spectral weight functions. We finally obtain,

$$S^{xx}(\underline{k},\omega) = \frac{S}{2}\ [\ \frac{E(\underline{k}) - 2\ B(\underline{k})}{\omega(\underline{k})}\ ]\ \{\ [\ n_{\underline{k}} + 1\ ]\ \delta[\ \omega - \omega(\underline{k})\ ] +$$

$$n_{\underline{k}}\ \delta[\ \omega + \omega(\underline{k})\ ]\ \}$$

$$S^{yy}(\underline{k},\omega) = \frac{S}{2}\left[\frac{E(\underline{k}) + 2\,B(\underline{k})}{\omega(\underline{k})}\right]\{\,[\,n_{\underline{k}} + 1\,]\,\delta[\,\omega - \omega(\underline{k})\,] + n_{\underline{k}}\,\delta[\,\omega + \omega(\underline{k})\,]\,\} \qquad (5.4.11)$$

$$S^{xy}(\underline{k},\omega) = -\frac{1}{2i}\{\,[\,n_{\underline{k}} + 1\,]\,\delta[\,\omega - \omega(\underline{k})\,] + n_{\underline{k}}\,\delta[\,\omega + \omega(\underline{k})\,]\,\}$$

where the Bose factor, n_k, was defined in Eqn.(1.5.14).

The algebra involved in obtaining these spectral weights is very simple so we have omitted the details here.

In the next section we write down the results obtained for the polarisation, etc.

5.5 Results

For convenience we write,

$$\begin{aligned} F(\underline{k},\omega) &= F^{(+)}(\underline{k},\omega) + F^{(-)}(\underline{k},\omega) \\ \underline{G}(\underline{k},\omega) &= \underline{G}^{(+)}(\underline{k},\omega) + \underline{G}^{(-)}(\underline{k},\omega) \end{aligned} \qquad (5.5.1)$$

where (+) denotes spin-wave creation or neutron energy loss and (−) denotes spin-wave annihilation or neutron energy gain. Substituting the spectral weights, Eqn.(5.4.11), into Eqns.(5.2.5) and (5.2.6), gives,

$$F^{(\pm)}(\underline{k},\omega) = \frac{S}{2}\{\,(\,1 + K'^{2}_{z}\,)\,\frac{E(\underline{k})}{\omega(\underline{k})} + (\,K'^{2}_{x} - K'^{2}_{y}\,)\,\frac{2\,B(\underline{k})}{\omega(\underline{k})} \mp 2P\,K'^{2}_{z}\,\}\,[\,n_{\underline{k}} + \frac{1}{2} \pm \frac{1}{2}\,]\,\delta[\,\omega \mp \omega(\underline{k})\,] \qquad (5.5.2)$$

and,

$$\underline{G}^{(\pm)}(\underline{k},\omega) = \frac{S}{2}\{\,P(\,-1 + K'^{2}_{z} - 2K'^{4}_{z}\,)\,\frac{E(\underline{k})}{\omega(\underline{k})} + P(\,K'^{2}_{x} - K'^{2}_{y}\,) \times (\,-1 - 2K'^{2}_{z}\,)\,\frac{2\,B(\underline{k})}{\omega(\underline{k})} \pm 2K'^{2}_{z}\,\}\,[\,n_{\underline{k}} + \frac{1}{2} \pm \frac{1}{2}\,] \times$$

$$\delta[\ \omega \mp \omega(\underline{k})\ ] \qquad (5.5.3)$$

Then, using Eqn.(5.2.3), the z component of the polarisation of the scattered beam is,

$$P'^{\pm}_z = \{\ P(\ -1 + K'^2_z - 2K'^4_z\ )\ E(\underline{k}) + P(\ K'^2_x - K'^2_y\ )\ (\ -1 - 2K'^2_z\ ) \times 2B(\underline{k}) \pm 2K'^2_z\ \omega(\underline{k})\ \}\ \{\ (\ 1 + K'^2_z\ )\ E(\underline{k}) + (\ K'^2_x - K'^2_y\ ) \times 2B(\underline{k}) \mp 2P\ K'^2_z\ \omega(\underline{k})\ \} \qquad (5.5.4)$$

where $(\underline{P}')^{+}$ is the polarisation of neutrons scattered with energy loss $\omega(\underline{k})$ and $(\underline{P}')^{-}$ is the polarisation of neutrons scattered with energy gain $\omega(\underline{k})$.

We will discuss these results and their implications for our five special cases, of Sec.5.3, in the next section.

5.6 Discussion

We refer to the five models discussed in Sec.5.3. For models (A) and (B), $B(\underline{k})=0$ and Eqns.(5.5.2) and (5.5.4) reduce to,

$$F^{(\pm)}(\underline{k},\omega) = \frac{S}{2}\ \{\ (\ 1 + K'^2_z\ ) \mp 2P\ K'^2_z\ \}\ [\ n_{\underline{k}} + \frac{1}{2} \pm \frac{1}{2}\ ] \times \delta[\ \omega \mp \omega(\underline{k})\ ] \qquad (5.6.1)$$

and,

$$P'^{\pm}_z = \{\ P(\ -1 + K'^2_z - 2K'^4_z\ ) \pm 2K'^2_z\ \} \times \{\ (\ 1 + K'^2_z\ ) \mp 2P\ K'^2_z\ \}^{-1} \qquad (5.6.2)$$

which agree with previous results, for example Eqn.(10.153) of Marshall and Lovesey (1971). We conclude that for this linear spin-wave theory, it is not possible to distinguish between exchange anisotropy and single-site anisotropy for an easy-axis system using polarisation analysis.

For model (C),

$$B(\underline{k}) = \frac{1}{2} DS \left(1 - \frac{1}{2S} \right)^{1/2} \qquad (5.6.3)$$

which is independent of wave vector $\underline{k}$, and for model (D),

$$B(\underline{k}) = \frac{1}{2} \eta rJS \, \gamma(\underline{k}) \qquad (5.6.4)$$

which depends on the wave vector $\underline{k}$ through the geometric function $\gamma(\underline{k})$, defined in Eqn.(5.4.4). Since the neutron scattering wave vector $\underline{K}$ differs from $\underline{k}$ by a reciprocal lattice vector $\underline{\tau}$, it is possible, in principal, to vary $\underline{K}'$ and $\underline{k}$ independently by varying $\underline{\tau}$. Hence for any $\underline{k}$ we can vary $\underline{K}'$, measure P_z' and calculate $B(\underline{k})$ from Eqn.(5.5.4). The dependence of $B(\underline{k})$ on $\underline{k}$ then gives us a means of distinguishing between single-site and exchange anisotropies for an easy-plane system. In fact it is not even necessary to polarise the incident neutron beam since for P=0 Eqn.(5.5.4) becomes,

$$P'^{\pm}_{z} = \pm 2K'^{2}_{z} \, \omega(\underline{k}) \, \{ (1 + K'^{2}_{z}) E(\underline{k}) + (K'^{2}_{x} - K'^{2}_{y}) 2B(\underline{k}) \}^{-1} \qquad (5.6.5)$$

This is helpful from an experimental point of view. In principle it should be possible to obtain the wave vector dependence of $B(\underline{k})$ from the spin-wave dispersion, Eqn.(5.4.8). However, for small values of the anisotropy $\omega(\underline{k})$ depends on $[B(\underline{k})]^2$ whereas $(P_z')^{\pm}$ depends on $B(\underline{k})$ so we expect polarisation analysis to give a better determination of $B(\underline{k})$.

For all these models there are two special cases for which the x and y components of the polarisation of the scattered beam, that we have not written down expressions for in this thesis, vanish. One such case is $K_z=0$, which gives $P_z'=-P$ and a cross-section independent of P, from Eqns.(5.5.2) and (5.5.4). This is not very useful. The other case is $K_x=K_y=0$ and is more interesting since Eqn.(5.5.2) reduces to,

$$F^{(\pm)}(\underline{k},\omega) = S\{ \frac{E(\underline{k})}{\omega(\underline{k})} \mp P \} \, [n_{\underline{k}} + \frac{1}{2} \pm \frac{1}{2}] \, \delta[\omega \mp \omega(\underline{k})] \qquad (5.6.6)$$

For models (A) and (B), if P=1 then the cross-section for spin-wave creation vanishes, i.e. $F^{(+)}(\underline{k},\omega)=0$, and if P=-1 the cross-section for spin-wave annihilation vanishes. For models (C) and (D) both the cross-sections for spin-wave creation and annihilation are non-zero for $P=\pm 1$. This provides a means of distinguishing between easy-axis and easy-plane systems.

If $B(\underline{k})$ is measured for model (E) with the magnetic field along any one direction, it gives the difference between the exchange interactions for the other two directions.

We mention that there are many other Hamiltonians that can be studied using this method. For example, Dobrzynski and Bytonski (1980) have used it to study Hamiltonians with dipole-dipole interactions.

In the next section we will discuss the dependence of our results on the transformation to boson operators used.

5.7 Dependence of Results on Boson Transformation

In this section we consider the question of whether our results of Sec.5.5 are dependent on the transformation from spin operators to boson operators. We work with model (C) as an example since we have already studied this model in Ch.4. The transformation of Lindgard and Kowalska (1976), Eqn.(4.2.10), gives the quadratic boson Hamiltonian,

$$H = \sum_{\underline{k}} \{ E(\underline{k})\, a^{+}_{\underline{k}} a_{\underline{k}} + B(\underline{k}) (a_{\underline{k}} a_{-\underline{k}} + a^{+}_{\underline{k}} a^{+}_{-\underline{k}}) \}$$

$$E(\underline{k}) = 2rJS [1 - \gamma(\underline{k})] + D(S - \tfrac{1}{2}) + h \qquad (5.7.1)$$

$$B(\underline{k}) = rJS \frac{DS}{2rJS + h} (1 - \frac{1}{2S}) \gamma(\underline{k})$$

This $B(\underline{k})$ depends on $\underline{k}$ unlike the $B(\underline{k})$ obtained previously, Eqn.(5.6.3). This seems to contradict our arguments in Sec.5.6 concerning how to distinguish between single-site and exchange anisotropies for easy-plane systems. However, when we calculate the spectral weights using this transformation the factors $\gamma(\underline{k})$ cancel in such a way that the expressions for the cross-section and polarisation have the same form as Eqns.(5.5.2) and (5.5.4) with $B(\underline{k})$ replaced by,

$$B'(\underline{k}) = \tfrac{1}{2} DS(1 - \frac{1}{2S}) \qquad (5.7.2)$$

so the conclusions of the previous section still hold. We do not go into details of the calculation using this transformation since they are essentially the same as those in Sec.5.4.

Our conclusion here contradicts that of Lovesey and Steiner (1981) since they did not use the full transformation in calculating the cross-section and polarisation.

We suggest that the conclusions of Sec.5.6 are in fact independent of the transformations to boson operators that can be used.

5.9 Experimental Work

Finally in this chapter we mention briefly some early experimental work, testing our predictions, by Kakurai et al. (1984) on $CsNiF_3$. These neutron scattering experiments show conclusively that the system is easy-plane but for the range of wave vectors over which the experiment was done there was very little differences between the predicted polarisations for single-site and exchange anisotropies and they were effectively indistinguishable. Results for higher temperatures seemed to show that the system was becoming more isotropic as the temperature was increased. However these last results are currently in dispute.

CHAPTER 6: FERMI FLUID SYSTEM

6.1 Introduction

In the previous chapters we have been studying spin waves in localised ferromagnetic systems using a Green function equation-of-motion method to calculate the spectral weight. In this chapter we study a Fermi fluid, which is a very different system, for example fermion operators are used instead of boson operators. However, we will still use the equation-of-motion method for calculating Green functions described in Sec.2.2.

The goal of this chapter is to calculate the particle density autocorrelation function. We are concerned primarily with density fluctuations and hence focus on the operator c^+c, where c^+ and c are the fermion creation and annihilation operators that we will discuss later in this section. We go beyond the RPA (Pines and Bohm 1952) using an equation-of-motion for density fluctuations. This is a new approach to the task of including lifetime effects.

Fermi liquid theory is usually applied to physical systems such as liquid ^{3}He, the electron gas and electrons in metals, and hence itinerant ferromagnets, for example iron and nickel. Such systems show interesting features for the fermion momenta close to the Fermi momentum. These fermions all have spin 1/2 and we will work with this value of the spin throughout. We will not go into the details of Fermi liquid theory in this section but will merely give the necessary background for the problem in this chapter. A more detailed review is given by, for example, Levin and Valls (1983). We will also present some results for non-interacting fermions.

We denote our fermion creation and annihilation operators by $c^+_{a\sigma}(t)$ and $c_{a\sigma}(t)$ respectively, such operators are discussed in detail by Abrikosov et al. (1963) and Fetter and Walecka (1971). The subscript a is the momentum and σ is the spin. These are Heisenberg operators, as in Eqn.(1.2.1), and they anticommute so that,

$$\{ c_{a\sigma}, c_{b\sigma'} \} = \{ c^+_{a\sigma}, c^+_{b\sigma'} \} = 0 \qquad (6.1.1)$$

$$\{ c_{a\sigma}, c^{+}_{b\sigma'} \} = \delta_{ab} \delta_{\sigma\sigma'}$$

where the anticommutator of two operators A and B is defined,

$$\{ A, B \} = AB + BA \tag{6.1.2}$$

The operators in Eqn.(6.1.1) have the same value of time.

The thermal averages, defined in Eqn.(1.2.2), of the products of two fermion operators are,

$$\begin{aligned} &< c_{a\sigma} c_{b\sigma'} > = < c^{+}_{a\sigma} c^{+}_{b\sigma'} > = 0 \\ &< c^{+}_{a\sigma} c_{b\sigma'} > = \delta_{ab} \delta_{\sigma\sigma'} f_{a\sigma} \end{aligned} \tag{6.1.3}$$

For non-interacting fermions $f_{a\sigma}$ is given by a Fermi distribution,

$$f_{a\sigma} = \{ \exp[(\varepsilon_{a\sigma} - \mu_{\sigma}) / T] + 1 \}^{-1} \tag{6.1.4}$$

where $\varepsilon_{a\sigma}$ is the energy of the fermion and μ_{σ} is the chemical potential. We usually take the energies to be independent of spin, and,

$$\varepsilon_{a} = \frac{a^2}{2m} \tag{6.1.5}$$

where m is the mass of the fermion. The chemical potential is calculated from,

$$N = \sum_{a,\sigma} f_{a\sigma} \tag{6.1.6}$$

and is independent of spin. N is the total number of fermions.

We define the particle density fluctuation operator,

$$n_{q\sigma}(p) = c^{+}_{p+q\sigma} c_{q\sigma} - \delta_{p0} f_{q\sigma} \tag{6.1.7}$$

which is the fluctuation of $c^{+}_{p+q\sigma} c_{q\sigma}$ from its thermal average. Also,

$$n(p) = \sum_{q,\sigma} n_{q\sigma}(p) \tag{6.1.8}$$

will be a useful operator in our calculation. We will usually work with the time Fourier transforms of these operators, i.e.,

$$n_{q\sigma}(p;\omega) = \int_{-\infty}^{\infty} dt\ e^{i\omega t}\ n_{q\sigma}(p) \tag{6.1.9}$$

and,

$$n(p;\omega) = \int_{-\infty}^{\infty} dt\ e^{i\omega t}\ n(p) \tag{6.1.10}$$

The Green functions used to calculate the particle density autocorrelation function are,

$$\begin{aligned} G_{q\sigma}(p,t) &= \langle\langle\, n_{q\sigma}(p,t);\ n(-p)\, \rangle\rangle \\ G(p,t) &= \sum_{q,\sigma} G_{q\sigma}(p,t) \\ &= \langle\langle\, n(p,t);\ n(-p)\, \rangle\rangle \end{aligned} \tag{6.1.11}$$

and their time Fourier transforms,

$$\begin{aligned} G_{q\sigma}(p,\omega) &= \langle\langle\, n_{q\sigma}(p);\ n(-p)\, \rangle\rangle_{\omega} \\ G(p,\omega) &= \sum_{q,\sigma} G_{q\sigma}(p,\omega) \\ &= \langle\langle\, n(p);\ n(-p)\, \rangle\rangle_{\omega} \end{aligned} \tag{6.1.12}$$

where the notation is defined in Eqns.(2.1.1) and (2.1.3). From these Green functions we obtain all our physical results. We see immediately that this problem is more complicated than our previous ones since $G(p,\omega)$ is a four–particle Green function and the elementary excitations of the system involve two fermions, rather than one boson as in previous chapters. It is well known that it is impossible to create and annihilate single fermions so this is not unexpected.

For non–interacting fermions the Hamiltonian describing the system is,

$$H = \sum_{k,\sigma} \varepsilon_k c^{+}_{k\sigma} c_{k\sigma} \qquad (6.1.13)$$

It is easy to calculate the non-interacting Green function, $G^{(0)}(p,\omega)$, using this Hamiltonian and the equation-of-motion method described in Sec.2.2 and the result is,

$$G^{(0)}(p,\omega) = \sum_{q,\sigma} f_{q\sigma} \left\{ \frac{1}{\omega + \varepsilon_q - \varepsilon_{p+q}} - \frac{1}{\omega + \varepsilon_{p+q} - \varepsilon_q} \right\} \qquad (6.1.14)$$

Because G(p,t) is a causal Green function it satisfies a dispersion relation, Eqn.(2.1.4), and we only need to calculate either the real or imaginary part. For the latter we find,

$$\mathrm{Im}\, G^{(0)}(p,\omega) = -\pi \sum_{q,\sigma} f_{q\sigma} \{ \delta(\omega + \varepsilon_q - \varepsilon_{p+q}) - \delta(-\omega + \varepsilon_q - \varepsilon_{p+q}) \} \qquad (6.1.15)$$

using Eqn.(2.1.12) and the fact that the δ-function is an even function of its argument.

It is simple to evaluate this expression in the high and low temperature limits. Since $f_{q\sigma}$ is independent of the spin and N is large, we can write,

$$\sum_{q,\sigma} \rightarrow \frac{2V}{(2\pi)^3} \int d^3q \qquad (6.1.16)$$

where the integral is taken over the volume of the system.

The high temperature limit, in which quantum effects are negligible, is given by,

$$T \rightarrow \infty , \quad \mu / T \rightarrow -\infty \qquad (6.1.17)$$

Hence,

$$f_{q\sigma} \rightarrow \exp[(\mu - \varepsilon_q) / T] \qquad (6.1.18)$$

i.e. a Boltzmann distribution. Eqn.(6.1.6) becomes,

$$N = \frac{2V}{(2\pi)^3} \int d^3q \exp[(\mu - \varepsilon_q) / T] \tag{6.1.19}$$

Since ε_q depends only on q^2, we can transform to spherical polar coordinates and do the integration to obtain,

$$\exp(\mu / T) = \frac{4N}{V} (\frac{\pi}{2mT})^{3/2} \tag{6.1.20}$$

where we have used the result,

$$\int_0^\infty dq\, q^2 \exp(-aq^2) = \frac{1}{4} \frac{1}{a} (\frac{\pi}{a})^{1/2} \tag{6.1.21}$$

The first term on the right-hand side of Eqn.(6.1.15) becomes,

$$-\pi \exp(\mu/T) \frac{2V}{(2\pi)^3} \int d^3q \exp(\frac{-q^2}{2mT}) 2m\, \delta(2m\omega - p^2 - 2\underline{p}.\underline{q}) \tag{6.1.22}$$

and the second term is obtained from this by $\omega \rightarrow -\omega$. We choose the z-axis to lie parallel to $\underline{p}$ and work in cylindrical polar coordinates since the integrand is invariant under rotations about this axis.

Then,

$$\begin{gathered} \int d^3q \;\rightarrow\; 2\pi \int_{-\infty}^{\infty} dq_z \int_0^\infty \frac{1}{2} d(q_\rho)^2 \\ q_\rho^2 = q^2 - q_z^2 \end{gathered} \tag{6.1.23}$$

and the integrand in Eqn.(6.1.22) is easy to evaluate. Eqn.(6.1.15) becomes,

$$\mathrm{Im}\, G^{(0)}(p,\omega) = - \frac{N}{p} (\frac{\pi m}{2T})^{1/2} \{ \exp(\frac{-Q^2}{2mT}) - \exp(\frac{-Q'^2}{2mT}) \} \tag{6.1.24}$$

where,

$$\begin{gathered} Q = \frac{m\omega}{p} - \frac{p}{2} \\ Q' = - \frac{m\omega}{p} - \frac{p}{2} \end{gathered} \tag{6.1.25}$$

The low temperature degenerate Fermi fluid limit is given by, using Eqn.(6.1.6) to calculate μ,

$$T \to 0 \ , \quad \mu \to \varepsilon \ = \frac{1}{2m} \left(\frac{3\pi^2 N}{V} \right)^{2/3} \qquad (6.1.26)$$

Hence,

$$f_{q\sigma} = \begin{cases} 0 \text{ for } \varepsilon_q > \mu \\ 1 \text{ for } \varepsilon_q < \mu \end{cases} \qquad (6.1.27)$$

Hence the range of integration is effectively reduced to the sphere,

$$q < p_f = \left(\frac{3\pi^2 N}{V} \right)^{1/3} \qquad (6.1.28)$$

when the integrand contains the factor $f_{q\sigma}$.

The expression for Im $G^{(0)}(p,\omega)$ in Eqn.(6.1.15) is easy to evaluate, transforming to cylindrical polar coordinates again. One way of writing the results is,

$$\begin{aligned} \text{Im } G^{(0)}(p,\omega) &= 0 \ , & p_f^2 &< Q^2 \\ \text{Im } G^{(0)}(p,\omega) &= -\frac{mV}{4\pi p} \left(p_f^2 - Q^2 \right) \ , & Q^2 &< p_f^2 < Q'^2 \qquad (6.1.29) \\ \text{Im } G^{(0)}(p,\omega) &= -\frac{m^2 V\omega}{2\pi p} \ , & p_f^2 &> Q'^2 \end{aligned}$$

The conditions $p_f^2 < Q^2$, etc. correspond to regions in the p–ω plane (Lovesey 1980). These are well known results.

In the next section we add interaction terms into the Hamiltonian.

6.2 Hamiltonian

We write our Hamiltonian in the form,

$$H = \sum_{k,\sigma} \varepsilon_k \, c^+_{k\sigma} \, c_{k\sigma} + \sum_k I(k) \, \rho(k) \, \rho(-k) \qquad (6.2.1)$$

where the particle density operator is,

$$\rho(k) = \sum_{q,\sigma} c^{+}_{k+q\sigma}\, c_{q\sigma} \tag{6.2.2}$$

and I(k) is the spatial Fourier transform of the particle interaction. The other parameters and operators were defined in Sec.6.1 and the first term in the Hamiltonian is the non-interacting Hamiltonian, H_0, of Eqn.(6.1.13). The second term can be written,

$$\sum_{kqq'} \sum_{\sigma\sigma'} I(k)\, c^{+}_{q+k\sigma}\, c_{q\sigma}\, c^{+}_{q'-k\sigma'}\, c_{q'\sigma'} \tag{6.2.3}$$

so it represents the scattering of two fermions with initial momenta q and q', and final momenta q+k and q'-k. The interaction I(k) depends only on the momentum transfer, k, and I(-k)=I(k), and the spins of the fermions are unchanged.

One problem is deciding what momentum dependence the interaction should have. If the only interaction between the fermions is a Coulomb interaction then I(k) is proportional to $(1/k^2)$. If we have a contact interaction, proportional to $\delta(R)$ where R is the distance between the fermions, then I(k) is a constant, independent of k.

We note that $\rho(k)$, in Eqn.(6.2.2), is related to n(k), defined in Eqn.(6.1.8). The relation is,

$$\rho(k) = n(k) + N\,\delta_{k0} \tag{6.2.4}$$

We will derive some results for a system described by this Hamiltonian in the following sections.

6.3 Calculation of $n_{q\sigma}(p,\omega)$

In this section we discuss our calculation of the spectrum of spontaneous fluctuations, $n(p,\omega)$, outlining the approximations as we make them. Our aim is to construct an approximation that embodies the RPA and includes the effects of particle lifetimes.

First we consider the equation-of-motion for a product of two fermion operators,

$$i\,\partial_t\, c^+_{\alpha\sigma}\, c_{\beta\sigma} = [\, c^+_{\alpha\sigma}\, c_{\beta\sigma},\, H\,] \tag{6.3.1}$$

From the first term in the Hamiltonian, H_0, we obtain,

$$[\, c^+_{\alpha\sigma}\, c_{\beta\sigma},\, H_0\,] = (\, \varepsilon_\beta - \varepsilon_\alpha\,)\, c^+_{\alpha\sigma}\, c_{\beta\sigma} \tag{6.3.2}$$

where we have used the anticommutation relations, Eqn.(6.1.1), to normal order the operators and to interchange two creation or annihilation operators.

We choose to write the second term in our Hamiltonian as,

$$\sum_{kq\sigma'} I(k)\, \rho(-k)\, c^+_{q+k\sigma'}\, c_{q\sigma'} \tag{6.3.3}$$

and make the approximation that $\rho(-k)$ in this term commutes with c^+c. This scheme greatly simplifies the calculation. It is a semi-classical approximation and we show that it readily reproduces the standard RPA. We find,

$$[\, c^+_{\alpha\sigma}\, c_{\beta\sigma},\, \sum_{kq\sigma'} I(k)\, \rho(-k)\, c^+_{q+k\sigma'}\, c_{q\sigma'}\,] =$$

$$\sum_{k} I(k)\, (\, c^+_{\alpha\sigma}\, c_{\beta-k\sigma} - c^+_{\alpha+k\sigma}\, c_{\beta\sigma}\,)\, \rho(-k) \tag{6.3.4}$$

In Sec.6.8 we will find that the exact result for this commutator, not making the above approximation, can be written,

$$\sum_{k} 2I(k)\, [\, c^+_{\alpha\sigma}\, \rho(-k)\, c_{\beta-k\sigma} - c^+_{\alpha+k\sigma}\, \rho(-k)\, c_{\beta\sigma}\,] \tag{6.3.5}$$

Hence the terms that we have neglected are of the forms, after ordering the operators,

$$\sum_{k} I(k)\, c^+_{\alpha\sigma}\, c_{\beta\sigma}\;, \quad \sum_{k} I(k)\, c^+_{\alpha-k\sigma}\, c_{\beta-k\sigma} \tag{6.3.6}$$

at this stage. The factor of two in Eqn.(6.3.5) arises from taking the commutator with $\rho(-k)$ as well as with $\rho(k)$.

Then, setting $\alpha=p+q$, $\beta=q$, Eqn.(6.3.1) gives,

$$i\partial_t n_{q\sigma}(p) = (\varepsilon_q - \varepsilon_{p+q}) n_{q\sigma}(p) + I(-p) (f_{p+q\sigma} - f_{q\sigma}) n(p) + \sum_k I(k) [n_{q-k\sigma}(p+k) - n_{q\sigma}(p+k)] \rho(-k) \tag{6.3.7}$$

using the definition of $n_{q\sigma}(p)$, Eqn.(6.1.7).

Taking the Fourier transform of this equation gives,

$$(\omega + \varepsilon_{p+q} - \varepsilon_q) n_{q\sigma}(p,\omega) = I(p) (f_{p+q\sigma} - f_{q\sigma}) n(p,\omega) + \frac{1}{2\pi} \int_{-\infty}^{\infty} du \sum_k I(k) [n_{q-k\sigma}(p+k,u) - n_{q\sigma}(p+k,u)] \rho(-k,\omega-u) \tag{6.3.8}$$

where $\rho(k,\omega)$ is the time Fourier transform of $\rho(k)$.

In the standard Random Phase Approximation, or RPA, all terms involving momentum $\underline{k}$, except k=0, are neglected in Eqn.(6.3.8). Hence, in this approximation,

$$(\omega + \varepsilon_{p+q} - \varepsilon_q) n_{q\sigma}(p,\omega) = I(p) (f_{p+q\sigma} - f_{q\sigma}) n(p,\omega) \tag{6.3.9}$$

Using an equation-of-motion method, as will be described in Sec.6.4, then gives,

$$G(p,\omega) = \chi^{(0)}(p,\omega) + \chi^{(0)}(p,\omega) I(-p) G(p,\omega) \tag{6.3.10}$$

or,

$$G(p,\omega) = \chi^{(0)}(p,\omega) / \{ 1 - I(-p) \chi^{(0)}(p,\omega) \} \tag{6.3.11}$$

where,

$$\chi^{(0)}(p,\omega) = \sum_{q\sigma} (f_{p+q\sigma} - f_{q\sigma}) (\omega + \varepsilon_{p+q} - \varepsilon_q)^{-1} \tag{6.3.12}$$

We will see that the main difference between these RPA results and the results of our calculation is that we obtain a self-energy in the denominator of our dynamic susceptibility, from which it should be possible to study lifetime effects.

In our calculation, however, we iterate Eqn.(6.3.8) once, i.e. we replace $n_{q-k\sigma}(p+k,u)$ and $n_{q\sigma}(p+k,u)$ by their expressions to order I, obtained from Eqn.(6.3.8). We obtain,

$$(\omega + \varepsilon_{p+q} - \varepsilon_q) n_{q\sigma}(p,\omega) = I(-p) (f_{p+q\sigma} - f_{q\sigma}) n(p,\omega) +$$

$$n_{q\sigma}(p,\omega) \int_{-\infty}^{\infty} du \sum_k I(k) I(-k) F_1(k,\omega-u) [\frac{1}{u + \varepsilon_{p+q} - \varepsilon_{q+k}} +$$

$$\frac{1}{u + \varepsilon_{p+q+k} - \varepsilon_q}] - \int_{-\infty}^{\infty} du \sum_k I(k) I(-k) n_{q+k\sigma}(p,\omega) F_1(k,\omega-u)$$

$$\times [\frac{1}{u + \varepsilon_{p+q} - \varepsilon_{q+k}} + \frac{1}{u + \varepsilon_{p+q+k} - \varepsilon_q}] \qquad (6.3.13)$$

where the spectral function of prime interest is,

$$F_1(k,v) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dt\, e^{ivt} < \rho(-k,t) \rho(k) > \qquad (6.3.14)$$

and we have replaced products of the form $[\rho(k,u)\rho(k',u')]$ by their thermal averages in obtaining Eqn.(6.3.13).

We then neglect the term in Eqn.(6.3.13) involving $n_{q+k\sigma}(p,\omega)$ except for k=0. Such terms correspond to fluctuations in $n_{q\sigma}(p,\omega)$, which is itself a fluctuation, as shown in Eqn.(6.1.7). Clearly we are retaining terms neglected by the RPA, however.

We then make the replacement,

$$\sum_k \quad \rightarrow \quad \sum_k{}' = \sum_{k \neq 0} \qquad (6.3.15)$$

which has no effect since terms with k=0 in Eqn.(6.3.13) cancel.

Finally,

$$(\omega + \varepsilon_{p+q} - \varepsilon_q) n_{q\sigma}(p,\omega) = I(-p) (f_{p+q\sigma} - f_{q\sigma}) n(p,\omega) +$$

$$\frac{1}{2\pi}\, n_{q\sigma}(p,\omega) \int_{-\infty}^{\infty} du \sum_{k}{}' \; I(k)\; I(-k)\; F_1(k,\omega-u)\; \left[\frac{1}{u + \varepsilon_{p+q} - \varepsilon_{q+k}} + \frac{1}{u + \varepsilon_{p+q+k} - \varepsilon_{q}} \right] \qquad (6.3.16)$$

In the next section we use this approximate result to calculate the Green function $G(p,\omega)$ of Eqn.(6.1.12).

6.4 Calculation of G(p,ω)

Using the result,

$$< [\, n_{q\sigma}(p),\; n(-p) \,] > \; = f_{p+q\sigma} - f_{q\sigma} \qquad (6.4.1)$$

which is easily derived from the anticommutation relations, Eqn.(6.1.1), and thermal averages of fermion operators, Eqn.(6.1.3), along with the result for $n_{q\sigma}(p,\omega)$, Eqn.(6.3.16), we can write an expression for $G_{q\sigma}(p,\omega)$ immediately, since,

$$\omega\, G_{q\sigma}(p,\omega) = \; < [\, n_{q\sigma}(p),\; n(-p) \,] > + \ll [\, n_{q\sigma}(p),\; H \,];\; n(-p) \gg_{\omega} \qquad (6.4.2)$$

from Eqn.(2.2.3). The result is,

$$[\, \omega + \varepsilon_{p+q} - \varepsilon_{q} - \Sigma_{q\sigma}(p,\omega) \,]\; G_{q\sigma}(p,\omega) =$$

$$(\, f_{p+q\sigma} - f_{q\sigma} \,)\; [\, 1 + I(-p)\; G(p,\omega) \,] \qquad (6.4.3)$$

where,

$$\Sigma_{q\sigma}(p,\omega) = \int_{-\infty}^{\infty} du \sum_{k}{}' \; I(k)\; I(-k)\; F\,(k,\omega-u) \;\times$$

$$\left[\frac{1}{\omega - u + \varepsilon_{p+q} - \varepsilon_{q+k}} + \frac{1}{\omega - u + \varepsilon_{p+q+k} - \varepsilon_{q}} \right] \qquad (6.4.4)$$

is the self–energy, and,

$$F(k,v) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dt\ e^{ivt} < n(k,t)\ n(-k) > \qquad (6.4.5)$$

We note that, for k≠0, $F(k,v)$ is the same as $F_1(k,v)$ of Eqn.(6.3.14).

The fluctuation-dissipation theorem then is,

$$F(k,v) = -\frac{1}{\pi} \{ 1 - e^{-v/T} \}^{-1} \ \mathrm{Im}\ G(k,v) \qquad (6.4.6)$$

by arguments similar to those for deriving Eqn.(2.1.6).

We define the dynamic susceptibility by,

$$\chi(p,\omega) = \sum_{q\sigma} (f_{p+q\sigma} - f_{q\sigma}) \{ \omega + \varepsilon_{p+q} - \varepsilon_q - \Sigma(p,\omega) \}^{-1} \qquad (6.4.7)$$

Then, using Eqn.(6.4.3),

$$G(p,\omega) = \chi(p,\omega) + I(-p)\ \chi(p,\omega)\ G(p,\omega) \qquad (6.4.8)$$

or,

$$G(p,\omega) = \chi(p,\omega) \ / \ [\ 1 - I(-p)\ \chi(p,\omega)\ ] \qquad (6.4.9)$$

Hence we have expressions for $G(p,\omega)$ in terms of $\Sigma_{q\sigma}(p,\omega)$ and for $\Sigma_{q\sigma}(p,\omega)$ in terms of $\mathrm{Im}\ G(k,u)$, etc. We do not have an equation for $G(p,\omega)$ or $\Sigma_{q\sigma}(p,\omega)$ that we can solve easily. In the next section we will make some more simple approximations in an attempt to obtain an expression which can be evaluated. We choose to calculate $\mathrm{Im}\Sigma_{q\sigma}(p,\omega)$, which is, using Eqns.(6.4.4) and (6.4.6),

$$\begin{aligned}\mathrm{Im}\ \Sigma_{q\sigma}(p,\omega) = \sum_k{}' \ I(k)\ I(-k)\ \{\ [\ 1 + n(\omega+\varepsilon_{p+q}-\varepsilon_{q+k})\ ] \times \\ \mathrm{Im}\ G(k,\omega+\varepsilon_{p+q}-\varepsilon_{q+k}) + [\ 1 + n(\omega+\varepsilon_{p+q+k}-\varepsilon_q)\ ] \times \\ \mathrm{Im}\ G(k,\omega+\varepsilon_{p+q+k}-\varepsilon_q)\ \}\end{aligned} \qquad (6.4.10)$$

where,

$$n(u) = \{ \exp(\frac{u}{T}) - 1 \}^{-1} \qquad (6.4.11)$$

and we have used the δ-function obtained from taking the imaginary part of ,

$$\frac{1}{\omega - u + \varepsilon_{p+q} - \varepsilon_{q+k}} + \frac{1}{\omega - u + \varepsilon_{p+q+k} - \varepsilon_{q}}$$

to do the integration over the variable u.

Re $\Sigma_{q\sigma}(p,\omega)$ is obtained from the dispersion relation, Eqn.(2.1.4), and we can then obtain $G(p,\omega)$ from $\Sigma_{q\sigma}(p,\omega)$.

6.5 First Approximation to Im $\Sigma_{q\sigma}(p,\omega)$

We wish to explore the features of the self-energy and the ramifications for the spectrum by calculating Im $\Sigma_{q\sigma}(p,\omega)$ from Eqn.(6.4.10). As a first approximation we replace Im $G(k,u)$ on the right-hand side by its non-interacting value, Eqn.(6.1.15). In principle, we should be able to substitute the new expression for $G(k,u)$ obtained back into the equation and iterate to obtain better approximations to $G(k,u)$. In practice we will stop after the first iteration. Then,

$$\text{Im}\ \Sigma_{q\sigma}(p,\omega) = \int_{-\infty}^{\infty} du\ [\ 1 + n(u)\ ] \sum_{k}{}' \ I(k)\ I(-k)\ \text{Im}\ G^{(0)}(k,u)\ \times$$

$$[\ \delta(\ \omega - u + \varepsilon_{p+q} - \varepsilon_{q+k}\ ) + \delta(\ \omega - u + \varepsilon_{p+q+k} - \varepsilon_{q}\ )\ ] \qquad (6.5.1)$$

We have retained the integration over u in this expression for convenience as it may not be simplest to do the u integration first.

Using the expression for ε_a, Eqn.(6.1.5), we can write the arguments of the δ-functions as,

$$\omega - u + \varepsilon_{p+q} - \varepsilon_{q+k} = \frac{-1}{2m}\ \{\ (\ \underline{k} + \underline{q}\ )^2 - 2m(\ \omega - u\ ) - (\ \underline{p} + \underline{q}\ )^2\ \}$$

$$\omega - u + \varepsilon_{p+q+k} - \varepsilon_q = \frac{1}{2m} \{ (\underline{k} + \underline{p} + \underline{q})^2 + 2m(\omega - u) - q^2 \} \qquad (6.5.2)$$

We have to integrate over all wave vectors $\underline{k}$. The first of these expressions is invariant under rotations of $\underline{k}$ about $\underline{q}$ and the second is invariant under rotations about $(\underline{p}+\underline{q})$. Hence it is convenient to work in cylindrical polar coordinates taking the z-axis to lie along $\underline{q}$ in the first case and $(\underline{p}+\underline{q})$ in the second. We denote the coordinates (k_z, k_ρ, ϕ) given by,

$$\begin{aligned} k_x &= k_\rho \cos(\phi) \\ k_y &= k_\rho \sin(\phi) \end{aligned} \qquad (6.5.3)$$

and we have,

$$\int d^3k = \int_0^{2\pi} d\phi \int_{-\infty}^{\infty} dk_z \int_0^{\infty} k_\rho \, dk_\rho \qquad (6.5.4)$$

and the integration over ϕ gives a factor of (2π).

Hence we have, from Eqn.(6.5.1), and using Eqn.(6.1.16) to transform the sum into an integral,

$$\text{Im}\ \Sigma_{q\sigma}(p,\omega) = \frac{mV}{(2\pi)^2} \int_{-\infty}^{\infty} du \,[\, 1 + n(u) \,] \int_{-\infty}^{\infty} dk_z \int_0^{\infty} d(k_\rho^2)\, I(k) \times$$

$$I(-k)\ \text{Im}\ G^{(0)}(k,u) \{ \delta(k_\rho^2 + k_z^2 + 2qk_z - p^2 - 2\underline{p}.\underline{q} - 2m[\omega - u])$$

$$+ \delta(k_\rho^2 + k_z^2 + 2|\underline{p}+\underline{q}|k_z + p^2 + 2\underline{p}.\underline{q} + 2m[\omega - u]) \} \qquad (6.5.5)$$

where,

$$k = (k_\rho^2 + k_z^2)^{1/2} \qquad (6.5.6)$$

and we are assuming that the interaction $I(k)$ depends only on the magnitude of $\underline{k}$ and not on its direction.

The δ-functions in the integrand can be used to do one of the three integrations in Eqn.(6.5.5). Because of the form of the arguments of the δ-functions it is probably not sensible to use them to do the k_z integration.

Doing the k_ρ integration gives,

$$\mathrm{Im}\,\Sigma_{q\sigma}(p,\omega) = \frac{mV}{(2\pi)^2}\int_{-\infty}^{\infty} du\,[\,1+n(u)\,]\int_{-\infty}^{\infty} dk_z\,\{\,I(k_1)\,I(-k_1)\,\times$$

$$\mathrm{Im}\,G^{(0)}(k_1,u)\,\theta(\,k_1^2-k_z^2\,) + I(k_2)\,I(-k_2)\,\mathrm{Im}\,G^{(0)}(k_2,u)\,\times$$

$$\theta(\,k_2^2-k_z^2\,)\,\} \qquad (6.5.6)$$

$$k_1^2 = 2m(\,\omega-u\,) - 2qk_z + p^2 + 2\underline{p}.\underline{q}$$

$$k_2^2 = 2m(\,\omega-u\,) - 2|\underline{p}+\underline{q}|k_z - p^2 - 2\underline{p}.\underline{q}$$

We can then get rid of the θ-functions by changing the integration ranges since, for example, $k_1{}^2 > k_z{}^2$ places restrictions on the allowed values of k_z and u.

Hence,

$$\mathrm{Im}\,\Sigma_{q\sigma}(p,\omega) = \frac{mV}{(2\pi)^2}\,\{\int_{-\infty}^{\omega+(\underline{p}+\underline{q})^2/2m} du\,[\,1+n(u)\,]\,\times$$

$$\int_{-q-[(\underline{p}+\underline{q})^2+2m(\omega-u)]^{1/2}}^{-q+[(\underline{p}+\underline{q})^2+2m(\omega-u)]^{1/2}} dk_z\,I(k_1)\,I(-k_1)\,\mathrm{Im}\,G^{(0)}(k_1,u)\,+$$

$$\int_{\omega-q^2/2m}^{\infty} du\,[\,1+n(u)\,]\int_{-|\underline{p}+\underline{q}|-[q^2-2m(\omega-u)]^{1/2}}^{-|\underline{p}+\underline{q}|+[q^2-2m(\omega-u)]^{1/2}} dk_z I(k_2)\,\times$$

$$I(-k_2)\,\mathrm{Im}\,G^{(0)}(k_2,u)\,\} \qquad (6.5.7)$$

or, equivalently,

$$\mathrm{Im}\,\Sigma_{q\sigma}(p,\omega) = \frac{mV}{(2\pi)^2}\,\{\int_{-\infty}^{\infty} dk_z\int_{-\infty}^{\omega+(-k_z^2-2qk_z+p^2-2\underline{p}.\underline{q})/2m} du\,\times$$

$$[\,1+n(u)\,]\,I(k_1)\,I(-k_1)\,\mathrm{Im}\,G^{(0)}(k_1,u)\; + \int_{-\infty}^{\infty} dk_z\,\times$$

$$\int_{\omega+(k_z^2+2|\underline{p}+\underline{q}|k_z+p^2+2\underline{p}.\underline{q})/2m}^{\infty} du \; [\; 1 + n(u)\;]\; I(k_2)\; I(-k_2) \times$$

$$\operatorname{Im} G^{(0)}(k_2,u) \tag{6.5.8}$$

These expressions are clearly difficult to evaluate in general. We will consider what they give in the high and low temperature limits in the next section.

6.6 High and Low Temperature Limits

The high temperature limit is given by T→∞. We will work to lowest order in (1/T) throughout. To this order,

$$1 + n(u) = T\,/\,u \tag{6.6.1}$$

from Eqn.(6.4.11), and,

$$\operatorname{Im} G^{(0)}(k,u) = -N\left(\frac{\pi m}{2T^3}\right)^{1/2}\frac{u}{k} \tag{6.6.2}$$

from Eqns.(6.1.24) and (6.1.25).

Substituting these expressions into Eqn.(6.5.7) gives,

$$\operatorname{Im} \Sigma_{q\sigma}(p,\omega) = -\frac{mVN}{(2\pi)^2}\left(\frac{\pi m}{2T}\right)^{1/2}\left\{\frac{1}{q}\int_{-\infty}^{\omega+(\underline{p}+\underline{q})^2/2m} du \times \right.$$

$$\left.\int_{x_1}^{x_2} dk\; I(k)\; I(-k) \;+\; \frac{1}{|\underline{p}+\underline{q}|}\int_{\omega-q^2/2m}^{\infty} du \int_{y_1}^{y_2} dk\; I(k)\; I(-k)\right. \tag{6.6.3}$$

where,

$$x_1 = |\; q - [\; (\underline{p}+\underline{q})^2 + 2m(\omega-u)\;]^{1/2}\; |$$

$$x_2 = q + [\; (\underline{p}+\underline{q})^2 + 2m(\omega-u)\;]^{1/2} \tag{6.6.4}$$

$$y_1 = |\; |\underline{p}+\underline{q}| - [\; q^2 - 2m(\omega-u)\;]^{1/2}\; |$$

$$y_2 = |\underline{p}+\underline{q}| + [\, q^2 - 2m(\omega-u)\,]^{1/2}$$

We consider the special case,

$$I(k) = \begin{cases} I \text{ for } k < k_{max} \\ 0 \text{ otherwise} \end{cases} \qquad (6.6.5)$$

In this case the integrals in Eqn.(6.6.3) are easy to evaluate but messy because of the integration limits. For example, we have to consider whether x_1 and x_2 are less than or greater than k_{max} for each value of u. We omit these details. The result is,

$$\text{Im}\ \Sigma_{q\sigma}(p,\omega) = - \frac{NV}{(2\pi)^2} \left(\frac{2\pi m}{T} \right)^{1/2} I^2\, k_{max}^2 \qquad (6.6.6)$$

which is independent of p, q and ω but depends on the high momentum cut-off k_{max} and if we let k_{max} go to infinity then Im $\Sigma_{q\sigma}(p,\omega)$ diverges. It seems that the interaction of Eqn.(6.6.5) is not very useful.

The low temperature limit is given by T=0. Then, using Eqn.(6.4.11),

$$1 + n(u) = 1 \qquad (6.6.7)$$

and Im $G^{(0)}(k,u)$ is given by Eqn.(6.1.29). The integrand in Eqn.(6.5.7), or Eqn.(6.5.8), has a simple form that is easy to integrate for the interaction in Eqn.(6.6.5). However, the conditions $p_f{}^2 < Q^2$, etc. in Eqn.(6.1.29) cause the integration ranges in the integrals of Eqns.(6.5.7) and (6.5.8) to have to be split up. In fact, there are so many cases to take account of that we were not able to obtain a useful expression for Im $\Sigma_{q\sigma}(p,\omega)$, even for the form of I(k) in Eqn.(6.6.5)

6.7 Expansion in (1/ω)

For a Fermi liquid system such as the one we are considering there are sum rules. In terms of F(k,u), Eqn.(6.4.5), one such sum rule is,

$$\int_{-\infty}^{\infty} du\ F(k,u) = S(k) \tag{6.7.1}$$

where the structure factor, S(k), is defined,

$$S(k) = < n_{-k}\ n_{k} > \tag{6.7.2}$$

Another is,

$$\int_{-\infty}^{\infty} du\ u\ F(k,u) = \frac{k^2}{2m} \tag{6.7.3}$$

More of these sum rules are derived by Pines and Nozieres (1966). They are obtained by taking moments of the correlation function F(k,u). Using Eqn.(6.4.6) we can also write them in terms of the Green function G(k,u).

In this section we expand G(p,ω) in (1/ω) and make use of these moments relations and other known information on Fermi liquid systems to assess the features of the G(p,ω) that we have obtained and also to attempt to place some restrictions on the momentum dependence of the interaction I(k).

Expanding $\Sigma_{q\sigma}(p,\omega)$ of Eqn.(6.4.4) in powers of (1/ω) and using the sum rules of Eqns.(6.7.1) and (6.7.3) gives,

$$\Sigma_{q\sigma}(p,\omega) = \frac{2}{\omega} \sum_{k}{}' \ I(k)\ I(-k)\ S(k) + \frac{1}{\omega^2} \sum_{k} \ I(k)\ I(-k) \times$$

$$\{ \frac{k^2}{m} - \frac{(\ p^2 + 2p.q\ )}{m} S(k)\ ] + O(1/\omega^3) \tag{6.7.4}$$

Then, expanding $\chi(p,\omega)$, Eqn.(6.4.7), in (1/ω),

$$\frac{1}{N}\ \chi(p,\omega) = \frac{p^2}{m\omega^2} + \frac{1}{\omega^4} \{ \frac{6p^2}{m} \sum_{k}{}' \ I(k)\ I(-k)\ S(k) \ + \frac{p^6}{4m^3} +$$

$$\frac{2p^4}{m^2} <KE> \} + O(1/\omega^6) \tag{6.7.5}$$

$$<KE> = \frac{3}{2mp^2} \frac{1}{N} \sum_{q\sigma} f_{q\sigma} (\underline{p}.\underline{q})^2$$

Finally, expanding $G(p,\omega)$ of Eqn.(6.4.9), using the above result, gives,

$$G(p,\omega) = \chi_p \{ \omega_0^2 / \omega^2 + \omega_0^2 \omega_1^2 / \omega^4 + O(1/\omega^6) \} \qquad (6.7.6)$$

where,

$$\omega_0^2 \chi_p = \frac{p^2}{m}$$

$$\omega_1^2 = (\frac{p^2}{2m})^2 + 4(\frac{p^2}{2m}) <KE> + 6 \sum_k{}' I(k) I(-k) S(k) + \frac{p^2}{m} I(-p) \qquad (6.7.7)$$

We have chosen to define the functions ω_0, ω_1 and χ_p for ease of comparison with other results on Fermi liquids. For example, there is the result,

$$\omega_1^2 = (\frac{p^2}{2m}) \{ (\frac{p^2}{2m}) + 4<KE> \} + \Omega^2(p) \qquad (6.7.8)$$

where (Lovesey 1975),

$$\Omega^2(p) = (\frac{n_0}{m}) \int d^3r \, g(r) [1 - \cos(\underline{p}.\underline{r})] \, \partial_{zz} V(r) \qquad (6.7.9)$$

where $V(r)$ is a pair potential and $g(r)$ is a pair distribution function. We will not need to know the definitions or forms of these functions here. We note that as $p \to 0$, $\Omega^2(p) \to 0$.

Comparing Eqns.(6.7.7) and (6.7.8) we have,

$$\Omega^2(p) = \frac{p^2}{m} I(-p) + 6 \sum_k{}' I(k) I(-k) S(k) \qquad (6.7.10)$$

The second term on the right-hand side of this equation is a positive constant. Hence we do not have the required result that $\Omega^2(p) \to 0$ as $p \to 0$ unless,

$$I(p) \rightarrow -\frac{6m}{p^2} \sum_k{}' \; I(k)\; I(-k)\; S(k) \qquad (6.7.11)$$

which diverges as p→0.

Hence our result for $G(p,\omega)$ cannot be correct for a general momentum dependence of the interaction $I(k)$. We have not been able to discover which approximation in our calculation is not valid.

Finally, in the next section we consider a perturbative calculation on our Hamiltonian.

6.8 Comparison With Perturbative Calculation

In this section we attempt to increase our understanding of the problem by doing a perturbative calculation. Using our Hamiltonian, Eqn.(6.2.1), we calculate the Green function $G(p,\omega)$ as an expansion in powers of the interaction I. We write the second term in the form of Eqn.(6.2.3) and use the equation-of-motion method described in Sec.2.2. The equation-of-motion for $G_{q\sigma}(p,\omega)$ becomes,

$$\begin{aligned} (\omega + \varepsilon_{p+q} - \varepsilon_q)\, G_{q\sigma}(p,\omega) &= f_{p+q\sigma} - f_{q\sigma} + \sum_{kk'\sigma'} 2\, I(k) \times \\ \{ &\ll c^+_{p+q\sigma}\, c^+_{k+k'\sigma'}\, c_{k\sigma'}\, c_{q+k\sigma};\, n(-p) \gg_\omega - \\ &\ll c^+_{p+q+k\sigma}\, c^+_{k'-k\sigma'}\, c_{k'\sigma'}\, c_{q\sigma};\, n(-p) \gg_\omega \} \qquad (6.8.1) \end{aligned}$$

using the anticommutation relations, Eqn.(6.1.1), and the thermal averages of fermion operators, Eqn.(6.1.3).

If we want $G(p,\omega)$ to first order in I then we need to calculate the six-particle Green functions of the form,

$$\ll c^+_{\alpha\sigma}\, c^+_{\beta\sigma'}\, c_{\gamma\sigma'}\, c_{\delta\sigma};\, n(-p) \gg_\omega \qquad (6.8.2)$$

to zeroth order in I, so replace H by H_0 in the equation-of-motion for this Green function. Using,

$$< c^{+}_{\alpha\sigma}\, c^{+}_{\beta\sigma'},\, c_{\gamma\sigma'},\, c_{\delta\sigma} > = \delta_{\alpha\delta}\, \delta_{\beta\gamma}\, f_{\alpha\sigma}\, f_{\beta\sigma'} -$$

$$\delta_{\sigma\sigma'}\, \delta_{\alpha\gamma}\, \delta_{\beta\delta}\, f_{\alpha\sigma}\, f_{\beta\sigma} \qquad (6.8.3)$$

from Wick's theorem, we find after a little algebra that, to first order in I,

$$G_{q\sigma}(p,\omega) = G^{(0)}_{q\sigma}(p,\omega)\ \{\ 1 + 2I(p)\ G^{(0)}(p,\omega) + \sum_{k}{}'\ 2I(k) \times$$

$$[\ (\ f_{p+q+k\sigma} - f_{q+k\sigma}\ )\ (\ \omega + \varepsilon_{p+q} - \varepsilon_{q}\ )^{-1} -$$

$$G^{(0)}_{q+k\sigma}(p,\omega)\ ]\ \} \qquad (6.8.4)$$

where,

$$G^{(0)}_{q\sigma}(p,\omega) = (\ f_{p+q\sigma} - f_{q\sigma}\ )\ (\ \omega + \varepsilon_{p+q} - \varepsilon_{q}\ )^{-1} \qquad (6.8.5)$$

The corresponding result in our calculation, if we sum over q and σ in this equation, from expanding G(p,ω) in Eqn.(6.4.8) to order I is,

$$G(p,\omega) = G^{(0)}(p,\omega)\ \{\ 1 + I(-p)\ G^{(0)}(p,\omega)\ \} \qquad (6.8.6)$$

The factor of 2 in Eqn.(6.8.4) was accounted for in Sec.6.3. The other terms that we have neglected in Eqn.(6.4.8) are those neglected by the RPA.

To work to order I^2 in the calculation of G(p,ω) we must calculate the Green function in Eqn.(6.8.2) to order I. The calculation is straightforward. However, we have not been able to write down the result in a form that can easily be compared to our results of Sec.6.4.

We conclude that there are still problems needing to be dealt with in this calculation. Clearly the terms involving k in Eqn.(6.8.4) cannot be obtained from expanding the G(p,ω) of Eqn.(6.4.9), using Eqn.(6.4.7) to define χ(p,ω), to first order in I unless the self-energy contains first order terms in I. However, we cannot obtain the form of G(p,ω) in Eqn.(6.4.9) by doing any finite order of perturbation theory. Such a form clearly contains information on singularities in G(p,ω), which are important physically. Hence we do not pursue a perturbative calculation further.

It is obvious that there is much work still to be done on the problem of this chapter.

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