MANY BODY THEORY OF FERROMAGNETIC RESONANCE IN METALS AND ALLOYS

A Thesis

Submitted by

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for the Degree of Doctor of Philosophy of the University of London.

September 1971

ABSTRACT

In this thesis the problem of ferromagnetic resonance linewidths in metals is treated by methods which assume that the energy absorption from the electromagnetic field is carried in the material by spin waves. The linewidth is then explained in terms of the spin wave damping rates. In the first part of the thesis a discussion is given of this connection between spin wave damping rates and ferromagnetic resonance widths. Simple criteria are given for the calculation of the one from the other. The remainder of the thesis is concerned with the calculation of spin wave spectra and linewidths in metals and alloys using different models of magnetism and different damping mechanisms.

CONTENTS

CHAPTER 1

MACROSCOPIC DESCRIPTION OF FERROMAGNETIC RESONANCE

In this chapter a discussion of the macroscopic approach to ferromagnetic resonance is given. Although the calculations of this thesis are microscopic calculations, the conceptual interpretation is still the same as in the macroscopic theory. The correlation function approach can in fact still be used, where $\theta(t)\langle[\underline{M}(t), \underline{M}(0)]\rangle$ is evaluated by using the equation of motion for $\underline{M}(t)$. In the microscopic approach $\hat{\underline{M}}(t)$ is expressed in terms of other operators. However, the conventional approach is used here, where the ferromagnet is considered as a continuous medium characterized by a magnetic moment $\underline{M}(\underline{r},t)$ which depends on position and time. In equilibrium $\underline{M}$ is independent of position. The fundamental concepts are that of the resonance frequency and the linewidth, the first of these including the effect of the demagnetizing fields. The macroscopic theory gives good results for the resonance frequency, but leads to an incorrect analytic form for the correlation functions. The microscopic theory places the calculation of damping on a more secure theoretical basis.

The Equation of Motion for the Magnetization of a System of Non-Interacting Spins (1)

A homogeneously magnetized sample is characterized by a magnetization vector $\underline{M}$, which depends on the temperature and the external field. (This assumes there is no domain structure.) $\underline{M}$ is equal to the sum of the magnetic moments of the electrons in a unit volume, and is parallel to the magnetic field $\underline{H}$. The magnetic moment of the electron $\underline{\mu}$ is associated with the spin $\underline{s}$, where $\underline{\mu} = -\gamma\underline{s}$, $\gamma = \frac{g|e|}{2m_o c}$. $\therefore$ $\underline{M}$ is

similar to the total angular momentum of a rigid body, and in analogy one can write the equation of motion for $\underset{\sim}{M}$ as

$$\frac{d\underset{\sim}{M}(t)}{dt} = -\gamma \{\underset{\sim}{M} \wedge \underset{\sim}{H}\} \tag{1.1}$$

where $\underset{\sim}{H}$ is the external field, and $\underset{\sim}{M} \wedge \underset{\sim}{H}$ is the external torque.

Consider an ellipsoidal isotopic ferromagnetic specimen, on which a weak homogeneous field $\underset{\sim}{h}\{\underset{\sim}{h}(t) << \underset{\sim}{H}_o\}$, (which changes harmonically in time with a frequency ω, and acts in the xy plane) is superimposed on a constant magnetic field $\underset{\sim}{H}_o$ directed along the z axis, which is sufficient to destroy any domain structure. If there is no skin effect, $\underset{\sim}{h}(t)$ will be the same over the whole sample, and the equation of motion will be the same at each point of the medium.

Let

$$\underset{\sim}{M}(t) = \underset{\sim}{M}_o + \underset{\sim}{m}(t) \qquad |\underset{\sim}{m}(t)| << M_o \underset{\sim}{k}$$

where

$$\underset{\sim}{H}_o = H_o \underset{\sim}{k} \tag{1.2}$$

$\underset{\sim}{m}$ is small and varies harmonically.

Then, discarding terms of order $\underset{\sim}{m} \wedge \underset{\sim}{h}$, from equation (1.1) one has

$$\frac{d\underset{\sim}{M}(t)}{dt} = -\gamma \underset{\sim}{M}_o \wedge \underset{\sim}{h} - \gamma \{\underset{\sim}{m} \wedge \underset{\sim}{H}_o\} \tag{1.3}$$

Then

$$\underset{\sim}{m} = \underset{=}{\chi} \cdot \underset{\sim}{h} \tag{1.4}$$

where $\underset{=}{\chi}$ is the susceptibility tensor, remembering that the equations are now linear, one finds

$$\chi_{xx} = \chi_{yy} = \chi_o \frac{\omega_o^2}{\{\omega_o^2 - \omega^2\}} \qquad \chi_o = \frac{M_o}{H_o} \tag{1.5}$$

from (1.3) and (1.4)

$$\chi_{xy} = -\chi_{yx} = (-i)\,\chi_o \frac{\gamma\,\omega}{\omega_o^2 - \omega^2} \qquad \omega_o = \gamma H_o \tag{1.6}$$

where

$$\begin{aligned} m_x &= \chi_{xx} h_x + \chi_{xy} h_y \\ m_y &= \chi_{yy} h_y + \chi_{yx} h_x \\ m_z &= 0 \ . \end{aligned} \tag{1.7}$$

If the electromagnetic wave is polarized, i.e. $h\pm = h_x \pm i h_y = h_o\, e^{\pm i\omega t}$ and $m\pm = m_x \pm i m_y$

$$\begin{aligned} m_+ &= \chi_+ h_+ = \chi_o \frac{\omega_o}{\omega_o - \omega} h_+ \\ m_- &= \chi_- h_- = \chi_o \frac{\omega_o}{\omega_o - \omega} h_- \end{aligned} \tag{1.8}$$

This analysis is only good for ω well away from ω_o, but does indicate a resonance near ω_o. To make sense of the analysis one must include the energy loss processes.

Effective Internal Field and the Resonance Frequency

The various interactions in a ferromagnetic metal can be taken into account by assuming that the spins responsible for ferromagnetism precess not only in the external field $\underline{H}_o$, but in an effective field $\underline{H}_{eff}$ composed of an external and internal contribution[1]

$$\frac{d\underset{\sim}{m}(t)}{dt} = -\gamma \{\underset{\sim}{m}(t) \wedge \underset{\sim}{H}_{eff}\} \qquad (1.9)$$

$H_{eff} - H_o$ causes the resonance frequency to shift relative to ω_o. In a state of thermodynamic equilibrium the direction of $\underset{\sim}{M}$ coincides with H_{eff}, whose magnitude is determined by the free energy per unit volume F

$$H_M = -\frac{\partial F}{\partial M} \qquad H_\theta = H_\phi = 0 \; . \qquad (1.10)$$

In this case the components H_θ and H_ϕ of the effective field are absent. The equilibrium orientation of the vector M defined by θ_o and ϕ_o can be found from the equations

$$\frac{\partial F}{\partial \theta} = 0 \; , \qquad \frac{\partial F}{\partial \phi} = 0 \qquad (1.11)$$

$$\Rightarrow \theta_o \text{ exists} \qquad \Rightarrow \phi_o \text{ exists}$$

By examining oscillations about this position one can then find an expression for the resonance frequency[2].

The Effect of Demagnetizing Fields on the Resonance Frequency

These arise because of surface magnetization. The field inside the sample is not $\underset{\sim}{H}_o$, but $\underset{\sim}{H}_o$ minus the field due to surface magnetic charges. For a general surface of second degree with principal axis parallel to the x,y,z axes the demagnetizing factors are N_x, N_y, N_z. The H_{eff} is given by

$$\begin{aligned} (H_E)_x &= -N_x \, m_x(t) \\ (H_E)_y &= -N_y \, m_y(t) \qquad (1.12) \\ (H_E)_z &= H_z - N_z \, M_z(t) \; . \end{aligned}$$

Then as before let $\underline{m}(t)$ and $\underline{h}(t) = (h_x, h_y, 0)$ be the oscillating parts of $\underline{M}$ and $\underline{H}$

$$\frac{d\underline{M}}{dt} = -\gamma \{\underline{M} \wedge \underline{H}_{eff}\} \tag{1.9}$$

From (1.9) and (1.12) one obtains, and assuming $\underline{m}(t) = \underline{m}(0)e^{i\omega t}$

$$\therefore\ i\omega m_x = \{-\gamma\}\{m_y(H_o - N_z M_o) - M_o(h_y - N_y m_y)\}$$

$$i\omega m_y = \{-\gamma\}\{M_o(h_x - N_x m_x) - m_x(H_o - N_z M_o)\}$$

$$\therefore\ i\omega m_x = (-\gamma) -\gamma \{M_o(h_x - N_x m_x) - m_x(H_o - N_z M_o)\}$$

$$\times (i\omega)^{-1}\{H_o - N_z M_o + N_y M_o\} + \gamma M_o h_y$$

$$\therefore\ -\omega^2 m_x = \gamma^2 M_o h_x (H_o - N_z M_o + N_y M_o) - m_x\gamma^2\{N_x M_o - H_o + N_z M_o\}$$

$$\{H_o - N_z M_o + N_y M_o\} + i\omega\gamma M_o h_y$$

$$-\omega^2 m_x = -[H_o + (N_y - N_z)M_o]\{(N_x - N_z)M_o - H_o\}\gamma^2 m_x$$

$$+ [H_o + (N_y - N_z)M_o] M_o h_x + i\omega\gamma M_o h_y$$

$$\therefore\ \chi_{xx}(\omega) = \frac{\chi_o}{\{1 \mp (\frac{\omega}{\omega_{res}})^2\}} \tag{1.13}$$

$$\text{Where}\quad \omega_{res} = \gamma \{[H_o + (N_y - N_z) M_o][H_o + (N_x - N_z) M_o]\}^{\frac{1}{2}} \tag{1.14}$$

$$\text{and}\quad \chi_o = \frac{M_o}{H_o + (N_x - N_z)M_o} \tag{1.15}$$

This is still only valid for ω well away from ω_{ϖ}. However, when damping

is included ω_o is seen to be the resonance frequency. $(\omega_o \equiv \omega_{res})$

For a cylinder

$$N_x = N_y = 2\pi \quad : \qquad N_z = 0$$

$$\therefore \quad \omega_{res} = \gamma (H_o + 2\pi M_o)$$

Sphere

$$N_x = N_y = N_z = 0$$

$$\omega_{res} = \gamma H_o$$

Plane (xz plane)

$$N_z = N_x = 0 \qquad N_y = 4\pi$$

$$\omega_{res} = \gamma \left\{H_o \left[H_o + 4\pi M_o\right]\right\}^{\frac{1}{2}} = \gamma \left\{B_o H_o\right\}^{\frac{1}{2}} \tag{1.16}$$

Phenomenological Approach to Damping in the Equation of Motion for the Magnetization

One wants to find an equation of motion for the magnetization which leads to the correct shape for the resonance absorption line. It is in the calculation of the linewidth of the resonance that the importance of ferromagnetic resonance lies. The idea is to calculate the width of the resonance resulting from relaxation mechanisms which one postulates. Then one may learn about the interactions present in the ferromagnetic substance. A macroscopic theory can often be an important guide to microscopic calculations.

The relaxation may be caused by interactions within the spin system, (magnetic dipole interaction), by interaction between the spin system and the lattice, etc. The presence of the different interactions can be taken into account formally by adding to the R.H.S. of the equation of motion a relaxation term which describes the damping.

$$\frac{d\underset{\sim}{M}}{dt} = -\gamma\,[\underset{\sim}{M} \wedge \underset{\sim}{H}] + \underset{\sim}{R}(\underset{\sim}{M} \cdot \underset{\sim}{H}) \qquad (1.17)$$

The vector $\underset{\sim}{R}$ can be looked on as a total moment of friction forces. Then $\underset{\sim}{M} \cdot \frac{d\underset{\sim}{M}}{dt} \neq 0$, and $|\underset{\sim}{M}|$ is not constant as before. The selection of $\underset{\sim}{R}$ is a matter of educated guesswork.

The suggestion of Landau is[2]

$$\frac{d\underset{\sim}{M}}{dt} = -\gamma\{\underset{\sim}{M} \wedge \underset{\sim}{H}\} - \frac{\lambda}{|\underset{\sim}{M}|^2}\ \underset{\sim}{M} \wedge \{\underset{\sim}{M} \wedge \underset{\sim}{H}\} \qquad (1.18)$$

λ characterizes the relaxation frequency.

The length of $\underset{\sim}{M}$ remains constant when in motion, reflecting the independence of the magnetization of a single domain sample from the external field at temperatures below the Curie temperature. The relaxation term characterizes the torque striving to return the magnetization to its equilibrium position. When $\underset{\sim}{H} = \underset{\sim}{H}_o$, i.e. no r.f. field, one obtains the solution

$$\begin{aligned} M_x &= M_\rho\, e^{-t/\zeta} \cos \omega_o t \\ M_y &= M_\rho\, e^{-t/\zeta} \sin \omega_o t \qquad (1.19) \\ M_z &= M_\rho \left(1 - \left(\frac{M_\rho}{M}\right) e^{-2t/\zeta}\right)^{\frac{1}{2}} \end{aligned}$$

where

$$\tau = \frac{|\underset{\sim}{M}|}{\lambda H_o}$$

is the relaxation time

$$\omega_o = \gamma H_o$$

is the precession frequency.

The magnetization vector moves along a spiral and gradually approaches the equilibrium value. Widening of the ferromagnetic absorption line is due to the finiteness of the relaxation time of the transverse component of the magnetic moment.

Solution of the Damping Equation (3)

The equation of motion is

$$\frac{d\underset{\sim}{M}}{dt} = -\gamma \{\underset{\sim}{M} \wedge \underset{\sim}{H}\} - \frac{\alpha\gamma}{|\underset{\sim}{M}|} M \wedge \{\underset{\sim}{M} \wedge \underset{\sim}{H}\} \qquad (1.20)$$

Then

$$\underset{\sim}{M} = M_o \underset{\sim}{k} + \underset{\sim}{m}(t) \qquad \underset{\sim}{m}(t) = |\underset{\sim}{m}| e^{i\omega t} \qquad (1.21)$$

(1.20) and (1.21) give

$$i\omega m_x = -\gamma \{m_y H_o - M_o h_y\} + \gamma\alpha \{H_o m_x - H_x M_o\}$$

$$i\omega m_y = -\gamma \{M_o h_x - m_x H_o\} + \gamma\alpha \{h_y M_o - H_o m_y\}$$

$$i\omega m_y \left(1 + \frac{H_o \gamma\alpha}{i\omega}\right) = -\gamma \{M_o h_x - m_x H_o\} + \gamma\alpha\, h_y M_o$$

$$\therefore \quad m_y = \frac{-\gamma \{M_o h_x - m_x H_o\}}{(i\omega)\left(1 + \frac{H_o \gamma\alpha}{i\omega}\right)} + \frac{\gamma\alpha\, h_y M_o}{\left(1 + \frac{H_o \gamma\alpha}{i\omega}\right)(i\omega)}$$

$$\therefore \quad i\omega m_x \left(1 + \frac{H_o \gamma\alpha}{i\omega}\right) = + \frac{\gamma^2 H_o}{(i\omega)} \frac{M_o h_x}{\left(1 + \frac{H_o\gamma\alpha}{i\omega}\right)} - \frac{\gamma^2 H_o^2 m_x}{i\omega\left(1 + \frac{H_o\gamma\alpha}{i\omega}\right)}$$

$$- \frac{\gamma^2 H_o^2 \alpha M_o h_y}{i\omega\left(1 + \frac{H_o\gamma\alpha}{i\omega}\right)} + \gamma\alpha h_x M_o + \gamma M_o h_y$$

$$\therefore \quad -\omega^2\left(1 + \frac{H_o\gamma\alpha}{i\omega}\right)m_x + \frac{\gamma^2 H_o^2}{\left(1 + \frac{H_o\gamma\alpha}{i\omega}\right)} m_x = \left(\frac{\gamma^2 H_o M_o}{\left(1 + \frac{H_o\gamma\alpha}{i\omega}\right)} + i\omega\gamma\alpha M_o\right) hx$$

$$+ \left(- \frac{\gamma^2 H_o^2 \alpha M_o}{\left(1 + \frac{H_o\gamma\alpha}{i\omega}\right)} + i\omega\gamma M_o\right) h_y$$

$$\therefore \quad \{- \omega^2 + H_o^2\gamma^2\alpha^2 + \gamma^2 H_o^2 + 2i\omega H_o\gamma\alpha\} m_x$$

$$= \{\gamma^2 H_o^2 \psi_o + H_o^2\gamma^2\alpha^2\chi_o + i\omega\gamma\alpha H_o\chi_o\} h_x$$

$$+ \{i\omega\gamma H_o\chi_o\} h_y$$

$$\therefore \quad \text{If} \quad \omega_{res} = (1 + \alpha^2)^{\frac{1}{2}} \gamma H_o = \omega_r \qquad (1.22)$$

$$\chi_{xx}(\omega) = \frac{\omega_r^2 + i\omega\gamma\alpha H_o\chi_o}{\{\omega_r^2 - \omega^2 + 2i\omega H_o\gamma\alpha\}} \qquad (1.23)$$

$$\chi_{xy}(\omega) = \frac{i\omega\gamma H_o\chi_o}{\omega_r^2 - \omega^2 + 2i\omega H_o\gamma\alpha} \qquad (1.24)$$

There is no longer a singularity at $\omega = \omega_r$, only a peak. This expression is then true for all ω providing (1.20) is true.

CHAPTER 2

THE SKIN EFFECT AND FERROMAGNETIC RESONANCE IN METALS

Simple Spin Wave Theory (4)

As we have seen above a ferromagnet can be described by a magnetization vector $\underset{\sim}{M}(\underset{\sim}{r})$. At absolute zero the thermodynamically stable state is such that $\underset{\sim}{M}(\underset{\sim}{r}) = \underset{\sim}{M}_o$, a vector constant over the whole sample. This state minimizes the exchange energy.

The higher energy states of the system are therefore states of non uniform magnetization. Let us consider those states where $\underset{\sim}{M}(\underset{\sim}{r})$ is close to $\underset{\sim}{M}_o$, i.e. $\underset{\sim}{M}(\underset{\sim}{r}) = \underset{\sim}{M}_o + \Delta\underset{\sim}{M}(\underset{\sim}{r})$ and such that only the direction of the magnetization changes from point to point.

Let us consider an isotropic ferromagnet in an external field $\underset{\sim}{H}_o$. The equilibrium magnetization $\underset{\sim}{M}_o$ is then parallel to $\underset{\sim}{H}_o$. A deviation of $\underset{\sim}{M}$ from $\underset{\sim}{M}_o$ causes a rise in energy/unit volume equal to

$$- \{(\underset{\sim}{M} - \underset{\sim}{M}_o) \cdot \underset{\sim}{H}_o\} \qquad (2.1)$$

and at the same time there is an increase in the exchange energy which is determined by the magnetization gradients, and is equal to

$$\frac{A}{|M_o|^2} \{(\nabla M_x)^2 + (\nabla M_y)^2 + (\nabla M_z)^2\} \qquad (2.2)$$

where A is the exchange energy interaction constant.

The total energy of the non uniform magnetized state is from (2.2) and (2.1)

$$H = \int_V \left\{ \frac{A}{|M_o|^2} \{(\nabla M_x)^2 + (\nabla M_y)^2 + (\nabla M_z)^2\} - \right.$$

$$\left. \{(\underset{\sim}{M}(\underset{\sim}{r}) - \underset{\sim}{M}_o) \cdot \underset{\sim}{H}_o\} \right] d^3\underset{\sim}{r}$$

If

$$\underset{\sim}{H}_o = |H_o|\underset{\sim}{k} \quad ; \quad M_x, M_y << M_o \quad ;$$

$$M_z \simeq M_o\{1 - \frac{M_x^2 + M_y^2}{2M_o^2}\} \tag{2.3}$$

To quadratic terms in M_x (harmonic approximation)

$$H = \int \left\{ \frac{A}{|M_o|^2} \{(\nabla M_x)^2 + (\nabla M_y)^2\} + H_o \frac{\{M_x^2 + M_y^2\}}{2M_o} \right\} d^3\underset{\sim}{r}$$

Put $M^{\pm} = M_x \pm iM_y$

$$\therefore H = \int \left\{ \frac{A}{|M_o|^2} \{\nabla M^+ \nabla M^-\} + \frac{H_o}{2M_o} M^+ M^- \right\} d^3\underset{\sim}{r} \tag{2.5}$$

Defining new coordinates b_k, b_k^+ by

$$M^-(\underset{\sim}{r}) = \left(\frac{2\mu M_o}{V}\right)^{\frac{1}{2}} \sum_{\underset{\sim}{K}} b_{\underset{\sim}{K}} e^{i\underset{\sim}{k}\cdot\underset{\sim}{r}} \tag{2.6}$$

$$M^+(\underset{\sim}{r}) = \left(\frac{2\mu M_o}{V}\right)^{\frac{1}{2}} \sum_{\underset{\sim}{K}} b_k^* e^{-i\underset{\sim}{k}\cdot\underset{\sim}{r}}$$

One finds that

$$H = \sum_{\underset{\sim}{K}} \left(\frac{2\mu A}{M_o} k^2 + \mu H_o\right) b_k^* b_k \tag{2.7}$$

If then one wrote out the equation of motion in terms of the b_k's, the b_k's would vary harmonically in time. Further, any motion can be expressed as a linear combination of these coordinates. This classical calculation concerns us only in the sense that it is a guide to a quantum mechanical calculation. The classical field $M(\underset{\sim}{r})$ must be replaced by operators $\hat{M}(\underset{\sim}{r})$ and instead of complex conjugate fourier amplitudes b_k and b_k^* we introduce hermitean conjugate operators $\hat{b}_k$ and $\hat{b}_k^+$. The commutation relations which define the statistics of the ferromagnons can be derived from those of the total angular momentum $\hat{I}$.

$$[\hat{I}_i, \hat{I}_j] = i\varepsilon_{ijk}\hat{I}_k \qquad i, j, k = 1, 2, 3 \quad (2.8)$$

Define

$$\hat{M} = \int \hat{M}(\underset{\sim}{r})\, d^3r = -\mu \hat{I}$$

$$\therefore \quad \hat{M}_y\hat{M}_x - \hat{M}_x\hat{M}_y = i\mu \hat{M}_o \qquad (2.9)$$

$$\therefore \quad \int \{\hat{M}_y(\underset{\sim}{r})\hat{M}_x(\underset{\sim}{r}') - \hat{M}_x(\underset{\sim}{r}')\hat{M}_y(\underset{\sim}{r})\}\, d^3\underset{\sim}{r} d^3\underset{\sim}{r}' = i\mu|M_o| \int \delta(\underset{\sim}{r}-\underset{\sim}{r}')\, d^3\underset{\sim}{r}\, d^3\underset{\sim}{r}' \qquad (2.10)$$

The integrands must be equal since this is true for any volume. Therefore

$$\hat{M}^+(\underset{\sim}{r})\hat{M}^-(\underset{\sim}{r}') - \hat{M}^-(\underset{\sim}{r}')\hat{M}^+(\underset{\sim}{r}) = 2\mu|M_o|\, \delta(\underset{\sim}{r}-\underset{\sim}{r}') \qquad (2.11)$$

and using the fourier expansions we get

$$\hat{b}_{\underset{\sim}{k}}\hat{b}^+_{\underset{\sim}{k}'} - \hat{b}^+_{\underset{\sim}{k}'}\hat{b}_{\underset{\sim}{k}} = \delta_{\underset{\sim}{k}\underset{\sim}{k}'} \quad . \qquad (2.12)$$

The Hamiltonian of the system is then

$$\hat{H} = \sum_{\underset{\sim}{k}} \left\{\frac{A}{M_o} k^2 + \mu H_o\right\} \hat{b}^+_{\underset{\sim}{k}}\hat{b}_{\underset{\sim}{k}} \qquad (2.13)$$

and is equivalent to a set of oscillators.

Therefore $\hat{n}_k = \hat{b}_k^+ \hat{b}_k$ can take on any integer value $n_k = 0, 1, 2 \ldots$.

The mean number of magnons with an energy ε_k is defined by the Bose-Einstein distribution

$$\bar{n}_k = \frac{1}{(e^{\varepsilon_k/kT} - 1)} \qquad \varepsilon_k = \frac{A}{M_o} k^2 + \mu H_o \qquad (2.14)$$

The possible energy levels are then

$$E(n_k) = \sum_k \varepsilon_k n_k \qquad n_k = 0, 1, 2 \ldots \qquad (2.15)$$

and all expectation values can be worked out from the fundamental matrix elements

$$\begin{aligned} (n_k|\hat{b}_k(t)|n_k + 1) &= (n_k + 1)^{\frac{1}{2}} e^{-i\varepsilon_k t/h} \\ (n_k|\hat{b}_k^+(t)|n_k - 1) &= (n_k)^{\frac{1}{2}} e^{i\varepsilon_k t/h} \end{aligned} \qquad (2.16)$$

At low temperatures (low energy of excitation) when only a few magnons are excited, this is an accurate picture of the ferromagnet. The individual magnons of given wave vectors $\underset{\sim}{k}$ are termed spin waves. In this temperature range ferromagnetic resonance can be regarded as excitation of spin waves by the external r.f. field. The resonance frequency is then determined from the frequency of the most excited magnon (in number). The line width can then be determined from the decay time of the magnons.

To see this explicitly, let us examine the behaviour of a system of magnons with energy given by the formula above in a high frequency alternating magnetic field.

The energy of interaction with $\underset{\sim}{M}(\underset{\sim}{r})$ is

$$\hat{W} = \int h_x M_x d^3\underset{\sim}{r} \tag{2.17}$$

This can be regarded as a perturbation causing quantum transitions between the energy levels. If h_o does not depend on r, then

$$\hat{W} = + \int \left(\frac{\mu_o M}{2}\right)^{\frac{1}{2}} h_x \sum_{\underset{\sim}{K}} (b_k^+ + b_k)\, \delta_{k,0} \tag{2.18}$$

First order perturbation theory gives the transition rate as

$$|< 1 \mid \hat{W} \mid 2 >|^2 = |< 1,k \mid \hat{W} \mid 2k' >|^2 \tag{2.19}$$

Then because of the form of $\hat{W}$, $\underset{\sim}{k} = \underset{\sim}{k}'$, and since $\underset{\sim}{k} = 0$ in the ground state at $T = 0$, only $\underset{\sim}{k} = 0$ magnons are excited. (At finite temperatures this result would have to be multiplied by $\bar{n}_k$, as the probability that the kth mode is occupied.) Therefore only $\underset{\sim}{k} = 0$ magnons can be excited. The selection rule is thus $\Delta n_{k=0} = \pm 1$. These selection rules define the resonance frequency, because of the conservation of energy, as

$$\hbar\omega_o = \mu H = \varepsilon_{K=0}$$

Non-uniform spin waves can be excited as a consequence of two effects. Firstly there may be a non-uniform magnetic field. Secondly as the specimen has boundaries, those modes for which $\int M d^3r$ is non-zero may be excited as standing mode spin waves.

The first case is always realized in a metal ferromagnet in which the skin effect implies that the radio frequency field can only penetrate the metal for a finite distance. In this case the radio frequency field is not uniform in the sample.

Then

$$\underset{\sim}{h}(\underset{\sim}{r}) = \sum_{\underset{\sim}{p}} h(\underset{\sim}{p})\, e^{i\underset{\sim}{p}\cdot\underset{\sim}{r}}$$

$$h(\underset{\sim}{p}) = \int d^3\underset{\sim}{r}\; h(\underset{\sim}{r})\, e^{-i\underset{\sim}{p}\cdot\underset{\sim}{r}} \qquad (2.20)$$

$$\therefore \quad \hat{W} = -\left(\frac{\mu M_o}{2}\right)^{\frac{1}{2}} \sum_{\underset{\sim}{k},\underset{\sim}{p}} h(\underset{\sim}{p})\, \{b_{\underset{\sim}{p}} + b^{+}_{\underset{\sim}{p}}\}\, \delta_{\underset{\sim}{K},\underset{\sim}{p}} \qquad (2.21)$$

Therefore as $\hat{W}$ acts on the ground state, one can see that there is a finite probability for the excitation of spin waves with non-zero wave vector, in fact this probability is proportional to $|h(p)|^2$.

Let us suppose then that the magnetic field varies in accordance with the classical skin effect law, the penetration depth in the direction of the y axis being δ (the ferromagnetic metal occupying the space to the right of the plane y = 0).

$$h(\underset{\sim}{r}) = h_o\, e^{-y\frac{(1+i)}{\delta}} \qquad (2.22)$$

$$\therefore \quad h(\underset{\sim}{k}) = h_o\, \delta_{k_x=0}\, \delta_{k_z=0}\, \frac{1}{\left(\frac{1}{\delta}\right)^2 - i\left(k_y - \frac{1}{\delta}\right)}$$

$$|h(k)|^2 = \frac{h_o^{\,2}}{\left(\frac{1}{\delta}\right)^2 + \left(k_y - \frac{1}{\delta}\right)^2} \qquad (2.23)$$

Then the most probable spin wave mode to be excited will be that of wave vector $|k| = \frac{1}{\delta}$. The resonance frequency is then shifted from $\omega_o = \gamma H_o$ to

$$\omega_o = \gamma H_o + \frac{2A\gamma}{M_o}\left(\frac{1}{\delta}\right)^2 . \qquad (2.24)$$

A Self Consistent Treatment of the Skin Effect

In an analysis of ferromagnetic resonance one can take account of the skin effect by this simple method of assuming that the width is given by that of the spin wave of wave vector δ. As a better approximation one can use the simple theory discussed below for improving the estimate of the resonance linewidth as compared to the spin wave line width. For completeness sake we shall also point out the possibility of "spin wave resonance", which is a direct effect of the exchange mechanism acting in the region of the boundary, and also to point out under what conditions it is realized.

Let a ferromagnetic specimen in the form of a lamina be placed in a magnetic field $\underset{\sim}{H}$ parallel to its surface.

$$\underset{\sim}{H} = \underset{\sim}{H}_o + \underset{\sim}{h}\, e^{i\omega t} \tag{2.25}$$

where $\underset{\sim}{H}_o$ is a constant uniform field and $\underset{\sim}{h}$ is the amplitude of an alternating field of frequency ω perpendicular to $\underset{\sim}{H}_o$. Assuming that the electromagnetic field is attenuated as $e^{i(\underset{\sim}{k}\cdot\underset{\sim}{r})}$, one can find the propagation constant k from the Maxwell equations for a medium with complex magnetic permeability $\mu(\omega) = \mu_1 - i\mu_2$ as

$$k^2 = \frac{i4\pi\sigma\omega\mu(\omega)}{c^2} \tag{2.26}$$

where σ is the electrical conductivity, and c is the velocity of light. The reciprocal of the real part of k is the penetration depth δ where $\mu(\omega) = 1 + 4\pi\,\chi(\omega)$, and for a given specimen near the resonance frequency is given by (from equation (1.24))

$$\mu(\omega) = \frac{\{\omega_a^2 - \omega^2\}}{\{\omega_o^2 - \omega^2 + 2i\omega\Delta\omega\}} \qquad (2.27)$$

$$\omega_o = \gamma\sqrt{B_o h_o}$$

$$B_o = H_o + 4\pi M_o = H_o(1 + 4\pi \chi_o) \qquad (2.28)$$

$$\omega_a = \gamma B_o$$

and $\Delta\omega$ is the total line width which includes both the intrinsic linewidth $\Delta\omega_r$ and the exchange linewidth $\Delta\omega_e$.

At resonance ($\omega = \omega_o$) we have

$$\frac{1}{\delta} = k = \sqrt{\frac{4\pi\sigma\omega_o\mu_2(\omega_o)}{c}} \quad (a) \qquad (2.29)$$

$$\mu_2(\omega_o) = \frac{\Omega_o^2}{\omega_o\Delta\omega} \quad (b) \qquad \Omega_o = \gamma\sqrt{2\pi M_o}\, B_o \quad (c) \qquad (2.30)$$

If one ignores exchange effects, i.e. $\Delta\omega_e = 0$, then $\Delta\omega_r$ is usually given by a function of k' and ω, where $\underset{\sim}{k}'$ is a wave vector, i.e. $\Delta\omega_r \equiv \Delta\omega_r(\underset{\sim}{k}', \omega)$. Near resonance this equals $\Delta\omega_r(k, \omega_o)$, where k is of the order $\frac{1}{\delta}$. Then from (a), (b) and this expression one can determine a self consistent expression for $\Delta\omega_r$.

A Full Treatment of the Skin Effect: Justification of Approximations

A more detailed analysis[5] leads to what has been termed "spin wave resonance". We will consider this briefly here, at least so that we can make clear under what conditions one may expect either kind of resonance to occur. In the above discussion the three equations

considered were the magnetization equation of motion and two of Maxwell's equations. The two Maxwell equations were treated first, using the connection between the magnetization and the field derived separately from the first equation. Under certain conditions, however, one should solve all three equations together.

Put

$$\underset{\sim}{B} = \underset{\sim}{H} + 4\pi \underset{\sim}{M}$$

and the two Maxwell equations become

$$\begin{aligned} \text{Curl } \underset{\sim}{E} &= -\left(\frac{1}{c}\right)\left(\frac{\partial}{\partial t}\right)(\underset{\sim}{H} + 4\pi \underset{\sim}{M}) \\ \text{Curl } \underset{\sim}{H} &= \frac{4\pi\sigma}{c}\underset{\sim}{E} \end{aligned} \tag{2.31}$$

where one has used $\underset{\sim}{J} = \sigma\underset{\sim}{E}$, where $\underset{\sim}{J}$ is the current density and the displacement term has been neglected, essentially because of the high value of σ in a ferromagnetic metal.

The equation of motion of the magnetization vector $\underset{\sim}{M}$ is equation (1.9)

$$\frac{d\underset{\sim}{M}(t)}{dt} = -\gamma\{\underset{\sim}{M}(t) \wedge \underset{\sim}{H}_{eff}\} \tag{2.32}$$

If the magnetization varies with distance as it does if the skin depth is small then one must include the effects of the exchange energy. The exchange energy density[6] is equation (2.2)

$$\int \frac{A}{M_o^2}\{(\nabla M_x)^2 + (\nabla M_y)^2 + (\nabla M_z)^2\, d^3\underset{\sim}{r} = \int (\underset{\sim}{M} \cdot \underset{\sim}{H}_{eff})\, d^3\underset{\sim}{r}$$

Then

$$\underset{\sim}{H}_{eff} = -\frac{\partial H(r)}{\partial \underset{\sim}{M}_j} + \sum_\alpha \frac{\partial}{\partial r_\alpha}\left[\frac{\partial H(r)}{\left(\frac{\partial M_j}{\partial r_\alpha}\right)}\right] \qquad (2.33)$$

One finds

$$\underset{\sim}{H}_{ex} = \frac{2A}{M_o^2}\nabla^2 \underset{\sim}{M} \ . \qquad (2.34)$$

Including the normal kind of damping equation (2.32) becomes

$$\frac{1}{\gamma}\frac{d\underset{\sim}{M}}{dt} = \underset{\sim}{M} \times \left\{\underset{\sim}{H}_o + \frac{2A}{M_o^2}\nabla^2 \underset{\sim}{M} - \frac{\lambda}{\lambda M_o^2}\underset{\sim}{M} \times \underset{\sim}{H}\right\} \qquad (2.35)$$

where

$$\gamma = \frac{ge}{2mc} \ .$$

One solves these three equations for a plane sample parallel to the xz plane, the air metal boundary being at y = 0. The static magnetic field H_z is taken as parallel to the boundary. The applied microwaves are assumed to be plane waves normally incident upon the xy plane.

The fields are decomposed into a static component and a microwave component so that

$$\begin{aligned} \underset{\sim}{M} &= M_o \underset{\sim}{i}_z + \underset{\sim}{m}(t) \\ \underset{\sim}{H} &= H_o \underset{\sim}{i}_z + \underset{\sim}{h}(t) \qquad (2.36) \\ \underset{\sim}{E} &= \underset{\sim}{e}(t) \ . \end{aligned}$$

The microwave components are assumed to be proportional to $\exp(i\omega t - ky)$ in the metal and $\frac{|m|}{|M_s|}$, $\frac{|h|}{|H_o|}$ are assumed to be $<<1$.

The three equations can then be reduced to a system of three linear homogeneous equations for the unknowns m_y, m_x, h_x.

If one defines the following dimensionless quantities

$$\eta = \frac{H_o}{4\pi M_o} \; ; \qquad \Omega = \frac{\omega}{4\pi M_o \gamma} \; ; \qquad L = \frac{\lambda}{M_o \gamma}$$

$$\epsilon^2 = \frac{A}{2\pi M_o{}^2 \delta^2} \; ; \qquad K = k\epsilon\delta \; ; \qquad \delta = \frac{c^2}{(2\pi\omega\sigma)^{\frac{1}{2}}} \tag{2.37}$$

these three equations can be written as

$$\begin{aligned} (K^2 - 1 - \eta)m_y + (i\Omega + L\eta)m_z - \left(\frac{L}{4\pi}\right)k_x &= 0 \\ -(i\Omega + L\eta + L)m_y + (K^2 - \eta)m_x + \left(\frac{1}{4\pi}\right)h_x &= 0 \\ -8\pi i\epsilon^2 m_x + (K^2 - 2i\epsilon^2)h_x &= 0 \; . \end{aligned} \tag{2.38}$$

In order that these three equations possess a non vanishing solution the determinant of the coefficients must vanish. This requirement leads to the secular equation

$$K^6 - c_1 K^4 + c_2 K^2 - c_3 = 0 \; . \tag{2.39}$$

There are three solutions for K^2, and therefore three solutions whose real part is positive. These represent waves whose energy flow is into the metal. (The other solutions would be needed only in the case where there are reflected waves.) If n is a label for the three solutions, then one finds

$$\begin{aligned} m_{nx} &= u_n h_{nx} \\ m_{ny} &= v_n h_{nx} \end{aligned} \tag{2.40}$$

where u_n, v_n are functions of K_n^2 and c_1, c_2 and c_3. Then one finds that

$$e_{nz} = \left(\frac{c\,K_n}{4\pi\sigma\varepsilon\delta}\right) h_{nx}$$

$$h_{ny} = -4\pi\, v_n\, h_{nx} \quad . \tag{2.41}$$

The values m_x, etc., inside the metal are $m_x = m_{1x} + m_{2x} + m_{3x}$. These can all be expressed in terms of h_{1x}, h_{2x}, h_{3x}. Therefore for a given h_{ox} (in the air) one needs four equations at the boundary to determine h_{1x}, h_{2x} and h_{3x}. The equations lead to an expression for $Z = \left(\frac{e_z}{h_x}\right)_{y=0}$ which determines the energy flow into the ferromagnet. The actual experiments are analyzed using $\mu_{equiv} = \mu_1 - i\mu_2 = 2i\left(\frac{cZ}{\omega\delta}\right)^2$. It is shown in (6) that an approximate solution of the equations yields

$$\mu_{equiv} = \frac{\eta - \Omega^2 + i\Omega L + 2\varepsilon(1+i)}{\left[\eta - \Omega^2 + i\Omega L + \varepsilon(1+i)^2\right]^2} \tag{2.42}$$

If there is no exchange effect, $A = \varepsilon = 0$, and

$$\mu_{equiv} = \frac{1}{\left[\eta - \Omega^2 - i\Omega L\right]} \tag{2.43}$$

a result we have ($H_o << 4\pi M_o$), i.e. $\eta << 1$, obtained before by simply disregarding Maxwell's equations. If one disregards the phenomenological damping, i.e. $L = 0$

$$\mu_{equiv} = \frac{\eta - \Omega^2 + 2\varepsilon(1+i)}{\left[\eta - \Omega^2 + \varepsilon(1+i)\right]^2} \tag{2.44}$$

Here the linewidth and shape are essentially determined by σ and A, i.e. by the combined effect of eddy current dissipation and exchange.

The resonance field determined by the maximum in $\mu_2(\mu_{eq} = \mu_1 - \mu_2)$

$$\eta_o = \Omega^2 - \tfrac{2}{3}\,\epsilon \tag{2.45}$$

i.e. there is a shift by

$$\Delta H_o = \frac{8\pi}{3}\sqrt{\frac{A\sigma\omega}{c}} \tag{2.46}$$

For the line width ΔH determined by the equation $\mu_2(\eta_o + \tfrac{1}{2}\,\Delta\eta) = \tfrac{1}{2}\mu_2(\eta_o)$ one obtains

$$\Delta H \cong \tfrac{4}{3}\,\epsilon\ . \tag{2.47}$$

One may also note the important point that the line shape is assymmetric. The form for the phenomenological damping is symmetric. We show below that under certain conditions "ordinary spin wave resonance" can yield an assymmetric curve.

The results above are valid for η, Ω, L, $\epsilon^2 << 1$. This means that this type of resonance occurs at rather small frequencies ($\omega_o = (M_s\, H_o \gamma^2)^{\frac{1}{2}}$, since H_o is $<<M_o$. It occurs in samples for which the saturation magnetization is reached at rather low fields.

If the frequencies are much larger then one obtains ordinary spin wave resonance[7]. In this case the equations decouple into a magnetic solution and two non-magnetic waves.

If one rewrites the secular determinant for K^2 in terms of $K'^2 = K^2 - \eta$, one obtains the following form if $L = 0$ (damping is neglected) and

$$K'^6 + K'^4(\eta - 1) - \Omega^2 K'^2 - \Omega^2\eta + 2i\epsilon^2\,\Omega^2 = 0 \tag{2.48}$$

The approximate solutions of this equation are

$$K_1^2 = 2i\varepsilon^2 - \eta \tag{2.49}$$

which is the solution obtained from Maxwell's equations with permeability **1**. This solution has $m_x = m_y = 0$, and is non magnetic, and

$$K'^2_{2,3} = \pm \Omega \tag{2.50}$$

$$\therefore \frac{\omega}{4\pi M_s \gamma} = k^2 \frac{A}{2\pi M_s^2} + \frac{H_o}{4\pi M_s}$$

$$\therefore \omega = \frac{\gamma k^2 A 2}{M_s} + \gamma H_o \tag{2.51}$$

which is the dispersion relation for a spin wave.

Absorption from the Microwave Field in Terms of the Correlation Function

In Appendix (3) which demonstrates the connection of $\chi''(\underset{\sim}{k},\omega)$ or $\chi''(\underset{\sim}{r},\underset{\sim}{r}',\omega)$ with the absorption of energy, it is shown that the mean rate of energy flow at frequency ω into the sample is, equation (E-6)

$$\frac{d\bar{W}}{dt}(\omega) = \tfrac{1}{2} \int d\underset{\sim}{r} \int d\underset{\sim}{r}' \; h(\underset{\sim}{r}) \; \chi''_{mm}(\underset{\sim}{r},\underset{\sim}{r}': \omega) \; h(\underset{\sim}{r})\omega \tag{2.52}$$

If one considers a semi-infinite sample with $h(y) = e^{-y(1+i)_\delta}$ where δ is the skin depth, one can calculate this expression by fourier transforming the x and z variables and Laplace transforming the y variables using the convolution theorem. Then

$$\frac{d\bar{W}}{dt}(\omega) = \frac{4\pi}{2}\int_{-\infty}^{+\infty} dk_y \, |h(k_y)|^2 \, \chi''(|k_y|, \omega)\omega \qquad (2.53)$$

where one has assumed that $\chi(\underset{\sim}{r},\underset{\sim}{r}',\omega)$ is a function of $\underset{\sim}{r}-\underset{\sim}{r}'$. If, for instance

$$\chi''(|k|, \omega) = \frac{\Gamma(|k|, \omega)}{(\omega - Dk^2)^2 + \Gamma^2(|k| \omega)} \qquad (2.54)$$

Then

$$\frac{d\bar{W}}{dt}(\omega) = 2\pi \int_{-\infty}^{+\infty} dk_y \, |h(k_y)|^2 \frac{\Gamma(k_y, \omega)}{(\omega - Dk_y^2) + \Gamma^2(k_y, \omega)} \qquad (2.55)$$

$$= 2\pi \int_{-\infty}^{+\infty} dk_y \frac{|h_o|^2}{\left(k_y - \frac{1}{\delta}\right)^2 + \left(\frac{1}{\delta}\right)^2} \cdot \frac{\Gamma(k_y, \omega)}{(\omega - Dk_y^2) + \Gamma^2(k_y, \omega)} \qquad (2.56)$$

This expression shows that if $\Gamma(k_y, \omega) \gg \frac{1}{\delta}$ then

$$\frac{d\bar{W}}{dt}(\omega) = \frac{|h_o|^2 \, \Gamma(\frac{1}{\delta}, \omega)}{\left(\omega - D\left(\frac{1}{\delta}\right)^2\right) + \Gamma^2(\frac{1}{\delta}, \omega)} \qquad (2.57)$$

which yields a symmetric resonance curve. If Γ is $\ll \frac{1}{\delta}$ however

$$\frac{d\bar{W}}{dt}(\omega) \quad \frac{|h_o|^2}{\left(\sqrt{\frac{\omega}{D}} - \frac{1}{\delta}\right)^2 + \left(\frac{1}{\delta}\right)^2} \qquad (2.58)$$

and the resonance curve is asymetric with width determined by the skin depth. This corresponds to the two cases treated above.

CHAPTER 3

SPIN WAVES IN THE ITINERANT MODEL (7)

The Paramagnetic State

Spin waves and ferromagnetic resonance occur only in ferromagnetic systems, but in order to understand the structure of the ferromagnetic state one has to consider the properties in the paramagnetic state. The approach considered here can be taken towards both ferromagnetism and superconductivity. It consists of searching for those correlations which become singular in the paramagnetic state. For the ferromagnetic state these correlations are then considered to be non zero in a re-evaluation of the Hartree-Fock theory of the system where one uses the same Hamiltonian. This involves modifying the decoupling procedure in the usual Hartree-Fock procedure. From this one obtains a Green's function of modified form which describes the thermodynamic properties of the system, and a second order Green's function which describes the transport properties of the ferromagnetic state.

The ferromagnetic state is one in which there are strong electron-electron correlations, and these are caused by the electron-electron interaction. One can approach this through fermi liquid theory which is philosophically more satisfying, but here we shall use the independent particle theory, with Bloch or plane wave functions for the electrons. We approximate the electron correlations by a zero range on site repulsive interaction. Then the Hamiltonian of the system is

$$\hat{H} = \sum_{p} \epsilon_p \hat{a}_p^{+} \hat{a}_p + I \sum_{I} \hat{n}_{I\uparrow} \hat{n}_{I\downarrow} \qquad (3.1)$$

The ground state is, in the paramagnetic state, a state where all free

electron states are filled up to $p_F = \mu$, where μ is the chemical potential and p_F is the fermi momentum

$$p_F^3 = \frac{N}{V} 3\pi^2 h^3 \tag{3.2}$$

N is the total number of particles

V is the volume of the system

and at finite temperatures (as must be in the paramagnetic state when there can be ferromagnetism) the electrons are distributed according to

$$\bar{n}_p = \frac{1}{\{1 + e^{\beta(\epsilon_p - \mu)}\}} \quad . \tag{3.3}$$

We shall treat systems where $T_C << T_D$. T_C is the Curie Temperature and T_D is the degeneracy temperature, and we shall not consider weak ferromagnetism.

Under the effect of the electron interactions the second order Green's function $G_2^{+-}(x,x') = \langle T\{\hat{\psi}_\uparrow(x)\hat{\psi}^+_\downarrow(x)\hat{\psi}_\downarrow(x')\hat{\psi}^+_\uparrow(x')\}\rangle$ develops a singularity in its space and time fourier transform. This indicates that this correlation function is finite over large distances, and that there is an instability in the ground state of the system. This correlation function is related to the correlation function $\langle T\{M(\underset{\sim}{r},t)M(\underset{\sim}{r}',t')\}\rangle$ and hence by the fluctuation dissipation theorem to the generalized response function. So let us consider this function as it proves more convenient as it has a physical meaning.

If one considers the response of the system to an external magnetic field which varies both in time and space, $\underset{\sim}{h}(x,t)$, then the induced magnetization in the linear approximation is given by,

$$\langle \hat{M}^\alpha(\underset{\sim}{r},t)\rangle = \int d^3\,\underset{\sim}{x}' \int dt' \sum_\beta \chi^{\alpha\beta}(\underset{\sim}{x},\underset{\sim}{x}',t-t')\, h^\beta(\underset{\sim}{x}',t') \tag{3.4}$$

where,

$$\chi^{\alpha\beta}(\underset{\sim}{x},t) = i\,\theta(t) \langle [\hat{M}^{\alpha}(\underset{\sim}{x},t), \hat{M}^{\beta}(0,0)] \rangle \qquad (3.5)$$

where the operators and states are calculated in the unperturbed system. As expected, the linear response is determined by the unperturbed properties (correlations) of the system and vice versa. Further, if one introduces a complete set of states in between the $\hat{M}$ operators as is needed for its evaluation, one can see that this function samples all the excited states of the system. If there is a state amongst these that is a stationary state of the system, then this state will give the main contribution to this function at that energy. This is indicated by a pole in the fourier transform of this response function.

Looked at from this point of view, the form of the response function can tell us something about the excited states of the system. Elsewhere we shall discuss it as describing the absorption of energy, but in absorbing energy the system has to transfer to states of higher energy.

Now in the non-interacting limit where

$$\hat{H}_o = \sum_{p} \varepsilon_p \hat{a}^{+}_p \hat{a}_p \qquad (3.6)$$

the excited states are all single particle excitations. The response function is in this case given by

$$\chi^{o}_{q}(\omega) = \sum_{\underset{\sim}{p}} \frac{f_{p+q} - f_p}{(\varepsilon_{p+q} - \varepsilon_p - \omega - i\eta)} \qquad (3.7)$$

and is as expected a sum of contributions from all the single particle excitations, with due allowance for the pauli exclusion principle.

On considering the correlations one finds that the most important contributions come from coherent electron-hole scattering.

Then

$$\chi_q^{Int}(\omega) = \frac{\chi_q^o(\omega)}{\{1 - I\chi_q^o(\omega)\}} \quad . \tag{3.8}$$

In the limit $q \to 0$, $\omega \to 0$, one has (taking the limits from right to left as the order is important)

$$\lim_{\substack{q \to 0 \\ \omega \to 0}} \begin{cases} \text{Im } \chi_q^o(\omega) = 0 & (3.9) \\ \text{Re } \chi_q^o(\omega) = \nu(\varepsilon_F) & \text{The density of states at the Fermi level.} \end{cases}$$

Then

$$\lim_{\substack{q \to 0 \\ \omega \to 0}} \chi_q(\omega) = \chi_s = \frac{\chi_s^o}{1 - \bar{I}} \; ; \quad \bar{I} = I\nu(\varepsilon_F) \tag{3.10}$$

One can see from the above that $\chi_q(\omega)$ is singular when $1 = \bar{I}\chi_q(\omega)$, and since $R_e\ \chi_q^o(\omega)$ is a decreasing function of q and ω, a pole occurs first at $q = 0$. Therefore, one would expect the new ground state to be a uniform one in space (i.e. all spins aligned). One considers $\omega = 0$ because one is looking for a stationary state. So when $\bar{I} = 1$, the system becomes unstable, and a new state is formed. If $\chi(q)$ is large for $q = 0$, $\chi(r)$ has a long range part. Now at large separations $\langle M(\underset{\sim}{r})\, M(\underset{\sim}{r}')\rangle \equiv \langle M(r)\rangle\langle M(r')\rangle$ $\therefore$ $\langle M(r)\rangle$ is not zero and one has a finite magnetization vector which characterizes the ferromagnetic state. Therefore one can no longer consider $\langle \hat{\psi}_\uparrow^\dagger(x)\psi_\uparrow(x)\rangle_\wedge$ $-\langle \hat{\psi}_\downarrow^\dagger(x)\hat{\psi}_\downarrow(x)\rangle$ to be zero in the ground state. Since $\bar{I}$ depends on temperature through $\chi^o(0,0)$, the condition $\bar{I} = 1$ yields the Curie temperature of the system (Appendix C).

With this assumption in mind one can do a new Hartree-Fock calculation on the above Hamiltonian, and we shall do a rather crude form

$$\hat{H} = \sum_{p_s} \varepsilon_{p_s} \hat{a}^{\dagger}_{p_s} \hat{a}_{p_s} + I \sum_{I} \hat{n}_{I\uparrow} \hat{n}_{I\downarrow} \tag{3.11}$$

If $n_{I\uparrow}$ is replaced by its average value

$$H = \sum_{p_s} \varepsilon_{p_s} \hat{a}^{\dagger}_{p_s} \hat{a}_{p_s} + \sum_{I} I\langle \hat{n}_{I\uparrow} \rangle \hat{n}_{I\downarrow} + I \sum_{I} \hat{n}_{I\uparrow} \langle \hat{n}_{I\downarrow} \rangle \tag{3.12}$$

$$\therefore E_{p\uparrow} = \varepsilon_p + I \frac{\langle \hat{n}\downarrow \rangle}{N}$$

$$E_{p\downarrow} = \varepsilon_p + I \frac{\langle \hat{n}\uparrow \rangle}{N} \tag{3.13}$$

and where $\mu = E_{pf\uparrow} = E_{pf\downarrow}$. Therefore the two bands are split. There is now a direction in the problem, i.e. the direction of quantization. Therefore the response function is a non-diagonal tensor.

$$\chi_o^{+-}(q,\omega) = \frac{1}{N} \sum_{\underset{\sim}{q}} \frac{f_{p\downarrow} - f_{p+q\uparrow}}{\{\varepsilon_{p+q} - \varepsilon_p + \Delta - \omega - i\eta\}} \tag{3.14}$$

Δ is the exchange splitting energy $= \frac{I}{N} \{\langle n_{\downarrow} \rangle - \langle n_{\uparrow} \rangle\}$

$\chi_o^{+-}(q,\omega)$ now has a gap in its singularities, i.e. there are no excited states of the system in this region. At $q = 0$, the gap is Δ.

For the interacting system

$$\chi^{+-}(\underset{\sim}{q},\omega) = \frac{\chi_o^{+-}(\underset{\sim}{q},\omega)}{I - I\, \chi_o^{\pm}(\underset{\sim}{q},\omega)} \tag{3.15}$$

There is now the possibility that a pole may appear in the gap, and this pole corresponds to the propagation of a spin wave.

CHAPTER 4

SPIN WAVES AND FERROMAGNETIC RESONANCE IN A COUPLED LOCAL MOMENT-ELECTRON SYSTEM

As an introduction to a two band calculation and in its own right as a treatment of ferromagnetic resonance in an alloy we will briefly describe a calculation on the spin waves of a local moment-electron coupled system[8]. The system as a whole is assumed to be ferromagnetic. Take as a specific example iron in palladium, where the spins on the iron atoms are treated as localized spins, coupled to the itinerant d holes of the palladium.

Let

$$K(\underline{x}_I - \underline{x}_J, t-t') = -\theta(t-t')\langle[\hat{\sigma}^-(\underline{x}_I, t), \hat{\sigma}^+(\underline{x}_J, t')]\rangle \tag{4.1}$$

be the susceptibility function for the combined system, where

$$\hat{\sigma}^{\pm}(\underline{x},t) = e^{-i\hat{H}t}\,\hat{\sigma}^{\pm}(x\,0)\,e^{i\hat{H}t}$$
$$\hat{\sigma}^{\pm}(x) = \tfrac{1}{2}(\hat{\sigma}^x(x) \pm i\hat{\sigma}^y(x)) \tag{4.2}$$

and σ^x and σ^y are the components of the Pauli spin density for the d band holes

$$\hat{\sigma}(\underline{x}_J) = \frac{1}{N}\sum_{\substack{\underline{K},\underline{q}\\ \alpha\ \beta}} \hat{C}^{+}_{\underline{k}+\underline{q}\ \beta}\,\hat{C}_{\underline{k},\beta}\,e^{i\underline{q}.\underline{x}_J}\,\hat{\underline{\sigma}}_{\alpha\ \beta} \tag{4.3}$$

where N is the number of atoms, and

$$\hat{H} = \hat{H}_{pd} + \hat{H}_{INT}$$

the hamiltonian in the absence of the perturbing magnetic field. The interaction is that of a short range exchange interaction between the spins on the iron sites and the local spin density of the d holes around each site,

$$\hat{H}_{INT} = J \sum_i \hat{\underset{\sim}{\sigma}}(X_i^{Fe}) \cdot \hat{\underset{\sim}{S}}_i \qquad (4.4)$$

where J is an energy parameter measuring the effective exchange coupling. For $\hat{H}_{pd}$ one takes a short range interaction, single band model

$$\hat{H}_{pd} = \sum_{\underset{\sim}{k}\,\sigma} \varepsilon_{\underset{\sim}{K}} \hat{C}^{+}_{\underset{\sim}{K}\,\sigma} \hat{C}_{\underset{\sim}{K}\,\sigma} + I \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \qquad (4.5)$$

$$\hat{n}_{i\uparrow} = \frac{1}{N} \sum_{\underset{\sim}{k},\underset{\sim}{q}} e^{i\underset{\sim}{q}\cdot\underset{\sim}{X}_i} \hat{C}^{+}_{\underset{\sim}{k}+\underset{\sim}{q}\uparrow} \hat{C}_{\underset{\sim}{k}\uparrow} \qquad (4.6)$$

K(x,t) in fact only represents the itinerant electron part of the response of the coupled system to the external forces. The complete response, (in each calculation) is, not calculated, but one uses the fact that the spin wave eigenfrequencies are given by the poles of

$$K(\underset{\sim}{q},\omega) = \int_{-\infty}^{+\infty} dt\, e^{-i\omega t} \sum_{ij} e^{-i\underset{\sim}{q}\cdot(\underset{\sim}{X}_i - \underset{\sim}{X}_j)} K(\underset{\sim}{X}_i - \underset{\sim}{X}_j, t)$$

The partial response function has the same poles as the complete response function. In the calculation the random phase approximation is used to decouple the equations of motion, and only the spatially uniform contributions to the averages is used

$$\text{i.e. } \langle C^{+}_{k+q\uparrow} C_{k\uparrow} \rangle = \delta_{qo}\, n_{k\uparrow} \qquad (4.7)$$

Further $\hat{S}_i^z$ is replaced by $\langle \hat{S}_{\ell i}^z \rangle$ and sums over the impurity sites are replaced by an average over the ensemble of impurity sites X_i^{Fe}. Then it is found that[8]

$$K(\underset{\sim}{q},\omega) = \frac{\chi^o(\underset{\sim}{q},\omega)}{1 - \{I + \frac{2J^2R'}{(JR-\omega)}\}\chi^o(\underset{\sim}{q},\omega)} \tag{4.8}$$

$$\chi^o(\underset{\sim}{q},\omega) = \frac{1}{N}\sum_{\underset{\sim}{k}} \frac{n_{\underset{\sim}{k}\uparrow} - n_{\underset{\sim}{k}+\underset{\sim}{q}\downarrow}}{\{\omega - (\epsilon_{\underset{\sim}{k}} - \epsilon_{\underset{\sim}{k}+\underset{\sim}{q}}) - IR - 2JR'\}} \tag{4.9}$$

$$R = \frac{1}{N}\sum_{\underset{\sim}{k}} n_{k\downarrow} - n_{k\uparrow} \qquad R' = -\frac{N_{Fe}}{N}\langle S_z \rangle \tag{4.10}$$

IR + 2JR' is then the effective splitting of the d band due to the molecular field of both types of spins.

If an effective frequency dependent interaction constant

$$I_{eff}(\omega) = I + \frac{2J^2R'}{(JR-\omega)} \tag{4.11}$$

is introduced, then $K(q,\omega)$ is seen to be analogous to that of a pure ferromagnetic metal. We may rewrite it in an alternative form. Introducing the exchange enhanced susceptibility function

$$\chi(\underset{\sim}{q},\omega) = \frac{\chi^o(\underset{\sim}{q},\omega)}{\{1 - I\chi^o(\underset{\sim}{q},\omega)\}} \tag{4.12}$$

Then

$$K(\underset{\sim}{q},\omega) = \frac{(JR - \omega)\,\chi(\underset{\sim}{q},\omega)}{JR - 2J^2R'\,\chi(\underset{\sim}{q},\omega) - \omega} \tag{4.13}$$

Also

$$\lim_{\omega\to 0, q\to 0} \chi(\underset{\sim}{q},\omega) = \frac{R}{2JR'} = \chi_{\phi}(0,0) \qquad (4.14)$$

Then

$$K(\underset{\sim}{q},\omega) = \frac{(JR - \omega)\,\chi(\underset{\sim}{q},\omega)}{2J^2R'\{\chi(0,0) - \chi(\underset{\sim}{q},\omega)\} - \omega} \qquad (4.15)$$

The poles of $K(\underset{\sim}{q},\omega)$ then occur at

$$\omega = 2J^2R'\{\chi(0,0) - \chi(\underset{\sim}{q},\omega)\} \qquad (4.16)$$

There are now two poles for each $\underset{\sim}{q}$, which is typical of a system of two coupled oscillating systems.

In the limit $q = 0$ we get

$$\omega\{JR + 2JR' - \omega\} = 0 \qquad (4.17)$$

$$\therefore \quad \omega_{ac} = 0 \quad \text{acoustic mode} \qquad (4.18)$$

$$\omega_{op} = JR + 2JR' \quad \text{optical mode} \qquad (4.19)$$

The frequency should be contrasted with the exchange splitting Δ of the magnetized d band which is

$$\Delta = IR + 2JR' \quad . \qquad (4.20)$$

Spin Wave Frequencies at finite q

One has

$$K(\underset{\sim}{q},\omega) = \frac{\chi^{o}(\underset{\sim}{q},\omega)}{1 - \left\{I + \frac{2J^2R'}{(JR-\omega)}\right\} \chi^{o}(\underset{\sim}{q},\omega)} \tag{4.21}$$

Therefore the poles occur when

$$1 = I_{eff}(\omega)\, \chi^{o}(\underset{\sim}{q},\omega) \tag{4.22}$$

$$1 = I_{eff}(\omega)\, \frac{1}{N} \sum_{\underset{\sim}{K}} \frac{n_{K\uparrow} - n_{K+q\downarrow}}{\left[\omega - (\varepsilon_{K+q} - \varepsilon_{K+q}) - IR - 2JR'\right]} \tag{4.23}$$

where

$$\Delta = IR + 2JR' \quad .$$

One expands the right hand side in powers of q, to obtain an expression near q = 0

$$1 = \frac{I_{eff}(\omega)}{(\omega - \Delta)} \frac{1}{N} \sum_{K} (n_{K\uparrow} - n_{K+q\downarrow}) \left\{1 - \frac{(\varepsilon_K - \varepsilon_{K+q})}{\omega - \Delta}\right\}^{-1}$$

$$= \frac{I_{eff}(\omega)}{(\omega - \Delta)} \frac{1}{N} \sum_{K} (n_{K\uparrow} - n_{K+q\downarrow})$$

$$+ \frac{I_{eff}(\omega)}{(\omega - \Delta)} \sum_{\underset{\sim}{K}} \frac{1}{2} \frac{(n_{K\uparrow} + n_{k\downarrow})(\underset{\sim}{q}.\nabla_k)^2\, \varepsilon(\underset{\sim}{k})}{(\omega - \Delta)}$$

$$- \frac{I_{eff}(\omega)}{(\omega - \Delta)} \sum_{\underset{\sim}{K}} \frac{(n_{k\uparrow} - n_{k+q\downarrow})(\underset{\sim}{q}.\nabla\varepsilon(k))^2}{(\omega - \Delta)^2} + O(q^4) \tag{4.24}$$

Multiplying through by $(\omega - \Delta)$, and using $\frac{1}{N}\sum_{\underset{\sim}{K}} (n_{K\uparrow} - n_{K+q\downarrow}) = R$, one can combine the L.H.S. with the first term on the R.H.S. to give

$$\omega(\omega_{op} - \omega) = I_{eff}(\omega)\,(JR - \omega)\Big\{\frac{1}{N}\sum_{\underset{\sim}{k}} \tfrac{1}{2}\,\frac{(n_{K\uparrow} + n_{K\downarrow})(\underset{\sim}{q}.\nabla_{\underset{\sim}{K}})^2\varepsilon(\underset{\sim}{k})}{(\omega - \Delta)}$$

$$- \sum_{\underset{\sim}{K}} \frac{(n_{K\uparrow} - n_{K+q\downarrow})}{(\omega - \Delta)^2}\;(\underset{\sim}{q}.\nabla\varepsilon(\underset{\sim}{k}))^2 + O(q^4)\Big\} \qquad (4.25)$$

and using $\varepsilon(\underset{\sim}{k}) = \varepsilon(-\underset{\sim}{k})$, and assuming cubic symmetry, one obtains

$$\omega(\omega_{op} - \omega) = \frac{1}{3}\,q^2(JR - \omega)\,\frac{1}{N}\sum_{\underset{\sim}{k}} \Big\{\tfrac{1}{2}\nabla_k^2\,\varepsilon_{\underset{\sim}{k}}\,\frac{(n_{k\uparrow} + n_{k\downarrow})}{(-1)(\omega - \Delta)}$$

$$- \frac{(n_{K\uparrow} - n_{K\downarrow})}{(\omega - \Delta)^2}\,(\nabla_{\underset{\sim}{K}}\,\varepsilon_K)^2\Big\} \qquad (4.26)$$

For the acoustic mode $\omega \cong 0$

$$\omega_{ac} = D_{ac}\,q^2 \qquad (4.27)$$

$$D_{ac} = \frac{1}{3}\,\frac{J}{\omega_{op}}\,\frac{1}{N}\sum_{\underset{\sim}{K}} \Big\{\tfrac{1}{2}\,\nabla_K^2\,\varepsilon_{\underset{\sim}{K}}(n_{K\uparrow} + n_{K\downarrow}) - (\nabla_{\underset{\sim}{K}}\,\varepsilon_{\underset{\sim}{K}})^2\,\frac{(n_{K\downarrow} - n_{K\uparrow})}{\Delta}\Big\} \qquad (4.28)$$

Damping due to Impurities (when the d band is Ferromagnetic or Paramagnetic)

In the form for $K(q,\omega)$, $\chi^o(\underset{\sim}{q},\omega)$ can be the susceptibility for exchange enhanced electrons with or without impurities. Further, when there is a magnetic field on there can be spin waves present above T_c.

If I is large enough, then the itinerant electrons are in the ferromagnetic state, and if there is impurity and spin orbit scattering[9], then from equation (A.44)

$$\chi_d^o(\underset{\sim}{q},\omega) = \frac{R}{\omega_o - IR - \mu H - 2JR' + \omega_L \frac{4}{3}\frac{i}{3\delta\ell_1} + B_1 q^2} \tag{4.29}$$

If $q = \gamma$ where γ is the skin depth, then this has the form

$$\chi_d^o(\underset{\sim}{q},\omega_o) = \frac{R}{\left\{\omega_o' - IR - 2JR' + \frac{i}{\tau_2}\right\}} \tag{4.30}$$

$$\frac{1}{\tau_2} = \omega_L \frac{4}{3}\frac{i}{3\delta\ell_1} + \mathrm{Im}B_1 \cdot \gamma^2 \tag{4.31}$$

where

$$\omega_o' = \omega_o - \mu H - \mathrm{Re}B_1\gamma^2$$

is the resonance frequency of the electron system. The poles of $K(q,\omega_o')$ are given by

$$1 = \left[I + \frac{2J^2R'}{(JR - \omega_o')}\right] \frac{R}{\left\{\omega_o' - IR - =JR' + \frac{i}{\tau_2}\right\}} \tag{4.32}$$

$$\therefore \quad 0 = \omega_o'(\omega_o' - 2JR' - JR + \frac{i}{\tau_2}) + JR\frac{i}{\tau_2}$$

$$\therefore \quad \omega_o' = \left[2JR' + JR + \frac{i}{\tau_2}\right] \pm \frac{\left\{(2JR' + JR + \frac{i}{\tau_2})^2 + 4.J^2R^2(\frac{1}{\tau_2})^2\right\}^{\frac{1}{2}}}{2} \tag{4.33}$$

One should remember that $\frac{1}{\tau_2}$ is $\alpha\ \omega_L = \mu H + 2JR'$.

In the case where $N(0)I \lesssim 1$, then the itinerant electrons are strongly paramagnetic.

$$\chi_d^o(\underset{\sim}{q},\omega) = \frac{(\Delta + i\gamma_1')}{(\omega - \Delta + i\gamma')} \tag{4.34}$$

From equation (A.34), where

$$\gamma' = \frac{4}{3\tau_1} + Dq^2\left(\frac{1-i\Gamma}{1+i\Gamma}\right) \qquad \Gamma = I\,\tau\,\Delta$$

$$\gamma_1' = N(0)\gamma' \qquad \text{and} \qquad q = \gamma$$

and in the paramagnetic region

$$\Delta = \frac{\omega_L}{1 - I} \qquad \omega_L = \mu_B H$$

$$\therefore\ \Delta = \omega_L + I\Delta\ . \tag{4.35}$$

The spin wave poles are again found from the expression

$$1 = \left(I + \frac{2J^2R'}{\{J\Delta - \omega'\}}\right) \frac{(-1)\{\Delta - i\gamma_1'\}}{\{\omega - \omega_L - I\Delta + i\gamma'\}} \tag{4.36}$$

$$\omega - \omega_L - I\Delta + i\gamma' = -I\Delta + i\gamma' I + \frac{2J^2R'}{(J\Delta - \omega')}(-\Delta + i\gamma_1')$$

$$\omega' = \omega - \mu H \qquad \omega_L = \mu H + 2JR'$$

$$\therefore\ \omega - \omega_L + i\gamma'(1 - I) = \frac{2J^2R'}{(J\Delta - \omega')}(-\Delta + i\gamma_1')$$

$$\therefore\ \omega'(\omega' - 2JR' - J\Delta) - i\gamma'(1 - I)) + i\gamma' J\Delta(1 - I)$$

$$= 2J^2R'\, i\gamma_1'$$

$$\omega'^2 - \omega'(2JR' - J\Delta - i\gamma'(1 - I)) + i\gamma'\{J\Delta(1 - I)\} = \{2J^2R'\}\gamma_1' \cdot \tag{4.37}$$

It may at first sight seem surprising that spin waves should exist above T_c. But when there is a magnetic field on, which splits the fermi surfaces for up and down spins, as long as I is finite there is an additional splitting due to the exchange interaction. The single particle excitations then start at $\omega_L + I\Delta$, whereas the resonance mode starts at ω_L.

One can see this in detail by looking at the one band susceptibility

(1) With a magnetic field:

$$\chi(\underset{\sim}{q},\omega) = \frac{\dfrac{-\Delta - i\gamma}{\omega' - \omega_L - I\Delta + i\gamma}}{1 - \dfrac{I(-\Delta + i\gamma)}{\omega' - \omega_L - I\Delta + i\gamma}} \tag{4.38}$$

$$= \frac{-\Delta + i\gamma}{\omega' - \omega_L + (1 - I)i\gamma} \tag{4.39}$$

The resonance then exists and starts at $\omega' = \omega_L$.

(2) No magnetic field:

Then ω_L and Δ are zero. $I \neq 0$, and

$$\chi(q,\omega) = \frac{i\gamma}{\{\omega' - \omega_L - (1 - I)i\gamma\}} \tag{4.40}$$

$$\text{Im } \chi(q,\omega) = \frac{i\gamma(\omega' - \omega_L)}{(\omega' - \omega_L)^2 + i\gamma^2} \tag{4.41}$$

which is not a resonance at all, and is zero for $\gamma = 0$.

In case (1) the resonance peak height is given by $\Delta(H)$ the magnetization, so the height of the resonance is much reduced from the ferromagnetic case, and is much broader because of the diffusion damping, which is however reduced by the (1 - I) factor as one approaches T_c from above.

Discussion of the Results of Damping Calculations

From equation (4.33) one can find the width of the resonance for the acoustic mode. In this case the mode has a frequency

$$\omega_o = \mu H \qquad \text{at} \quad q = 0 \ .$$

If $\frac{i}{\tau_2}$ is small, i.e. $\left|\frac{i}{\tau_2}\right| < 1$, then

$$\omega_o'^2 \ll \omega_o'$$

and

$$\omega_o' = \frac{JR \frac{i}{\tau_2}}{(2JR' + JR - \frac{i}{\tau_2})} \tag{4.42}$$

and

$$\Gamma = \frac{JR \frac{1}{\tau_2} (2JR' + JR)}{\left\{(2JR' + JR)^2 + \left(\frac{1}{\tau_2}\right)^2\right\}} \tag{4.43}$$

is the width of the acoustic mode. It may be noted that the condition $R \ll R'$ can not be used to simplify the calculation as $\frac{1}{\tau_2}$ is $\propto R'$. If $2JR' \gg \frac{1}{\tau_2}$ then

$$\Gamma = \frac{JR\,\frac{1}{\tau_2}}{(2JR' + JR)} \tag{4.44}$$

which, if $H \ll R'$ gives
$R \ll R'$

$$\Gamma = JR \cdot \frac{4}{3} \cdot \frac{1}{\delta \ell_1} + \left(\frac{JR\mu H}{2JR'} \cdot \frac{4}{3} \frac{1}{\delta \ell_1} \right) \tag{4.45}$$

where ℓ_1 is the spin orbit scattering length. In a pure ferromagnet without magnetic impurities JR is replaced by μH, and the last term is missing.

The case when the d band is nearly ferromagnetic can be worked out similarly.

CHAPTER 5

SPIN WAVES AND FERROMAGNETIC RESONANCE IN A TWO BAND MODEL OF A METAL

Two Band Calculation

If one considers a pure metal with two bands an s, and a d band say, one can carry out a calculation of the response along similar lines. One considers each band to have its own spin density, and each to have its own response function. Let us consider the spin waves to propagate in the d band. The s band can then be either paramagnetic or ferromagnetic.

One looks at the response of the d electrons, as the spin waves of the whole system appear as poles of this function.

One calculates the function

$$K(x - x', t - t') = - \theta(t-t')\langle[\hat{\sigma}_D^-(x,t), \hat{\sigma}_D^+(x',t')]\rangle \tag{5.1}$$

where

$$\hat{\sigma}_D(x) = \frac{1}{N_D} \sum_{\substack{\underset{\sim}{k} \\ \alpha}} \sum_{\substack{\underset{\sim}{q} \\ \beta}} \hat{C}^+_{d\ k+q\ \alpha}\ \hat{C}_{d\ \underset{\sim}{k}\ \beta}\ e^{i\underset{\sim}{q}\cdot\underset{\sim}{x}}\ \underset{\sim}{\sigma}_{\alpha\beta} \tag{5.2}$$

is the d band spin density operator.

Then, using the heisenberg equation of motion for the time dependence of an operator, one has

$$i\frac{\partial K'(t)}{\partial t} = \theta(t)\langle[[\hat{C}^{+}_{d\ \underset{\sim}{k}+\underset{\sim}{q}\downarrow}(t)\ \hat{C}_{k\uparrow}(t),\ \hat{H}_{d}],$$

$$\times\ \hat{C}^{+}_{d\ k'+q'\uparrow}(0)\ \hat{C}_{\underset{\sim}{k}'\downarrow}(0)] \qquad (5.3)$$

$$-\delta(t)\langle[\delta_{\underset{\sim}{k}+q,k'}\ \hat{C}^{+}_{d\ k'+q'\uparrow}\ C_{\underset{\sim}{k}\uparrow} - \delta_{k'+q',k}\hat{C}_{k+q\downarrow}\ C_{k\downarrow}]\rangle$$

(5.4)

where

$$K'(t) \equiv K'(k,k',qq') = \theta(t)\langle[\hat{C}^{+}_{d\ \underset{\sim}{k}+q\downarrow}(t)\ \hat{C}_{\underset{\sim}{k}\uparrow}(t),$$

$$\times\ C^{+}_{d\ K'+q'\uparrow}(0)\ C_{d\ k'\downarrow}(0)]\rangle$$

is an auxiliary function from which $K_1(q,\omega)$ can be calculated, this being the fourier transform of $K(x,t)$ (where the label $\mathcal{L}$ indicates that the fourier transform is a different function.) The Hamiltonian for the d band is taken as

$$H_D = \sum_{k\ \alpha} \varepsilon_{k\sigma}\ \hat{C}_{d\ \underset{\sim}{k}\sigma}\ C_{d\ \underset{\sim}{k}\sigma} + I_D \sum_{I} n^{d}_{I\uparrow}\ n^{d}_{I\downarrow} + J_{DS}\int d^3x\ \sigma_s(x).\sigma_d(x)$$

The contribution from the commutator is calculated in the random phase approximation, again picking out only spatially uniform commutators, and further replacing the operator σ^{z}_{s} by its thermal average. Then

$$\left(i\frac{\partial}{\partial t} - \{\varepsilon^{d}_{\underset{\sim}{k}+\underset{\sim}{q}} - \varepsilon^{d}_{\underset{\sim}{k}}\} - \frac{I_D}{N_D}\sum_{\underset{\sim}{k}''}(n_{k''\uparrow} - n_{\underset{\sim}{k}''\downarrow}) + 2J_{SD}\langle\sigma^{z}_{s}\rangle\right)K'(\underset{\sim}{k},\underset{\sim}{k}',\underset{\sim}{q}\underset{\sim}{q}'t)$$

$$= (n_{k\uparrow} - n_{k+q\downarrow})\left\{\delta(t) + \frac{I_D}{N_D}\sum_{K'} K(k'',k',q,q't)\right\}$$

$$+\ \theta(t)\frac{J_{SD}}{N_D}\sum_{K_1}\langle[C^{+}_{s\ \underset{\sim}{k}_1+q\downarrow}(t)\ \hat{C}_{s\ k_1\uparrow}(t),\ C^{+}_{d\ k'+q'\uparrow}C_{d\ k'\downarrow}(0)]\rangle$$

(5.5)

In order to express the time dependence of the correlation function involving the $C_s^+ C_s$ operators, one has to calculate its equation of motion within the r.p.a.

For the s band one uses the Hamiltonian

$$\hat{H}_s = \sum_{k\sigma} \hat{C}^{+s}_{k\sigma} \hat{C}^{s}_{k\sigma} \varepsilon^{s}_{ks} + J_{SD} \int d^3x \, \sigma_s(x) \cdot \sigma_d(x) \tag{5.6}$$

where one adds on the term $I_s \sum_I n^s_{I\uparrow} n^s_{I\downarrow}$ if one wants to consider the s band as magnetized. One obtains

$$\left(i \frac{\partial}{\partial t} - \{\varepsilon^s_{k_1+q} - \varepsilon^s_{k_1}\} - 2J_{SD}\langle\sigma^z_d\rangle\right) Y(k_1,q,t)$$

$$= \frac{J_{SD}}{N_s} \{n^s_{k_1+q\downarrow} - n^s_{k_1\uparrow}\} \sum_{k_2} K(k_2\ k'\ q\ q'\ t) \tag{5.7}$$

where

$$Y(k_1, k', q, q', t) = \theta(t)\langle[\hat{C}^+_{s\ k_1+q\downarrow}(t)\ \hat{C}_{s\ k_1\uparrow}(t)\ ,$$

$$\times\ \hat{C}^+_{d\ k'+q'\uparrow}\ \hat{C}_{d\ k'\downarrow}(0)]\rangle \tag{5.8}$$

In order to solve these coupled equations of motion, the fourier transform of Y and K' are introduced, Y_1 and K_1.

The above equation then becomes

$$\{\omega - (\varepsilon^s_{k_1+q} - \varepsilon^s_{k_1}) - 2J_{SD}\langle\sigma_d\rangle\}\ Y_1(k_1, k', q, q', \omega)$$

$$= \frac{J_{SD}}{N_s} \{n^s_{k_1+q\downarrow} - n^s_{k_1\uparrow}\} \sum_{k_2} K_1(k_2, k', q, q', \omega)$$

$$\therefore \sum_{\underset{\sim}{K}} Y_1(k_1, k, q, q', \omega) = J_{SD}\, \chi_o^s(\underset{\sim}{q},\omega) \sum_{k_2} K(\underset{\sim}{k}_2, \underset{\sim}{k}', q, q', \omega) \tag{5.9}$$

Further, the equation for $K_1'(k\ k'\ q, q', \omega)$ is

$$\left(\omega - \{\varepsilon^d_{k+q} - \varepsilon^d_k\} - I_D R_D + 2J_{SD} R_S\right) K_1(k, k', q, q', \omega)$$

$$= \{n^d_{k\uparrow} - n^d_{k+q\downarrow}\} + I_d\{n^d_{k\uparrow} - n^d_{k+q\downarrow}\} \sum_{k''} K_1'(k''\ k', q, q', \omega)$$

$$+ \chi_o^s(\underset{\sim}{q},\omega) \sum_{k_2} K_1(\underset{\sim}{k}_2, k', q, q', \omega)\, J_{SD} \tag{5.10}$$

where

$$R_d = \frac{1}{N_d} \sum_k (n^d_{k\uparrow} - n^d_{k\downarrow}) = \langle \sigma^z_d \rangle$$

$$R_s = \frac{1}{N_s} \sum_k (n^s_{k\uparrow} - n^s_{k\downarrow}) = \langle \sigma^z_s \rangle \tag{5.11}$$

Now

$$K_1(\underset{\sim}{q},\omega) = \frac{1}{N_D} \sum_{k\,k'} K_1(\underset{\sim}{k}, k', q, q', \omega) \tag{5.12}$$

$$\therefore K_1(\underset{\sim}{q},\omega) = \frac{\chi_o^d(\underset{\sim}{q},\omega)}{I - \chi_d^o(q,\omega)\{I + 2J_{sd}^2\, \chi_o^s(\underset{\sim}{q},\omega)\}} \tag{5.13}$$

where

$$\chi_o^d(\underset{\sim}{q},\omega) = \frac{1}{N_d} \sum_k \frac{n^d_{k\uparrow} - n^d_{k+q\downarrow}}{\{\omega - \{\varepsilon^d_k - \varepsilon^d_{k+q}\} - IR_d - 2J_{SD}R_S\}} \tag{5.14}$$

and

$$\chi_o^s(q,\omega) = \frac{1}{N_s}\sum_k \frac{n^s_{k\uparrow} - n^s_{k+q\downarrow}}{\{\omega - \{\epsilon^s_k - \epsilon^s_{k+q}\} - 2J_{SD}R_D\}} \qquad (5.15)$$

Spin Waves at q = 0

If an effective frequency dependent interaction

$$I'_{eff}(\omega) = I + J^2_{SD}\,\chi^s_o(q,\omega) \qquad (5.16)$$

is introduced, then $K_1(q,\omega)$ is seen to be analogous to that of a pure ferromagnetic metal.

For q = 0

$$\chi^o_s(q=0,\ \omega) = \frac{R_s}{(\omega - 2J_{sd}R_D)} \qquad (5.17)$$

and

$$\chi^o_d(q=0,\ \omega) = \frac{R_d}{(\omega - IR_d - 2J_{sd}R_s)} \qquad (5.18)$$

The spin wave frequencies are then given by the solutions to the equation

$$1 = \frac{-R_d}{\omega - IR_D - J_{SD}R_s}\left(I \mp J^2_{SD}\frac{R_s}{\omega - J_{SD}R_D}\right) \qquad (5.19)$$

$$\therefore\ \omega(\omega - JR - JR_d) = 0 \qquad (5.20)$$

$$\therefore \text{ at } q = 0 \qquad \omega_{ac} = 0$$

$$\omega_{op} = J(R_s + R_d) \tag{5.21}$$

At finite q the situation is more complicated than before because I_{eff} depends on q and ω.

For the calculation of the spin wave spectrum at finite q, one has to consider the eigenvalue equation

$$\mathcal{I} = (I + J^2 \chi_o^s(q,\omega) \chi_o^d(q,\omega) \tag{5.22}$$

$$= \sum_{\underset{\sim}{K}} \frac{n^d_{K\uparrow} - n^d_{K+q\downarrow}}{(\omega - IR_d - JR_s)} \left[I - \frac{(\varepsilon_K - \varepsilon_{K+q})}{(\omega - IR_D - JR_S)} \right]^{-1} \times \left[1 + j^2 \sum_{\underset{\sim}{K}} \frac{n^s_{K\uparrow} - n^s_{K+q\downarrow}}{(\omega - J_{sd}R_D)} \times \left(1 - \frac{(\varepsilon^s_K - \varepsilon^s_{K+q})}{(\omega - J_S R_D)} \right) \right] \tag{5.23}$$

$$\therefore I = \frac{R_d}{(\omega - IR_D - J_{sd}R_s)} \left(I + \frac{J^2 R_s}{(\omega - JR_d)} + \text{Terms } O(q^2) \right) \tag{5.24}$$

$$\therefore \omega(\omega - JR_s - JR_d) = J^2 \sum_K \left\{ \tfrac{1}{2} \nabla_K^2 \varepsilon^s_K \frac{(n^s_{K\uparrow} + n_{k\downarrow})}{(\omega - J_{SD}R_D)} - (\nabla_K \varepsilon^s_K) \frac{n^s_{K\uparrow} - n^s_{K\uparrow}}{(\omega - J_{SD}R_D)^2} \right.$$

$$+ \frac{1}{3q^2} I_{eff}(\omega, 0)(\omega - J_{SD}R_d) \sum_K \left(\tfrac{1}{2} \nabla_K^2 \varepsilon^d_K \frac{(n^d_K + n^d_K)}{(- IR_d - J_{sd}R_s)} - \right.$$

$$\left. \left. \frac{(\nabla_k \varepsilon^d_k)(n^d_{K\downarrow} - n^d_{K\uparrow})}{(\omega - IR_d - J_{sd}R_s)} \right) \right. \tag{5.25}$$

Therefore the acoustic mode has

$$\omega = D'_{ac}\, q \tag{5.26}$$

$$D'_{ac} = \frac{J^2}{J(R_S + R_D)} \sum_K \left(\tfrac{1}{2} \nabla_K^2 \varepsilon_K^s \frac{(n^s_{K\uparrow} + n^s_{K\downarrow})}{(\omega - J_{SD}R_D)} - (\nabla_K \varepsilon_K^s)^2 \frac{n^s_{K\downarrow} - n^s_{K\uparrow}}{(\omega - J_{SD}R_D)^2} \right)$$

$$+ \frac{(I\, JR_d + J^2 R_s)}{J(R_s + R_D)} \left(\sum_K \tfrac{1}{2} \nabla_K^2 \varepsilon_K^d \frac{(n^d_{K\uparrow} + n^d_{K\downarrow})}{(\omega - IR_d - J_{SD}R_S)} - \right.$$

$$\left. \times \frac{\nabla_K \varepsilon_K^d (n^d_{K\downarrow} - n^d_{K\uparrow})}{(\omega - IR_d - J_{sd}R_s)} \right) \tag{5.27}$$

ω''_{op}

The optical mode does not contribute to the microwave absorption, so will not concern us here.

Damping Effects in the Two Band Model

Here the d band is ferromagnetic and the s band is either paramagnetic or ferromagnetic, depending on whether there is exchange enhancement present in the s band.

(i) s band paramagnetic:

Spin wave poles derived from

$$1 = \left(I + J^2 \frac{(-R_s + i\gamma_1)}{(\omega - \mu H - JR_d + i\gamma)} \right) \frac{-R_d}{(\omega - \mu H - JR_s - IR_D)} \tag{5.28}$$

$$\omega^2 - \omega(J(R_s + R_d) - i\gamma) - J^2 R_s i\gamma_1 + J^2 i\gamma_1 R_d = 0 \quad (5.29)$$

$$\omega = J(R_s + R_d - i\gamma) \pm \left[(J(R_s + R_d) - i\gamma)^2 - 4(J^2((R_s + R_d)i\gamma_1)^2\right]^{\frac{1}{2}} \quad (5.30)$$

(ii) s band ferromagnetic:

The spin wave poles are derived from

$$\mathcal{L} = \left(I + \frac{J^2 R_s}{\{\omega - \mu H - JR_d - I_s R_s + \frac{i}{\tau_s}\}}\right) \frac{R_d}{\{\omega - \mu H - JR_s - IR_d + \frac{i}{\tau_d}\}} \quad (5.31)$$

$$\therefore \quad \omega' = \{J(R_s + R_d) + I_s R_s\} \pm \{(J(R_s + R_d) + I_s R_s\} + J^2 R_s \left(\frac{i}{\tau_s}\right)^2\}^{\frac{1}{2}} \quad (5.32)$$

where $\omega' = \omega - \mu H$, and where one has assumed that there is no damping due to impurity scattering in the d band. $\left(i.e.\ 1/\tau_d = 0\right)$

The interesting case is case (i), because one can consider the so-called bottleneck effect. This is roughly an idea which is claimed to explain the small resonance width in metals. The resonating spins are taken to be in the d band. No dissipating mechanism is said to exist for these spins, but as they are coupled to the s spins, damping of the s spins causes damping of the d spins. Further, if $\frac{1}{\tau_s}$ is the damping rate for s spins, the damping rate for the d spins is said to be $\frac{R_s}{R_d}\frac{1}{\tau_s}$ and since in the case where the s band is paramagnetic and the d band is ferromagnetic $R_d \gg R_s$, this damping is small, and hence the ferromagnetic resonance width is small.

In the above calculation $\frac{1}{\tau_s} \equiv \gamma$. In such a theory, however, $\frac{1}{\tau_s}$ is postulated and no expression is given for it. This analysis stands or falls on the form of $\chi_s(\omega)$. The form we use is

$$\chi_s(\omega) = \frac{(-R_s + i\gamma N(0))}{(\omega - \mu H - JR_d + i\gamma)} \qquad (5.32)$$

which as can be seen leads to a width

$$\propto \frac{J^3 \gamma (R_s + R_d)^2 N(0)}{\{J^2(R_s + R_d)^2 + \gamma^2\}}$$

$$\text{i.e. } \propto J\gamma N(0) \qquad (5.33)$$

The form usually taken is

$$\chi_s(\omega) = \frac{-R_s}{\{\omega - \mu H - JR_d + i\gamma\}} \qquad (5.34)$$

The width is

$$\propto \frac{J^2 R_s \gamma J(R_d)}{J^2 R_d^2} \qquad R_d \gg R_s$$

$$\propto \frac{J R_s}{R_d} \gamma \quad . \qquad (5.35)$$

Therefore, the important question that has to be answered is what is the correct form of $\chi_s(\omega)$ that has to be taken. In Appendix A, equation 33, and preceeding equations, it is shown that the first form should be taken as the correct form. For the case $q = 0$, $\gamma = \frac{4}{3}\frac{1}{\tau_{s.o}}$,

where $\tau_{s.o}$ is the spin orbit scattering time. For $q \neq 0$, $\chi_s(\underset{\sim}{q},\omega)$ has the same form providing that one takes q as equal to the skin depth.

CHAPTER 6

FERROMAGNETIC RESONANCE IN ALLOYS, USING THE HEISENBERG HAMILTONIAN FOR A FERROMAGNETIC ALLOY

The Heisenberg Hamiltonian can be adapted for use in alloys where some sites have magnetic moments and some do not. For instance, in FeCu, the iron atoms have moments and the copper atoms are assumed to carry no moment. The alloy is assumed to be a random one in the sense that one can replace the alloy by an ensemble of alloys all with the same concentration but with all possible distributions (in position) of the moment bearing sites. This is reasonable because the alloy itself can be considered to be made up of a large number of regions each still exhibiting macroscopic properties, but with different distributions of the moment bearing sites. One then carries out the dynamical calculation for one system and averages over all possible distributions following the methods of statistical mechanics.

The Hamiltonian for the alloy is then taken as

$$\hat{H} = -\mu H \sum_I \hat{S}_I^z c_i - \frac{1}{2} \sum_I \sum_J V(I-J)\, c_i \hat{S}_{i\sim i} \cdot c_j \hat{S}_{j\sim j} \qquad (6.1)$$

$\hat{S}_I$ is the spin operator on site I and is a vector operator;

I is the index label of the site, and for a three dimensional alloy I represents an ordered triplet (i_1, i_2, i_3)

$i_1, i_2, i_3 \in N$, where N is the set of integers;

H is the magnetic field applied to the system;

V(I-J) is the exchange interaction between sites I and J.

Equation (6.1) can be rewritten in the form

$$\hat{H} = -\mu H \sum_I \hat{S}_I c_i - \tfrac{1}{2} \sum_I \sum_{J \atop (I \neq J)} V(I-J)\,(c_i \hat{\underline{S}}_I - \langle c_i \hat{\underline{S}}_i \rangle)\cdot(\hat{\underline{S}}_j c_j - \langle c_j \hat{\underline{S}}_j \rangle) \tag{6.2}$$

$$+ \tfrac{1}{2} \sum_i \sum_j V(I-J) \langle c_i \hat{\underline{S}}_i \rangle \langle c_j \hat{\underline{S}}_j \rangle - \sum_i \sum_j V(I-J)\, c_i \underline{S}_i \langle c_j \underline{S}_j \rangle \quad .$$

Then one can write

$$\hat{H} = \hat{H}_o + \hat{H}_1 \tag{6.3}$$

where

$$\hat{H}_o = -\mu H \sum_I \hat{S}_i^z c_i - \sum_I \sum_J V(I-J)\, c_i \hat{S}_i^z \langle c_j S_j \rangle$$

$$+ \tfrac{1}{2} \sum_I \sum_J V(I-J) \langle c_i S_i \rangle \langle c_j S_j \rangle \quad . \tag{6.4}$$

$\langle c_i \hat{S}_i \rangle$ is independent of i and is equal to $c\langle S_i \rangle$.

This is the molecular field approximation to the Heisenberg Hamiltonian, $\hat{H}_1$ is treated by perturbation theory which one hopes converges. Usually such a perturbation expansion is an asymptotic series, but is divergent when all terms are considered. However, divergent series are sometimes amenable to certain summation techniques. These can be rigorous, e.g. Padé approximant techniques, but in solid state physics more intuitive methods are used, and hence these steps represent additional assumptions.

For the molecular field approximation one can derive the transition temperature of the alloy as follows. The free energy is

$$F^{(0)} = - \text{In Tr } e^{-\beta \hat{H}_o}$$

$$= - \text{In Tr EXP}\{- \beta\mu H \sum_I c_i \hat{S}_i^z - \sum_i \sum_j V(i-j)\, c_i \hat{S}_i \langle c_j \hat{S}_j \rangle$$

$$+ \tfrac{1}{2} \sum_i \sum_j V(I-j) \langle S_i \rangle \langle S_j \rangle c^2 \quad . \qquad (6.5)$$

Averaging over the c_i's

$$\langle F^o \rangle_{\text{alloy}} \equiv - \text{In Tr EXP}\{- \beta\mu Hc \sum_I S_i^z - \sum_I V(0)\, c^2 \langle S \rangle \hat{S}_i$$

$$- c^2 \beta \frac{V(0)}{2} \langle S \rangle^2\} \qquad (6.6)$$

Therefore

$$\langle F^o \rangle \equiv \frac{(y - \beta\mu H)^2}{2\beta V_o} - c \text{ In } \frac{\sinh(S+\frac{1}{2})y}{\sinh \frac{y}{2}} \qquad (6.7)$$

where

$$y = \beta(c\, V(0) \langle S \rangle + \mu H) \qquad (6.8)$$

Therefore

$$\langle F^o \rangle \equiv c\left\{\left[\frac{(y - \beta\mu H)^2}{2\beta c V_o}\right] - \text{In } \frac{\sinh(S+\frac{1}{2})y}{\sinh \frac{y}{2}}\right. \qquad (6.9)$$

where

$$y = \beta\{c\, V_o \langle S \rangle + \mu H\} \quad . \qquad (6.10)$$

The equilibrium state is given by

$$\frac{\partial \langle F^o \rangle}{\partial y} = 0 \quad .$$

Therefore

$$\langle S \rangle = \frac{(y - \beta\mu H)}{\beta c V_o} = b(y) \qquad (6.11)$$

$$b(y) = Tr \frac{\hat{S}_z \exp \hat{S}_z y}{Tr \exp \hat{S}_z y} = S\, B_s(S_y) \qquad (6.12)$$

$$= (S+\tfrac{1}{2}) \operatorname{Coth}(S+\tfrac{1}{2})y - \tfrac{1}{2} \operatorname{Coth} \frac{y}{2} \ . \qquad (6.13)$$

This is similar to the case where all sites are occupied except that V_o is replaced by cV_o. Therefore

$$T_c = cV_o \frac{S(S+1)}{3} \ . \qquad (6.14)$$

This model does not yield a critical concentration. This is to be expected as a critical concentration is due to the fall off of V(r) with distance, and yet in this simple molecular model the interaction is taken as a constant, which is reasonable only for small separations.

To proceed further to calculate the simplest changes in the spin wave spectrum one has to use either an equation of motion method or a diagram method. Both methods are complicated by the need to average over the sites, but a diagram method is to be preferred, as there is some hope of proving convergence and estimating the range of its validity, and furthermore it does possess a systematic way of calculating damping effects.

The decoupling procedure yields at best doubtful results and is probably useless for the calculation of damping as there are too many ways of decoupling the equations.

We use a form of the diagram technique due to Larkin et al[13,14] modified to take in the simplest corrections due to impurities.

Associating a factor c_r with each site spin $\hat{S}_r$, the analysis proceeds as in their paper.

The spin hamiltonian of the Heisenberg model is transformed to the usual fermion form. The operators $\hat{a}^+_{r\lambda}$ and $a_{r\lambda}$ represent the creation and annihilation of a particle in a state with co-ordinate r and a spin projection λ, and taking into account the fact that one, and only one, such particle is always on each site r, i.e. each spin is in a definite state with a definite z component. Then the hamiltonian becomes

$$\hat{H} = - \sum_{\substack{r \\ \lambda\lambda'}} \mu H \, c_r \, \hat{a}^+_{r\lambda} \, S_{\lambda\lambda'} \, a_{r\lambda'} - \tfrac{1}{2} \sum_{\substack{rr' \\ \lambda\lambda' \\ \nu\nu'}} V(r-r') \, c_r \, c_{r'}$$

$$(a^+_{r'\nu} \, S_{\nu\nu'} \, a_{r'\nu'})(a^+_{r\lambda} \, S_{\lambda\lambda'} \, a_{r\lambda'}) + g \sum_r c_r \Big(\sum_\lambda a^+_{r\lambda} \, a_{r\lambda} - 1\Big)^2 \qquad (6.15)$$

where $g \to \infty$ in the answer, and therefore since the hamiltonian is infinite unless the last term is zero, the states for which the number of particles in one site differs from unity make no contribution to the statistical properties of the system as the energy of such states would be infinite.

Then one can apply the usual perturbation theory to the above Hamiltonian. There are in effect two interaction terms and so each diagram is proportional to certain powers of g and V. Since g is to tend to infinite, one collects for each power of V all orders in g. It is important that the last term in the equation (6.15) is of the form of the interaction of particles located in a single unit cell. Therefore each connected diagram can be represented in the form of single cell diagrams connected by lines of interaction V(r-r'). Further, it follows that each block has one factor c_r associated with

it since $c_r^n = c_r$ where $(c_r = 0,1)$. Each line of interaction connects vertices of different blocks either $\hat{S}^z$ with $\hat{S}^z$, or $\hat{S}^+$ with $\hat{S}^-$. Since $g \to \infty$, in calculating a single cell block the problem reduces to the calculation of the statistical average of the T product of a certain number of single particle spin operators of the form $\hat{S}^\alpha(t) = e^{\hat{H}_o t} S^\alpha e^{-H_o t}$, and where one uses the interaction representation in the usual way. In the simplest approach $y = \beta(cV_o\langle S^z\rangle + \mu H)$, where c is the concentration. The unperturbed hamiltonian is the molecular field hamiltonian.

One uses the temperature form of the perturbation theory where one considers the time as a complex variable and calculates the correlation functions along the imaginary time axis from 0 to $i\beta$. All correlation functions are periodic with this period along this line. When one calculates the T products, the denominator $\mathrm{Tr}\, e^{-\beta\hat{H}_o}$ cancels out the disconnected diagrams, and therefore these diagrams have to be subtracted from the full T product of a string of spin operators.

The fourier component of a single cell block with n outgoing lines of interaction V is given by the expression

$$\Gamma^{\alpha_1 \cdots \alpha_n}(\omega_1 \cdots \omega_n) = \frac{k^n}{\beta^n} \int_0^\beta \prod_{j=1}^n dtj\, e^{i\omega tj} \langle \hat{T} \prod_{j=1}^n \hat{S}^\alpha(t_j)\rangle$$

$$- \sum_{m_1+m_2+\cdots m_k=n} [\Gamma^{\alpha_1 \cdots}_{m_1} \Gamma_{m_2} \cdots \Gamma^{\alpha}_{m_k}] \quad , \quad (6.16)$$

where $\hat{T}$ is the time ordering symbol, and $i\omega_m = 2\pi imT$ are the fourier frequencies used to expand the periodic calculation functions.

The graphical rules for calculating the blocks given below are based on the use of transposition relations among the spin operators (see Appendix G where some examples are given with their diagramatic representation).

The block Γ^n is represented by the aggregate of all diagrams with m vertices $\hat{S}^+$ and m vertices $\hat{S}^-$, and n-2m vertices $\hat{S}^z$. (This circumstance is due to the fact that $\underset{\sim}{S}.\underset{\sim}{S} = \frac{1}{2}(\hat{S}^+\hat{S}^- + \hat{S}^-\hat{S}^+) + \hat{S}_z\hat{S}_z$). Each $\hat{S}^+$ vertex has one outgoing line, each $\hat{S}^-$ vertex either one incoming line or two incoming and one outgoing line. Each S^z vertex has either one incoming or one outgoing line or no line at all. To each line there corresponds a Green's function

$$G(\omega_n) = \frac{¶}{y - i\beta\omega_n} .$$

The law of conservation of energy is fulfilled at each vertex. The sum of the incoming frequencies is equal to the sum of the outgoing frequencies. If the diagram splits into N singly connected diagrams, the total number of triple $\hat{S}^-$ vertices and $\hat{S}^z$ vertices on the continuous lines being ℓ, then the common factor of this diagram is $(-1)^\ell\, b^{N-1}$ where $b^{N-1}(y) = \frac{\partial}{\partial y^{N-1}} b(y)$.

The temperature correlation functions of the spins are defined as

$$K_{\alpha\gamma}(\underset{\sim}{k}, i\omega_n) = \frac{1}{2\beta}\int_{-\beta}^{+\beta} e^{i\omega_n t}\, dt \sum_{r_1} e^{i\underset{\sim}{k}.(r_1 - r_2)} \langle \hat{T}(c_{r_1} S^{\alpha}_{r_1}(t) - \langle S^{\alpha}\rangle)$$

$$(c_{r_2} \hat{S}^{\gamma}_{r_2}(0) - \langle S^{\gamma}\rangle)\rangle \qquad (6.17)$$

This function is represented by the aggregate of all singly connected diagrams with two vertices. (For an alloy this is an approximation.)

Denote by $\sum_{\alpha\gamma}(\underset{\sim}{k}, i\omega_n)$ the aggregate of all irreducible diagrams. Then the correlation functions can be written in the form

$$K_{zz}(\underset{\sim}{k}, i\omega_n) = \frac{\sum_{zz}(\underset{\sim}{k}, i\omega_n)}{1 - \beta V_K \sum(\underset{\sim}{k}, i\omega_n)} \tag{6.18}$$

$$K_{+-}(\underset{\sim}{k}, i\omega_n) = \frac{\sum_{+-}(\underset{\sim}{k}, i\omega_n)}{1 - \beta V(k) \sum(\underset{\sim}{k}, i\omega_n)} \quad . \tag{6.19}$$

For the case of a large radius of interaction and for low or high temperatures it is sufficient to restrict oneself to the simplest diagrams, i.e. Γ_2^{zz} and Γ_2^{+-}. In the alloy case, each vertex in the strong generating K_{zz} or K_{+-} has a c_γ attached to it. The random average is taken over all c_γ's but we keep only the term which is the product of the averages at each site. Therefore

$$K_{zz}(\underset{\sim}{k}, i\omega_n) = \delta_{no} \frac{b'}{1 - \beta V(\underset{\sim}{k}) b'} \tag{6.20}$$

$$K_{+-}(\underset{\sim}{k}, i\omega_n) = \frac{cb\, G(\omega_n)}{1 - \beta V_R\, cb\, G(\omega_n)} = \frac{(cb)}{(y - c\beta V_K b - i\beta\omega_n)} \tag{6.21}$$

This is the simplest approximation one can make. We will discuss improved approximations later.

Note that

$$b' = c\langle S_z^2\rangle - c^2 \langle S_z\rangle^2 \neq \frac{\partial}{\partial y} b(y) \tag{6.22}$$

and

$$y = \beta\{c\, V_o \langle S_z\rangle + \mu H\} \quad .$$

The excitation spectrum (collective modes) is determined by the poles

of the analytic continuation of $K_{+-}(\underset{\sim}{k}, i\omega_n)$ from the points $i\omega_n$ to the whole complex plane. The function $K_{+-}(\underset{\sim}{k}, \underset{\sim}{z})$ has a cut along the real axis, and the fourier transform of the retarded commutator (response function) is given by the boundary value $K_{+-}(\underset{\sim}{k}, \omega+i\varepsilon)$. A pole on the real axis represents an undamped spin wave, and if there is a pole in the analytic continuation of $K_{+-}(k, \omega+i\varepsilon)$ onto the second sheet and if this pole is not too far from the real axis then for intermediate times there is a damped spin wave.

In the above approximation, the pole occurs at

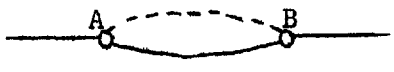
$$\omega = \varepsilon_{\underset{\sim}{K}} = c\, b(y)\, (V_o - V_k) + \mu H \quad . \tag{6.23}$$

Then if $V(k)$ has a Taylor series expanstion at $k = 0$

$$\omega = \varepsilon_K \cong c\, b(y)\, \{k^2\}\, V''(0) + \mu H \quad . \tag{6.24}$$

If $b(y) = \langle S_z \rangle$, then $\omega_{\underset{\sim}{k}}$ has an exponential temperature dependence at low temperatures where experiment indicates a power law. Further, we are interested in spin wave damping and one therefore has to take into account more diagrams which contribute to $\sum^{+-}$.

The diagram which contributes to spin wave damping is of the form



where A and B are vertex blocks $\langle S^+ S^- S^z \rangle$ and the line - - - - - represents a renormalized interaction

$$V^{zz}(\underset{\sim}{k}, i\omega_n) = \frac{\delta_{no}\, V(\underset{\sim}{k})}{\{1 - \beta V(k)\, b'\}} \tag{6.25}$$

and the solid line represents a spin wave propagator

$$V^{+-}(\underset{\sim}{k}, i\omega_n) = \frac{V(\underset{\sim}{k})}{1 - \beta V(\underset{\sim}{k})\ cb\ G_n(y)} \tag{6.26}$$

This diagram represents the expression

$$b(y)\ G_n^2(y)\ \beta\ b' \sum_{\underset{\sim}{q}} \frac{(V_{\underset{\sim}{q}-\underset{\sim}{k}} - V_{\underset{\sim}{q}})^2}{(\epsilon_{\underset{\sim}{q}} - i\omega_n)(1 - \beta\ V_{\underset{\sim}{k}-\underset{\sim}{q}}\ b')} \tag{6.27}$$

and gives a damping contribution

$$\pi\ b'\ \beta \sum_{\underset{\sim}{q}} \frac{(V_{\underset{\sim}{q}-\underset{\sim}{k}} - V_{\underset{\sim}{q}})^2}{(1 - \beta V_{\underset{\sim}{q}-\underset{\sim}{k}}\ b')}\ \delta(\epsilon_{\underset{\sim}{q}} - \omega)\ . \tag{6.28}$$

This damping represents scattering by fluctuations in $\langle S_z \rangle$ of the spin waves. At low temperatures b' is very small, and decreases to zero at $T = 0$ exponentially. In an alloy fluctuations in S_z occur as both temperature fluctuations and concentration fluctuations. The concentration fluctuations do not disappear at $T = 0$ and hence this form of damping can still be important in an alloy at low temperatures. Of course, near T_c this damping is very large, and one would similarly expect it to be very large near the critical concentration. Unfortunately, molecular field theory does not give a critical concentration and one can not therefore calculate the damping near to the critical concentration. The above expression would yield the damping only for concentrations where molecular field theory gives an adequate description of the magnetization.

However, assuming that this theory combined with a theory of a molecular field variety which yield a critical concentration would be correct, from experiment one can estimate the form of $K_{zz}(\underset{\sim}{k}, i\omega_n)$.

The function $K_{zz}(\underset{\sim}{r})$ varies exponentially with distance near to the critical concentration. If $K_{zz}(\underset{\sim}{r})$ goes as $e^{-\lambda r}$ then $V(\underset{\sim}{k})$ would seem to vary as k^2 and b' for the alloy would numerically be equal to $\frac{1}{\lambda}$, i.e. as b' becomes large λ would become small and the long range order would disappear. Assuming long wavelength spin waves still propagated with $b(y) = \langle S_z \rangle$ for the alloy, one would expect the damping to still be given by equation (6.28). This allows an estimation of the expected ferromagnetic resonance width from the neutron scattering experiments.

The damping integral involves replacing q by $\left(\frac{\omega-\mu H}{bV_o}\right)^{\frac{1}{2}}$ which is small in the case where one is interested in spin wave damping. Therefore $V_{\underset{\sim}{k}-\underset{\sim}{q}} - V_{\underset{\sim}{q}}$ can be expanded out as a Taylor's series keeping only terms up to q^2. Then

$$\Gamma(\underset{\sim}{k},\omega) = \frac{3\sqrt{6}}{2\pi r_o^2} \int_{-1}^{+1} \frac{b' V_o}{b(1 - \beta V_o b')} \left(\frac{\omega-\mu H}{bV_o}\right)^{\frac{1}{2}} \frac{k^4}{4}$$

$$\times \frac{(1 - 2\sqrt{t}y + 4ty^2)}{1 + x(1 + t + 2\sqrt{t}y)} \, dy \qquad (6.29)$$

where

$$y = \cos\theta \qquad x = \frac{\beta V_o b'}{1 - \beta V_o b'} \frac{k^2}{2} \qquad t = \frac{2(\omega-\mu H)}{k^2 b V_o}$$

Then

$$\Gamma(\underset{\sim}{k},\omega) = \frac{3\sqrt{6}}{2\pi r_o^3} \frac{b' V_o}{b(1 - \beta V_o b')} \left(\frac{\omega-\mu H}{bV_o}\right)^{\frac{1}{2}} \frac{k^4}{4}$$

$$\times f\left(\frac{\beta V_o b'}{1 - \beta V_o b'} \frac{k^2}{2} \, , \, \frac{2(\omega-\mu H)}{k^2 b V_o}\right) \qquad (6.30)$$

$$f(x,t) = \frac{(1 + xt)^2}{4 + 3\sqrt{t}} \ln\left[\frac{1 + x(1 + \sqrt{t})^2}{1 + x(1 - \sqrt{t})}\right] - \frac{1 + x(t + 1)}{x^2} \tag{6.31}$$

and

$$\lim_{x \to 0} f(x,t) = 1 + \frac{4}{3} t \quad . \tag{6.32}$$

The spin wave width is given by $\Gamma(k, \omega(k))$ where

$$\omega(k) = \mu H + cb\, V_o\, k^2$$

is the spin wave frequency for wave vector k.

This means that t = 1, and

$$b = c\langle S_z \rangle \qquad \text{and} \qquad b' = c\langle S_z^2 \rangle - c^2 \langle S_z \rangle^2 \quad .$$

Then for small k and temperatures which are not low, the spin wave damping is given by

$$\Gamma(k) = \left(\frac{3\sqrt{6}}{2\pi r_o^{\,3}}\right) \frac{\{c\langle S_z \rangle^2 - c^2 \langle S_z \rangle^2\}}{c\langle S_z \rangle (\{c\langle S_z \rangle^2 - c\langle S_z \rangle^2\}\beta - 1)} \frac{k^5}{4} \cdot \frac{7}{3} \tag{6.33}$$

For low temperatures $\langle S_z \rangle = S$ and one takes $V_{zz}(k) = V(k)$

$$\Gamma(k) = \left(\frac{3\sqrt{6}}{2\pi r_o^{\,3}}\right) \frac{7}{12} (1 - c)\, S \times k^5 \quad . \tag{6.34}$$

This is for a simple model of an alloy where c is near to one, and not near to the critical concentration. The expression for a general temperature is given in the simplest molecular field approximation by equation (6.33) where $\langle S_z \rangle$ is evaluated for the alloy.

In the molecular field model, however detailed a calculation one carries out, a critical concentration does not appear at zero temperature. However, as T_c is reduced by decreasing the concentration from c = 1, one can see that if the temperature is kept fixed then as the concentration is decreased the model predicts a change from the magnetic to the non-magnetic state at a certain concentration, at least for a certain range of temperatures. The absence of a critical concentration at T = 0 does not seem to be a consequence of the molecular field approximation but seems inevitable in the Heisenberg model unless V(r) has a finite range. The fact is that the $e^{-\beta H}$ factor means that at T = 0, as long as the spins feel the effect of V(r) from each other, the energy can be lowered by the spins aligning parallel to each other. While experimentally there is a critical concentration at fixed temperature, one could not confirm experimentally whether there was a critical concentration at zero temperature anyway. It may be noted at this point that the itinerant model seems more satisfactory in this respect. In this theory even at zero temperature I has to be greater than a certain value if the magnetic state is to occur. This is because there is both kinetic energy and potential energy in the problem. In the Heisenberg model there is no equivalent rise in kinetic energy at T = 0 if the spins are aligned parallel.

This work was embarked upon in order to consider ferromagnetic resonance in alloys. Neutron scattering experiments in FeCu alloys[19] indicate that the $\langle S_z^{(r)} S_z^{(0)} \rangle$ correlation function has the form $e^{-\lambda r}$ where $\lambda \equiv \lambda(\beta, c)$. Now in such systems one would expect the scattering of spin waves from the $\hat{S}_z$ fluctuations to be large and to contribute the main part of the ferromagnetic resonance linewidth. We will try to estimate this linewidth by using the previous theory as a phenomenological guide.

The correlation function $K_{zz}(\underset{\sim}{k},\omega)$ has the general form

$$\frac{b'\,\delta(\omega)}{\{1 - b'\,\beta V(k)\}} \quad . \tag{6.35}$$

The neutron experiments indicate a space form $K_{zz}(\underset{\sim}{r}) = e^{-\lambda r}$ const. We consider the temperature as fixed.

For low k one takes $K_{zz}(\underset{\sim}{r})$ as

$$\frac{\delta(\omega)\, b'}{1 - b'\beta_o \{V(0) + k^2\, V''(0)\}} \tag{6.36}$$

$$= \frac{\delta(\omega)\, b'}{\{1 - b'\beta_o\, V(0)\} + k^2\, V''(0)}$$

$$= \frac{\delta(\omega)}{\left\{\frac{1}{b'V''(0)} - \frac{\beta_o\, V(0)}{V''(0)}\right\} + k^2} \quad . \tag{6.37}$$

From this one can identify λ^2 as

$$= \left\{\frac{1}{b'\, V''(0)} - \frac{\beta_o\, V(0)}{V''(0)}\right\} \quad . \tag{6.38}$$

$K_{zz}(\underset{\sim}{k},\omega)$ then has the form

$$K_{zz}(\underset{\sim}{k},\omega) = \frac{\delta(\omega)}{(\lambda^2 + k^2)} \quad . \tag{6.39}$$

From this one can calculate $S_{zz}(\underset{\sim}{k},\omega)$ which is the function that occurs in the scattering cross-section for neutrons, by using the fluctuation dissipation theorem.

The neutron scattering experiments determine λ, and using these values of λ one can calculate the ferromagnetic resonance linewidth in such alloys. λ contains the concentration and temperature dependence.

The resonance width is given in terms of λ by

$$\Gamma(\underset{\sim}{k}) = \frac{3\sqrt{6}}{2\pi r_o^3} \cdot \frac{1}{\langle S_z \rangle} \cdot \frac{\frac{1}{\lambda(\beta,c)}}{1 - \beta V_o \frac{1}{\lambda(\beta,c)}} \frac{k^5}{4} \cdot \frac{7}{3}$$

$$= \frac{3\sqrt{6}}{2\pi r_o^3} \cdot \frac{1}{\langle S_z \rangle} \frac{1}{\{\lambda(\beta,c) - \beta V(0)\}} \cdot \frac{k^5}{4} \cdot \frac{7}{3} \qquad (6.40)$$

SUMMARY AND CONCLUSION

In this conclusion the main results of this thesis are discussed and possible applications and extensions of the work are pointed out.

In chapter one a brief discussion of the macroscopic theory is presented, so as to give a framework for the physical interpretation of the microscopic theory. It is pointed out that the macroscopic theory is sufficient to the task of calculating the resonance frequency, which is strongly modified by demagnetizing fields. This effect is due to the dipole-dipole interaction. The macroscopic theory however can not treat the linewidth problem, because damping processes are microscopic effects.

In chapter two a discussion of the skin effect in metals is given, and three approximate methods for the solution of this problem are presented. Each method allows a calculation of the ferromagnetic resonance linewidth to be made, starting from the spin wave width. The third method is in the context of the correlation function approach to the measurement of absorption. A detailed discussion of the difference between "spin wave resonance", where damping is due to eddy currents in the metal surface layers, and "ordinary spin wave resonance" where the spin waves excited are not coupled to the electromagnetic field, and damping is then due to the scattering of these spin waves. A simple criterion is stated which predicts when one should expect each kind to occur in metals.

In chapters four and five spin wave damping rates are derived for two models of magnetic systems. The damping mechanism treated is scattering of the spin waves (i.e. of the electrons which make up the coherent electron hole pair which is a spin wave) by impurities, via both a spin orbit interaction and an ordinary potential interaction. Both models are composed of two spin systems. Model (a) (chapter four) is a model of a dilute alloy in which magnetic impurities are present in a metal represented by a narrow d band of electrons. Model (b) (chapter five) is a two band

model (s and d bands) of a pure metal. The scattering off impurities is then taken to occur in the s band in (b), and in the d band in (a). The spin waves propagate in the d band in both cases but are coupled to the other spin system in each case by the exchange interaction, and expressions are derived for the spin wave lifetimes in both models. Within the framework of model (b) one can discuss the bottleneck effect for this system. This is said to occur in the case where the s band is paramagnetic, magnetization $\underline{M}_s$, and the d band is ferromagnetic, magnetization $\underline{M}_d$. Then if one introduces a damping mechanism in the s band with a lifetime τ_s, then the damping rate in the d band is claimed to be $\tau_d = \left(|\underline{M}_d| \times (|\underline{M}_s|)^{-1} \right) \tau_s$, and since $M_d >> M_s$, the decay of the d band magnetization can be much slower than that of the s band. In this theory a phenomenological form of the s band susceptibility is used. Within the framework of the theory in this thesis, if one takes the calculated form of the s band susceptibility function then the spin wave lifetime is not proportional to $\underline{M}_d \times (\underline{M}_s)^{-1}$. This result is claimed to be valid only for damping due to impurity scattering, and the question is left open for other mechanisms. There is probably a need for a further investigation of this whole problem in the case of a two band system. In this thesis, chapters three and five together with appendix A represent a comprehensive survey of spin waves in interacting electron systems. As well as the bottleneck effect being investigated, one could develop a full diagrammatic treatment of the s-d interaction in the presence of impurity scattering and the short range repulsive interaction responsible for magnetism, in both the ferromagnetic and paramagnetic state. In appendix A an attempt has been made to improve the method of evaluation of the discontinuity across the cut in the complex susceptibility. However the analytic properties of this function in the case where impurities are present need further investigation, since this function is not a geometric sum of terms where the frequency integral has been

carried out first, but a frequency integral over the sum of the diagrammatic terms.

In chapter six the problem of the dilute heisenberg model is treated. This is an interesting problem from a methodical point of view and has important physical applications to certain physical systems. It is made clear by the analysis that the existence of ferromagnetism does not require a rigorous periodicity in the distribution of the magnetic moments. This implies that this theory can treat both substitutional alloys, (where one component is magnetic) and amorphous ferromagnets. It could be extended to treat antiferromagnetic alloys, and alloys where both constituents are magnetic (by use of three or more exchange interactions).

It is shown in the analysis that the perturbation theory developed for the case of a pure ferromagnet can be developed purely in terms of operators fixed to a definite site in the lattice. The development does not make use of a fourier sum which would necessitate periodicity of the lattice. This means that the theory can be generalised to the case where some of the sites do have moments simply by restricting the sums over the lattice sites to those sites which are occupied. This means that the correlation functions lose their translational invariance and the average moment on a site depends on where the site is in the lattice.

An averaging procedure is introduced, which averages over all possible distributions of moments, which have a fixed number of occupied sites, because in a real physical system, different regions of the sample will have different distributions of moments, but with a fixed average concentration.

This method is then applied to discuss the NiCu system, in order to make a connection between neutron scattering experiments which measure the z-z spin correlation function, and spin wave damping which is postulated to be caused by scattering off the z-z spin fluctuations. At the same time of course one has put forward an interpretation of the neutron scattering results in such systems, and it is

shown how the neutron scattering cross section should vary near to the transition point. An expression is then derived for the spin wave damping which also depends on the concentration.

The method does yield a critical concentration at fixed finite temperature. From this method one can derive the way the magnetization depends on the concentration, as well as its dependence on the magnetic field and temperature.

As mentioned above this theory could be extended to treat antiferromagnetic alloys, and alloys with two constituents where both constituents are magnetic, by the use of three different exchange integrals.

As a final point, we note that in Appendix F a derivation is given of Van Hove's formula for the neutron cross section for the scattering of neutrons from magnetic systems. The approximations made are noted, and one can conclude that the use of the impulse approximation needs further investigation in a strongly interacting system. There seems a basic paradox between the use of the impulse approximation and a hamiltonian for the spin system in which the spins interact strongly with each other.

APPENDIX A

Discussion of the calculations of the magnetic susceptibility function for a system of electrons scattering from impurities.

The results in this Appendix are used in Chapters 5 and 6, and were derived in references 9 and 10.

The susceptibility for a system of electrons scattering from random impurities, without any electron-electron interactions, can be written in the form

$$\chi_{imp}(\underline{q},\omega_o) = i\int_{-\infty}^{+\infty} d\omega' \frac{\frac{1}{2\pi N(0)}\int G(p,\omega)G(\underline{p}+\underline{q},\omega+\omega_o)\frac{d^3p}{(2\pi)^3}}{1-\frac{1}{J}\frac{1}{2\pi N(0)}\int G(\underline{p},\omega)G(\underline{p}+q,\omega+\omega_o)\frac{d^3p}{(2\pi)^3}} \tag{A.1}$$

Then, when there is a short range exchange interaction between the electrons, if one ignores the self energy effects of such an interaction, one can write the total susceptibility in the form

$$\chi(\underline{q},\omega_o) = 2\mu_B^2 N(0)\frac{\chi_{imp}(\underline{q},\omega_o)}{1-N(0)\bar{V}_c\chi_{imp}(\underline{q},\omega_o)} \tag{A.2}$$

This really describes the multiple scattering of an electron and hole with opposite spins via the exchange interaction as they propagate and scatter off the impurities. One can see that when $J \to \infty$, and one has free electrons, $\chi(q,\omega_o)$ reduces to the usual exchange enhanced form. Further, when $\bar{V}_c = 0$, and $\omega_o = 0$, it reduces to the static susceptibility as calculated by De Gennes. De Gennes calculated the static susceptibility by performing the momentum integration first and then carrying out the frequency

integration which is the opposite order to that used in the free electron case. This method can be extended to the finite frequency case. This then shows that the above integral for $\chi_{imp}(\underset{\sim}{q},\omega_o)$ converges, and allows certain approximations to be made.

Evaluation of $\chi_{imp}(\underset{\sim}{q},\omega_o)$

First one evaluates the momentum integration. The Green's function for the system is[11]

$$G(\omega,\ r{:}r') \ = \ -\frac{m}{2\pi(r-r')}\, e^{iK(\omega)(r-r')} \qquad (A.3)$$

$$K(\omega) \ = \ \frac{i}{2\ell} + \operatorname{sgn}\omega \left(p_F^2 + 2m\omega - \frac{1}{4\ell^2}\right)^{\frac{1}{2}} \qquad (A.4)$$

Then

$$\int \frac{d^3p}{(2\pi)^3}\, G(\underset{\sim}{p},\omega)\ G(\underset{\sim}{p}+\underset{\sim}{q},\omega+\omega_o)$$

$$= \int d^3\underset{\sim}{r}\ G(r,\omega)\ G(r,\ \omega+\omega_o)\ e^{i\underset{\sim}{q}\cdot\underset{\sim}{r}} \qquad (A.5)$$

where $G(\underset{\sim}{r})$ is the Fourier transform of $G(\underset{\sim}{p})$ and is, of course, a different function although written the same in accordance with normal use in Physics.

$$\int d^3\underset{\sim}{r}\ G(\underset{\sim}{r},\omega)\ G(\underset{\sim}{r},\ \omega+\omega_o)\ e^{i\underset{\sim}{q}\cdot\underset{\sim}{r}}$$

$$= \int d^3\underset{\sim}{r}\ e^{i\underset{\sim}{q}\cdot\underset{\sim}{r}}\ \frac{m^2}{(4\pi)^2(r)^2}\ e^{i\{K(\omega)\ +\ K(\omega+\omega_o)\}|r|}$$

(A.6)

Performing the $|r|$ integration first one obtains

$$\int_{-1}^{+1} i\, d(\cos\theta)\, \frac{m^2}{4\pi 2}\, \frac{1}{q}\, \frac{\mathfrak{L}}{\{K(\omega) + K(\omega+\omega_o) + q\cos\theta\}}$$

$$= \frac{(i)m^2}{8\pi}\, \mathrm{Ln}\left[\frac{K(\omega) + K(\omega+\omega_o) + q}{K(\omega) + K(\omega+\omega_o) - q}\right] \qquad (A.7)$$

Then

$$\chi_{imp}(\underset{\sim}{q},\omega_o) = i \int_{-\infty}^{+\infty} d\omega' \, \frac{im^2}{4\pi^2 N(0)} \, \frac{\frac{\mathfrak{L}}{q}\, \mathrm{Ln}\left[\frac{K(\omega)+K(\omega+\omega_o)+q}{K(\omega)+K(\omega+\omega_o)-q}\right]}{1 - \frac{im^2}{4\pi^2 N(0)}\, \frac{\mathfrak{L}}{q}\, \frac{1}{\tau}\, \mathrm{Ln}\left[\frac{K(\omega)+K(\omega+\omega_o)+q}{K(\omega)+K(\omega+\omega_o)-q}\right]}$$

(A.8)

Now $K(\omega)$ changes sign at $\omega = 0$. Therefore, there are three ranges of integration in which $K(\omega) + K(\omega+\omega_o)$ are different functions. If one makes the substitution $y(\omega) = K(\omega) + K(\omega+\omega_o)$, one finds that the integrands reduce to the same form, whereas the path of integration is modified.

The non convergence at infinity is due to the fact that one has not cut off the momentum integration. This contribution is ignored. In fact, one notes that this contribution occurs in the first diagram, and this integral may be performed using a method which does the double integration in the other order and which de facto cuts off higher momentum values (Abrikosov). One can further show that doing the integral de Gennes way and throwing away the contribution at infinity leads to the same answer for the first diagram.

In the static case $\omega_o = 0$, $y(\omega) = 2K(\omega)$, and when ω_o is finite, the integration ranges $-\omega$ to $-\omega_o$ and 0 to $+\omega$ combine to give a very similar integration path.

First of all let us look at the static case. From the relation

$$K^2(\omega) - \frac{i}{\ell} K(\omega) - 2m\omega = 0 \qquad (A.9)$$

one finds that

$$d\omega = (K(\omega) - \frac{i}{2\ell}) \frac{dK(\omega)}{2m} \qquad (A.10)$$

$$K(\omega) = \frac{i}{2\ell} + \text{sgn } \omega\left(p_F^2 + 2m\omega - \frac{1}{4\ell^2}\right)^{\frac{1}{2}} \qquad \frac{1}{4\ell^2} \ll p_F^2 \qquad (A.11)$$

When ω is 0^+

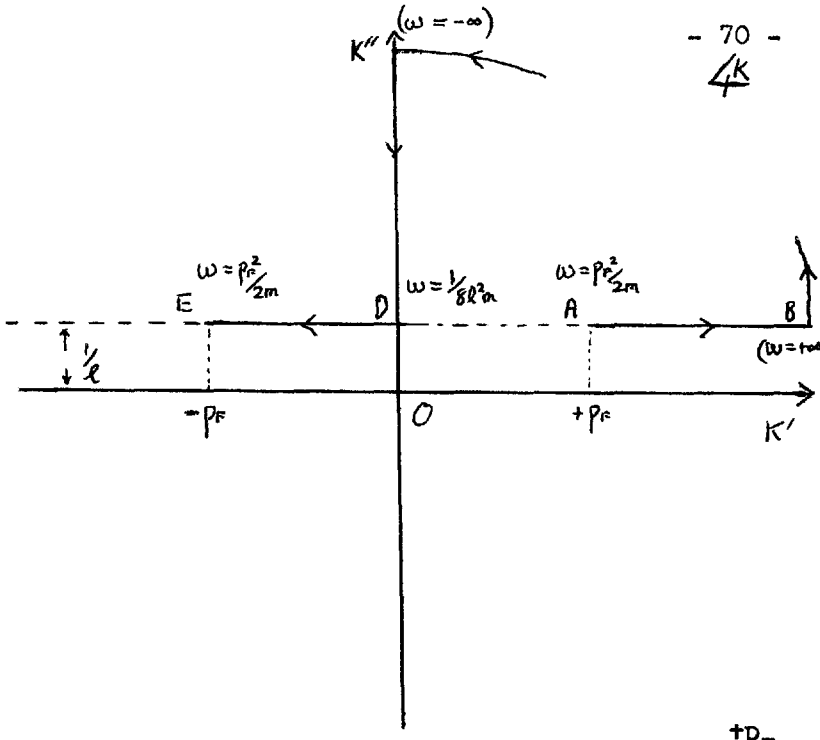
$$K(\omega) = \frac{i}{2\ell} + p_F \qquad (A.12)$$

as ω increases to $+\infty$, the square root remains +ve and $K(\omega)$ increases to ∞ along the line $\frac{i}{2\ell}$.

When ω is 0^-

$$K(\omega) = \frac{i}{2\ell} - p_F \qquad (A.13)$$

As ω decreases, the square root remains real until $\omega = -\frac{p_F^2}{2m}$, and the $K(\omega)$ is imaginary as $\omega \to \infty$. Therefore the path of integration is as in the diagram.



One can replace the path of integration by AE, because there is no pole inside the closed path. Then, adding AE to ED one obtains

$$\chi_{imp}(q,0) = (i)\int_{-p_F}^{+p_F} y\,\frac{dy}{m}\cdot\frac{\dfrac{im^2}{4\pi^2N(0)}\,\dfrac{1}{q}\,\mathrm{Ln}\left(\dfrac{y+q+\frac{i}{\ell}}{y-q+\frac{i}{\ell}}\right)}{1-\dfrac{im^2}{4\pi^2N(0)}\,\dfrac{1}{q}\,\dfrac{1}{\tau}\,\mathrm{Ln}\left(\dfrac{y+q+\frac{1}{\tau}}{y-q+\frac{i}{\ell}}\right)} \qquad (A.14)$$

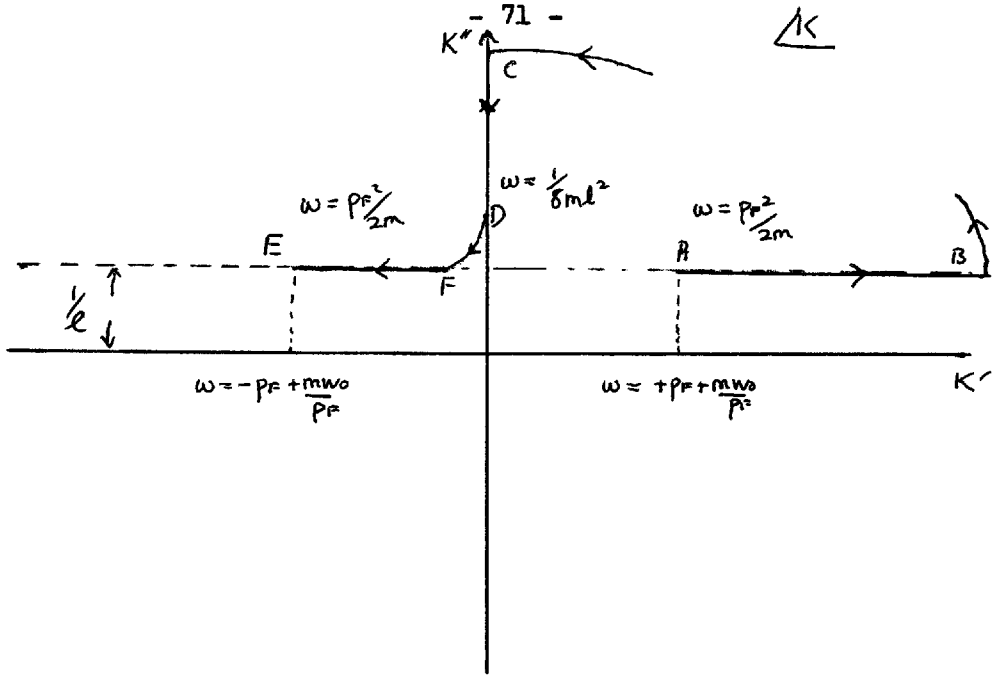
When $\omega_o \neq 0$, the change of variable is more complicated, but the path of integration only undergoes a slight modification. Putting

$$y(\omega) = K(\omega+\omega_o) + K(\omega) - \frac{i}{\ell} \qquad (A.15)$$

one finds that irrespective of the value of ω where $d\omega$ is taken

$$d\omega = \frac{1}{2m}\left(\frac{y}{2} - \frac{2(2m\omega_o)^2}{y^3}\right)dy \qquad (A.16)$$

The path of integration is shown in the diagram. As seen there is only a slight modification of the path, but there is an extra portion of the integral which corresponds to the region $-\omega_o$ to 0.



Then

$$\chi_{imp}(q,\omega_o) = (i)\int_{-p_F+\frac{m\omega_o}{p_F}}^{+p_F+\frac{m\omega_o}{p_F}} \frac{1}{2m}\left(\frac{y}{2} - \frac{2(2m\omega_o)^2}{y^3}\right)$$

$$\omega_o \ll \epsilon_F$$

$$\times \frac{\frac{im^2}{4\pi N(0)}\frac{1}{q}\ \mathrm{Ln}\left(\frac{y+q+\frac{i}{\ell}}{y-q+\frac{i}{\ell}}\right)}{1-\frac{i}{q\ell}\ \mathrm{Ln}\left(\frac{y+q+\frac{i}{\ell}}{y-q+\frac{i}{\ell}}\right)}\,dy$$

$$+\int_{-\omega_o}^{0} d\omega'\ \frac{im^2}{4\pi^2 N(0)}\ \frac{\frac{1}{q}\ \mathrm{Ln}\left(\frac{K(\omega)+K(\omega+\omega_o)+q}{K(\omega)+K(\omega+\omega_o)-q}\right)}{1-\frac{i}{q\ell}\ \mathrm{Ln}\left(\frac{K(\omega)+K(\omega+\omega_o)+q}{K(\omega)+K(\omega+\omega_o)-q}\right)}$$

(A.17)

The first term contributes terms of order $\frac{\omega_o^2}{\epsilon_F^2}$ and can be neglected, except that it equals $\chi(q,0)$. The second term gives terms of order $\frac{\omega_o}{\epsilon_F}$.

For $\omega_o \ll \varepsilon_F$

$$K(\omega+\omega_o) = \frac{i}{2\ell} + \mathrm{sgn}(\omega+\omega_o)\left(p_F + \frac{m(\omega+\omega_o)}{p_F}\right) \qquad (A.18)$$

Therefore in the region $-\omega_o < \omega < 0$

$$K(\omega) + K(\omega+\omega_o) = \frac{i}{2\ell} - p_F - \frac{m\omega}{p_F} + \frac{i}{2\ell} + p_F + \frac{m\omega}{p_F} + \frac{m\omega_o}{p_F}$$

$$= \frac{i}{\ell} + \frac{m\omega_o}{p_F} \qquad (A.19)$$

Therefore the last integral becomes

$$= \frac{\dfrac{\omega_o}{4\pi^2 N(0)}\dfrac{im^2}{q}\ \mathrm{Ln}\left(\dfrac{\frac{i}{\ell}+q+\frac{\omega_o}{V_f}}{\frac{i}{\ell}-q+\frac{\omega_o}{V_F}}\right)}{1 - \dfrac{i}{q\ell}\ \mathrm{Ln}\dfrac{\left(\frac{i}{\ell}+q+\frac{\omega_o}{V_F}\right)}{\left(\frac{i}{\ell}-q+\frac{\omega_o}{V_F}\right)}} \qquad (A.20)$$

$$\frac{m^2}{4\pi N(0)} = \frac{1}{V_F}$$

$\therefore$

$$\chi_{imp}(\underset{\sim}{q},\omega_o) = \chi_{imp}(q,0) + \frac{\dfrac{\omega_o}{qV_F}\ \mathrm{Ln}\left(\dfrac{\frac{i}{\ell}+q+\frac{\omega_o}{V_F}}{\frac{i}{\ell}-q+\frac{\omega_o}{V_F}}\right)}{1 - \dfrac{i}{q\ell}\ \mathrm{Ln}\left(\dfrac{\frac{i}{\ell}+q+\frac{\omega_o}{V_F}}{\frac{i}{\ell}-q+\frac{\omega_o}{V_F}}\right)}$$

$$= 1 + \frac{\omega_o}{qV_F} \frac{\operatorname{Ln}\left(\frac{i}{\ell} + q + \frac{\omega_o}{V_F}\right)}{1 - \frac{i}{q\ell} \operatorname{Ln}\left(\frac{\frac{i}{\ell} + q + \frac{\omega_o}{V_F}}{\frac{i}{\ell} - q + \frac{\omega_o}{V_F}}\right)} \qquad \text{(A.21)}$$

Then, with $u = \frac{\omega_o}{qV_F}$, and $u_o = \frac{1}{q\ell}$

$$\chi(\underset{\sim}{q},\omega_o) = 2\mu_B{}^2 N(0)\, \alpha(\underset{\sim}{q},\omega_o) \left(1 - \frac{i\omega_o}{2} \operatorname{Ln} \frac{u + iu_o - 1}{u + iu_o - 1}\right.$$

$$\left. \times - N(0)\, \bar{V}_i\, \alpha(q,\omega_o)\right)^{-1}$$

$$\alpha(q,\omega_o) = 1 - \frac{u + iu_o}{2} \operatorname{Ln}\left(\frac{u + iu_o + 1}{u + iu_o - 1}\right) \qquad \text{(A.22)}$$

When $g\ell \ll 1$

$$\chi(\underset{\sim}{q},\omega_o) = \frac{2\mu_B{}^2 N(0)}{1 - N(0)\bar{V}_c} \frac{Dq^2}{Dq^2 - i\omega_o} \qquad \frac{\omega_o}{qV_F} \ll 1$$

$$D = \frac{JV_F{}^2}{3(1 - N\bar{V}_c)} \qquad \text{(A.23)}$$

With a spin orbit interaction, the Green's function is of the same form except that the relaxation time is composed of two parts, one due to normal impurity scattering and one due to the spin orbit scattering

$$\frac{1}{\tau} = \frac{1}{\tau_o} + \frac{1}{\tau_1}$$

and

$$\chi_{imp}(\underset{\sim}{q},\omega_o) = i\int_{-\infty}^{+\infty} d\omega' \frac{J(\omega')(1 - \frac{1}{3\tau_1} J(\omega'))}{1 - \frac{1}{\tau_o} J(\omega)(1 - \frac{1}{3\tau_1} J(\omega'))} \tag{A.24}$$

The integral can be treated by the same contour method as before, and

$$\chi_{imp}(\underset{\sim}{q},\omega_o) = 1 + \frac{i\omega_o J(0,q,\omega_o)(1 - \frac{1}{3\tau_1} J(0,q,\omega_o))}{1 - \frac{1}{\tau_o} J(0,\underset{\sim}{q},\omega_o)(1 - \frac{1}{3\tau_1} J(0,q,\omega_o))} \tag{A.25}$$

$$J(0,\underset{\sim}{q},\omega_o) = \left(\frac{i}{2V_F q}\right) \mathrm{Ln}\left(\frac{\omega_o + \frac{i}{\tau} + V_F q}{\omega_o + \frac{i}{\tau} - V_F q}\right) \tag{A.26}$$

In the case where there is a magnetic field, the Greens function depends on the spin

$$G_o(r,\omega) = \frac{1}{|r|} e^{iK_\sigma(u)|r|}$$

$$K_\sigma(\omega) = \frac{i}{2\ell} + \mathrm{sgn}\omega\{p_{\sigma_F}^2 + 2m\omega\}^{\frac{1}{2}} \tag{A.27}$$

where

$$\frac{p_{F+}^2 - p_{F-}^2}{2m} = \mu H_o \quad . \tag{A.28}$$

The one defines

$$J_{+-}(q,\omega,\omega_o) = \frac{1}{2\pi N(0)} \frac{d^3p}{(2\pi)^3} G_+(\underset{\sim}{p},\omega)\, G_-(\underset{\sim}{p}+\underset{\sim}{q},\ \omega+\omega_o)$$

$$= \frac{i}{2V_F q} \mathrm{Ln} \frac{K_+(\omega) + K_-(\omega+\omega_o) + q}{K_+(\omega) + K_-(\omega+\omega_o) - q} \tag{A.29}$$

Then the corresponding transverse susceptibility $\chi^{+-}(\underset{\sim}{q},\omega_o)$ is given by

$$\chi^{+-}_{imp}(\underset{\sim}{q},\omega_o) = \frac{1 + i\omega_o\, J(0,\underset{\sim}{q},\omega_o-\Delta)(1 - \frac{1}{3\tau_1} J(0,\underset{\sim}{q},\omega_o-\Delta)}{1 - \frac{1}{\tau_o} J(0,\underset{\sim}{q},\omega_o-\Delta)(1 - \frac{1}{3\tau_1} J(0,\underset{\sim}{q},\omega_o-\Delta\ )} \tag{A.30}$$

where $\Delta = p_{F+}^2 - p_{F-}^2$

$$K_+(\omega) + K_-(\omega+\omega_o) = \frac{i}{\ell} - \left\{(p_{F+}^2 - p_{F-}^2) + p_{F-}^2 + 2m\omega\right\}^{\frac{1}{2}} \tag{A.31}$$

$$+ \left\{p_{F-}^2 + 2m(\omega+\omega_o)\right\}^{\frac{1}{2}}$$

$$\cong \frac{i}{\ell} + \frac{\omega_o - \Delta}{p_{F-}} \qquad p_{F-} \cong p_F \quad \text{for small splitting} \tag{A.32}$$

Then

$$\chi^{+-}_{imp}(0,\omega_o) = 2\mu_B^2 \frac{N(0)(-\Delta + \frac{4}{3}\frac{i}{\tau_1})}{\omega_o - \Delta + \frac{4}{3}\frac{i}{\tau_1}} \tag{A.33}$$

This and $\chi^{+-}_{imp}(q,\omega_o)$ is obtained by expanding $J(0,q,\omega_o)$ for $q\ell \ll 1$ as

$$J(0,q,\omega_o) \approx \frac{i}{2V_F}\left(\frac{1}{\frac{\omega_o-\Delta}{V_F} + \frac{i}{\ell}} + \frac{q^2}{3}\frac{1}{\left(\frac{\omega_o-\Delta}{V_F} + \frac{i}{\ell}\right)^3} + \cdots\right)$$

which gives

$$\chi^{+-}_{imp}(\underset{\sim}{q},\omega_o) = 2\mu_B^2 \frac{N(0)(-\Delta + i\gamma_1)}{\{\omega_o - \Delta + i\gamma_1\}} \tag{A.34}$$

$$\gamma_1 = \frac{4}{3}\frac{i}{\tau_1} + Dq^2 \left(\frac{1-i\Gamma}{1+i\Gamma}\right)$$

$$\Gamma = N(0)\,\bar{V}_c\,J\,\Delta$$

and

$$D = J\frac{V_F^2}{3} \quad .$$

Ferromagnetic Spin Susceptibility

The calculation is the same as for that when a magnetic field is present. Again in the ferromagnetic ground state $p_{F+} \neq p_{F-}$ and in fact they are related by the relation (see Appendix B)

$$\frac{1}{2m}\left(p_{F+}^2 - p_{F-}^2\right) = \omega_L + \frac{\bar{V}_c}{6\pi^3}\left(p_{F+}^3 - p_{F-}^3\right) \qquad (A.35)$$

Thus p_{F+} and p_{F-} depend on $\bar{V}_c$ and the strength of the magnetic field. Carrying through the contour integration as before, one obtains the result

$$\chi^{+-}_{imp}(\underset{\sim}{q},\omega_o) = i\int_{y(-\omega_o-)}^{y(0+)} dy\,\frac{i}{2m}\left(\frac{y}{2} - \frac{2\Delta^2}{y^3}\right)\frac{\operatorname{Ln}\dfrac{y+q+\frac{i}{\ell}}{y-q+\frac{i}{\ell}}}{1-\frac{i}{\ell}\operatorname{Ln}\left(\dfrac{y+q+\frac{i}{\ell}}{y-q+\frac{i}{\ell}}\right)} + i\int_{y(-\ {}_o+)}^{y(0-)} \frac{1}{2m}\left(\frac{y}{2} - \frac{2\Delta^2}{y^3}\right)\frac{\operatorname{Ln}\dfrac{y+q-\frac{i}{\ell}}{y-q+\frac{i}{\ell}}}{1-\frac{i}{\ell}\operatorname{Ln}\left(\dfrac{y+q+\frac{i}{\ell}}{y-q+\frac{i}{\ell}}\right)} \qquad (A.36)$$

for the case of simple impurities

$$y(\omega) = \text{Sgn } \omega+\omega_o \left(p_{F+}^2 + 2m\ \omega+\omega_o\right)^{\frac{1}{2}} + \text{Sgn } \omega \left(p_{F-}^2 + 2m\omega\right)^{\frac{1}{2}} \tag{A.37}$$

This integral can be carried out by expanding the integrand. Then

$$\chi^{+-}(q,0) = \frac{1}{2p_F}\left[\frac{3y_o^2 + \delta^2}{3y_o} - \frac{q^2}{3}\left[\frac{5y_o^2 - \delta^2}{5y_o^3}\right] + \ldots\right] \tag{A.38}$$

$$y_o = p_{F+} + p_{F-}$$

$$\delta = p_{F+} - p_{F-}$$

and

$$\chi_{imp}^{+-}(q,\omega_o) = \chi^{+-}(\underset{\sim}{q},0) + \frac{\delta\omega_o}{3V_F y_o^2} + \frac{\omega_o}{V_F\delta}\left[\frac{1 + \frac{q^2}{3}\left[\frac{i}{\ell} - \delta\right]^{-2}}{1 + \frac{iq^2}{3\delta\ell}\left[\frac{i}{\ell} - \delta^{-2}\right]}\right] \tag{A.39}$$

This gives the spin wave poles, since these are determined by the solutions to the equation

$$\mathbb{1} = N(0)\ \bar{V}_c\ \chi_{imp}^{+-}(\underset{\sim}{q},\omega_o) \tag{A.40}$$

and using (1)

$$N(0)\ \bar{V}_c\ \chi^{+-}(0,0) = \mathbb{1} - \omega_L$$

where

$$\frac{3y_o^2 + \delta^2}{3y_o} = \frac{p_{F+}^3 - p_{F-}^3}{p_{F+}^2 - p_{F-}^2} \tag{A.41}$$

The pole is at the frequency ω_o where

$$\omega_o = \omega_L + \alpha\Delta - \frac{i\omega_L}{\Delta}\bar{V}_c \frac{y_o^2 \ell}{24\pi^2}\left(\frac{1 - i\delta\ell}{1 + \delta\ell^2}\right) \qquad (A.42)$$

From these facts one can assume a form for $\chi^{+-}_{imp}(q,\omega_o)$ similar to the free electron form

$$\chi^{+-}_{imp}(\underset{\sim}{q},\omega_o) = \frac{\chi^{+-}_{imp}(q,0)}{\omega_o - \bar{V}_c\,\chi_{+-}(q,0) - \omega_L - Bq^2} \qquad (A.43)$$

When spin orbit scattering is included this is modified to

$$\chi^{+-}_{s.o.}(\underset{\sim}{q},\omega_o) = \frac{\chi^{+-}_{s.o.}(q,0)}{\omega_o - \bar{V}_c\,\chi_{+-}(q,0) - \omega_L + \omega_L \frac{4}{3}\frac{i}{3\delta\ell_1} + B_1 q^2} \qquad (A.44)$$

$$B_1 = B - \alpha\Delta\frac{4i}{3\delta\ell_1}$$

and

$$B = \alpha\Delta - \frac{i\omega_L}{\Delta}\frac{\bar{V}_c\, y_o^2\, \ell}{24\pi^2}\left(\frac{1 - i\delta\ell}{1 + \delta^2\ell^2}\right) \qquad (A.45)$$

APPENDIX B

Linear Response Theory

(Application of a weak external disturbance to a system in a steady state)

Suppose that before time (t_o) a system is described by a density matrix $\hat{\rho}$ which commutes with a time independent Hamiltonian $\hat{H}_o$. After time t_o, an external disturbance is applied which couples to the observable properties $\hat{A}_j(\underset{\sim}{r},t)$ of the system, described by an addition to the Hamiltonian of the form

$$\hat{H}(t) = -\int_V d^3\underset{\sim}{r} \sum_j \hat{A}_J(\underset{\sim}{r},t)\, a_j(\underset{\sim}{r},t) \qquad (B.1)$$

where the $a_J(\underset{\sim}{r},t)$ represent generalized external forces, e.g. Magnetic systems in a magnetic field

$$\hat{H}(t) = -\int_V d^3\underset{\sim}{r}\, \underset{\sim}{H}(\underset{\sim}{r},t) \cdot \underset{\sim}{\hat{M}}(\underset{\sim}{r},t) \qquad (B.1a)$$

where $H(\underset{\sim}{r},t)$ is an external spatially and time dependent magnetic field.

One calculates the expectation value at time t of the observable A_i, from the formula

$$Tr(\hat{\rho}(t)\, \hat{A}_I(\underset{\sim}{r},t)) = \langle \hat{A}_i(\underset{\sim}{r},t)\rangle_{N.E.} \qquad (B.2)$$

(N.E means non equilibrium)

If one assumes $\hat{A}_I(\underset{\sim}{r},t)$ does not depend on time explicitly, Then

$$\langle \hat{A}_I(\underset{\sim}{r},t)\rangle_{N.E.} = Tr\left(\hat{U}(t,t_o)\, \hat{\rho}\hat{U}^{-1}(t,t_o)\, \hat{A}_i(\underset{\sim}{r},t_o)\right) \qquad (B.3)$$

where $\hat{U}(t,t_o)$ is a unitary operator which describes the way the system changes in time and satisfies

$$i\hbar \frac{d}{dt} \hat{U}(t,t_o) = \left(\hat{H}_o + \hat{H}_{ext}(t)\right) \hat{U}(t,t_o)$$

$$\hat{U}(t_o,t_o) = 1$$

as the initial condition. One further assumes

$$\hat{U}(t,t_o) = \hat{U}_o(t,t_o)\, \hat{U}'(t,t_o)$$

where $\hat{U}_o$ satisfies

$$i\hbar \frac{d}{dt} \hat{U}_o = \hat{H}_o \hat{U}_o \qquad \text{i.e.} \quad \hat{U}_o = e^{i\hat{H}_o t} \quad \text{formally.}$$

Then

$$i\hbar \frac{d}{dt} \hat{U}'(t,t_o) = \{\hat{U}_o^{-1}(t,t_o)\, \hat{H}_{ext}(t)\, U_o(t,t_o)\}\, U'(t,t_o)$$

$$\therefore \quad i\hbar \frac{d}{dt} \hat{U}'(t,t_o) = H^I_{ext}(t)\, \hat{U}'(t,t_o) \ .$$

To first order this has the solution

$$\hat{U}'(t,t_o) = 1 + \frac{1}{i\hbar} \int_{t_o}^{t} H^I_{ext}(t')\, dt' + \ldots \qquad (B.4)$$

Denote by $\hat{A}^I(\underset{\sim}{r},t)$, the Heisenberg operators for the Hamiltonian $\hat{H}_o$

$$\hat{A}^I_i(\underset{\sim}{r},t) = \hat{U}_o^{-1}(t,t_o)\, \hat{A}_i(\underset{\sim}{r},t_o)\, \hat{U}_o(t,t_o) \qquad (B.5)$$

Therefore

$$\mathrm{Tr}\{\rho\, U^{-1}\, \hat{A}_i(\underset{\sim}{r},t_o)U\} = \mathrm{Tr}\, \{\rho U'^{-1}\, \hat{A}^I_i(\underset{\sim}{r},t)\, \hat{U}'\}$$

$$= \mathrm{Tr}\left(\rho\{\hat{A}^I + \frac{i}{\hbar} \sum_j \int d^3r' \int_{f_o}^{t} dt' \left(\hat{A}^I_i(\underset{\sim}{r},t),\, A^I_j(\underset{\sim}{r}',t')\right) \times a_j(\underset{\sim}{r}',t')\}\right) + \ldots$$

Dropping ~~subscript~~ superscript I

$$\langle \hat{A}_i(\underset{\sim}{r},t)\rangle_{N.E.} = \langle A_i(\underset{\sim}{r},t)\rangle + \frac{i}{\hbar}\sum_J \int d^3\underset{\sim}{r}' \int_{t_o}^{t} dt' \times \langle [\hat{A}_i^{I}(\underset{\sim}{r},t),\ \hat{A}_J^{I}(r',t')]a_j(\underset{\sim}{r}',t')\}]\rangle + \ldots \quad (B.6)$$

Defining the absorptive response as the commutator

$$\bar{\chi}''_{ij}(\underset{\sim}{r},\underset{\sim}{r}';\ t-t') \equiv \frac{1}{2\hbar}\langle [\hat{A}_i(\underset{\sim}{r},t),\ \hat{A}_j(\underset{\sim}{r}',t')]\rangle \quad (B.7)$$

$$= \int \frac{d\omega}{2\pi} e^{-i\omega(t-t')}\ \chi''_{ij}(\underset{\sim}{r},\underset{\sim}{r}',\omega) \quad (B.8)$$

[9]

Taking t_o as $-\infty$, and introducing the step function $\theta(t-t')$ one may write

$$\delta\langle \hat{A}_i(\underset{\sim}{r},t)\rangle = \sum_j \int d\underset{\sim}{r}' \int_{-\infty}^{+\infty} 2\ dt'\ \bar{\chi}''_{ij}(\underset{\sim}{r},\underset{\sim}{r}',t-t')\ a_j(\underset{\sim}{r}',t') \times i\ \theta(t-t') \quad (B.9)$$

Then define

$$\bar{\chi}_{ij}(\underset{\sim}{r},\underset{\sim}{r}',t-t') = 2i\ \theta(t-t')\ \bar{\chi}''_{ij}(\underset{\sim}{r},\underset{\sim}{r}',t-t') \quad (B.10)$$

$$\delta\langle \hat{A}_i(\underset{\sim}{r},t)\rangle = \sum_j \int dr' \int_{-\infty}^{+\infty} dt'\ \bar{\chi}_{ij}(\underset{\sim}{r},\underset{\sim}{r}',t-t')\ a_j(\underset{\sim}{r}',t') \ .$$

The step function $\theta(t-t')$ is here a symbolic expression of the causality condition.

Under certain conditions on $\bar{\chi}''_{ij}(\underset{\sim}{r},\underset{\sim}{r}',t-t')$ one can show that the fourier transform of $\bar{\chi}_{ij}(\underset{\sim}{r},\underset{\sim}{r}',t-t')$ is the boundary value as

z approaches the cut on the real axis from above of the sectionally holomorphic function

$$\chi_{ij}(\underset{\sim}{r},\underset{\sim}{r}',z) = \int \frac{d\omega'}{\pi} \frac{\chi''_{ij}(\underset{\sim}{r},\underset{\sim}{r}',\omega)}{(\omega' - z)} \qquad (B.11)$$

i.e.

$$\chi_{ij}(\underset{\sim}{r},\underset{\sim}{r}',\omega+i\varepsilon) = \chi'_{ij}(\underset{\sim}{r},\underset{\sim}{r}',\omega) + \chi''_{ij}(\underset{\sim}{r},\underset{\sim}{r}',\omega) \qquad (B.12)$$

where

$$\chi'_{ij}(\underset{\sim}{r},\underset{\sim}{r}',\omega) = P \int \frac{d\omega'}{\pi} \frac{\chi''_{ij}(\underset{\sim}{r},\underset{\sim}{r}',\omega)}{(\omega' - \omega)}$$

$$\chi''_{ij}(\underset{\sim}{r},\underset{\sim}{r}';\omega) = - P \int \frac{d\omega'}{\pi} \frac{\chi'_{ij}(\underset{\sim}{r},\underset{\sim}{r}',\omega')}{(\omega' - \omega)} \qquad (B.13)$$

In the case of magnetic systems which are dealt with in this thesis, the perturbing hamiltonian has the form (1a) and the response function is then

$$\bar{\chi}_{MM}(\underset{\sim}{r},\underset{\sim}{r}',t-t') = 2i\,\theta(t-t') \langle[\hat{M}(\underset{\sim}{r},t), \hat{M}(\underset{\sim}{r}',t')]\rangle \qquad (B.14)$$

For each model, of course, the ~~magnetization~~ magnetization operator has its own form. This function is calculated because the imaginary part gives the absorption of energy by the system from the external field. Further, if this function has a pole or sharp resonance in its fourier transform, then the absorption is associated with the existence of a collective mode of the system. As one can show, this function is associated both with the absorption of energy (dissipation) and with the dynamic behaviour of the system (fluctuation). This simple situation holds only in the linear approximation.

APPENDIX C

The Magnetization Relation in Hartree-Fock Theory

The interaction energy part of the hamiltonian is

$$\sum_I I\, n_{I\uparrow}\, n_{I\downarrow} \tag{C.1}$$

Therefore, at T = 0, the Hartree-Fock energy is

$$E = \frac{3}{5}\left(N_+ \frac{k_+^2}{2m} + N_- \frac{k_-^2}{2m}\right) + \frac{1}{V} N_+ N_- I \tag{C.2}$$

where $I = \frac{4\pi a}{m}$ and a is the s-wave scattering length of the short range repulsive interaction.

If there is a magnetic field as well, i.e. $N_o\ \omega$

$$E = \frac{3}{5}\left(N_+ \frac{k_+^2}{2m} + N_- \frac{k_-^2}{2m}\right) + \omega_L(N_+ - N_-) + \frac{1}{V} N_+ N_- I \tag{C.3}$$

where

$$N_+ + N_- = N$$

$$N_+ = \frac{4}{3}\pi k_+^3 \ .$$

k_+ and k_- are fermi momenta for up and down spin bands respectively. One then minimizes the energy with respect to k_+ and k_-, subject to the constraint above

$$\text{i.e.} \quad \lambda(k_+^3 + k_-^3 - k_F^3) = 0 \tag{C.4}$$

One minimizes

$$E + \lambda(k_+^3 + k_-^3 - k_F^3) = 0 \tag{C.5}$$

to obtain two equations

$$\frac{3}{2} k_{\pm}^2 + \frac{2a}{\pi} k_{\pm}^2 k_{+}^3 - 3\lambda k_{\pm}^2 = 0 \qquad (C.6)$$

or

$$\frac{3}{2} (k_{+}^2 - k_{-}^2) = \frac{2a}{\pi} (k_{+}^3 - k_{-}^3) \quad . \qquad (C.7)$$

The critical strength occurs when this has a solution and $k_{+} \neq k_{-}$. When $k_{+} \neq k_{-}$ one can divide by $(k_{+} - k_{-})$ to obtain

$$\frac{3}{2} (k_{+} + k_{-}) = \frac{2a}{\pi} (k_{+} - k_{-} + k_{+}k_{-}) \qquad (C.8)$$

At the critical strength $k_{+} = k_{-} = k_{F}$. Therefore

$$\frac{3}{2} 2k_F = \frac{2a}{\pi} 3k_F^2 \Rightarrow k_F a = \frac{\pi}{2} \qquad (C.9)$$

Complete alignment $(k_{-} = 0)$ is obtained when

$$k_{+} = \frac{3\pi}{4a} \qquad (C.10)$$

$$\text{i.e. } k_F a = \frac{\pi}{a} \frac{3}{2} \frac{4}{3}$$

At finite temperatures this has to be modified by the addition of Fermi factors in the energy, each spin band being distributed in a Fermi Dirac distribution. A simpler model for finite temperatures envisages the interaction strength increasing with decreasing temperature to reach its critical value at $T = T_c$.

With a magnetic field on, the corresponding relation to equation (C.7) is

$$\frac{3}{2} (k_{+}^2 - k_{-}^2) = m\omega_L \beta + \frac{2a}{\pi} (k_{+}^3 - k_{-}^3) \quad . \qquad (C.11)$$

This theory is at T = 0, and shows that a substance is ferromagnetic at T = 0 if I has a certain minimum value in that substance. If I is above this value, then the substance becomes ferromagnetic at a finite temperature.

To see this one looks at the paramagnetic susceptibility

$$\chi(q,z) = \frac{\chi^{o}(q,z)}{1 - I\,\chi^{o}(q,z)} \quad . \qquad \text{(C.12)}$$

The substance becomes ferromagnetic when the static susceptibility becomes very large or unbounded.

This happens when $1 = I\,\chi(0,0)$

$$\chi(0,0) = \left(\frac{\partial n}{\partial \mu}\right)_{T} \qquad \text{n is the density} \qquad \text{(C.13)}$$

where μ is the chemical potential.

$$\therefore \quad 1 = I \left(\frac{\partial n}{\partial \mu}\right)_{T=0} \left(1 - \frac{\pi^2}{12} \frac{1}{\beta^2 \mu_{T=0}}\right) \qquad \beta = 1/kT \qquad \text{(C.14)}$$

is the temperature at which this occurs. Therefore

$$k_B T_c \equiv \frac{2\sqrt{3}}{\pi} \frac{h^2 k_F^2}{2m} \left(\frac{2k_F a - \pi}{2k_F a}\right)^{\frac{1}{2}} \qquad \text{(C.15)}$$

Therefore T_c is > 0 when $k_F a > \frac{\pi}{2}$.

The calculations in this thesis are carried out at T = 0, for a system which is paramagnetic or ferromagnetic at T = 0. Variations in temperature can be taken into account in a simple way by considering I to be temperature dependent, e.g. one considers $\left(\frac{\partial n}{\partial \mu}\right)_{T} = f(T) \left(\frac{\partial n}{\partial \mu}\right)_{T=0}$, and redefines I as If(T). This can give one some idea of what happens as a paramagnetic system approaches the transition point without doing a full calculation.

In the strongly paramagnetic region, from (C.11) one has for $k_+ \equiv k_-$, $k_+ - k_- = x$

$$\frac{3}{2} 2k_F \, x = 3m\omega_L + \frac{2a}{\pi} \times 3k_F^2 \qquad \text{(C.11)}$$

$$\therefore \quad x = \frac{m\omega_L}{(k_F - \frac{2a}{\pi} k_F^2)} \qquad \text{(C.16)}$$

$$\therefore \quad \Delta = \frac{k_+^2 - k_-^2}{2m} = \frac{\mu_B H}{(I - \frac{2a}{\pi} k_F)} \qquad \text{(C.17)}$$

The critical value for magnetism, occurs when $1 = \frac{2a}{\pi} k_F$. Hence this expression only holds for a less than its critical value.

APPENDIX D

The Fluctuation - Dissipation Theorem

For most cases the stationary ensemble which characterizes the system is canonical.

The density matrix is

$$\hat{\rho} = e^{-\beta\hat{H}}/Tr\{e^{-\beta\hat{H}}\} \quad . \tag{D.1}$$

The time translation property of the operators and cyclical permutation of operators under atrace sign imply

$$Tr\{e^{-\beta\hat{H}}\,\hat{A}_I(\underset{\sim}{r},t)\,A_j(\underset{\sim}{r}',t')\} = Tr\{\hat{A}_i(\underset{\sim}{r},t+i\beta h)\,e^{-\beta\hat{H}}\,A_J(\underset{\sim}{r},t')\}$$

$$= Tr\{e^{-\beta\hat{H}}\,\hat{A}_J(\underset{\sim}{r}',t')\,\hat{A}_I(\underset{\sim}{r},t+i\beta h)\} \tag{D.2}$$

Further

$$Tr\{e^{-\beta\hat{H}}\,A_I(\underset{\sim}{r},t)\}$$

is independent of time. If the fourier transform of

$$\langle(A_I(\underset{\sim}{r},t) - \langle A_I(\underset{\sim}{r},t)\rangle)(A_J(\underset{\sim}{r}',t') - \langle A_J(\underset{\sim}{r}',t')\rangle)\rangle \tag{D.3}$$

denoted by $S_{IJ}(\underset{\sim}{r},\underset{\sim}{r}':\omega)$ exists

$$S_{IJ}(\underset{\sim}{r},\underset{\sim}{r}',\omega) = e^{\beta h\omega}\,S_{JI}(\underset{\sim}{r},\underset{\sim}{r}',\omega) \tag{D.4}$$

and since

$$\chi''_{IJ}(\underset{\sim}{r},\underset{\sim}{r}',\omega) = \frac{1}{2h}\left[S_{IJ}(\underset{\sim}{r},\underset{\sim}{r}',\omega) - S_{JI}(\underset{\sim}{r},\underset{\sim}{r}',\omega)\right] \tag{D.5}$$

$$\chi''_{IJ}(\underset{\sim}{r},\underset{\sim}{r}',\omega) = \frac{1}{2h}\left(1 - e^{-\beta h\omega}\right) S_{IJ}(\underset{\sim}{r},\underset{\sim}{r}',\omega) \qquad (D.6)$$

This is a form of the fluctuation dissipation theorem as χ''_{IJ} is a measure of the dissipation and S_{IJ} a measure of the fluctuations in the system.

APPENDIX E

Identification of $\chi''(\omega)$ with the Dissipation of Energy in a System

The work done on a system is given by the explicit rate of change of the Hamiltonian with time. The rate at which work is done on the system is given by the explicit rate of change of the expectation value of the hamiltonian.

$$-\frac{\partial}{\partial t}\langle\hat{H}\rangle = -\frac{\partial W}{\partial t} = \sum_I \int \langle\hat{A}_I(\underset{\sim}{r},t)\rangle_{N.E.}\ \overset{o}{a}_I(\underset{\sim}{r},t)\ d^3\underset{\sim}{r} \tag{E.1}$$

$$= \sum_I \int \langle A_I(\underset{\sim}{r},t)\rangle_{Eq}\ \overset{o}{a}_I(\underset{\sim}{r},t)\ d^3\underset{\sim}{r}$$

$$+ \sum_{IJ} \int d^3\underset{\sim}{r} \int d^3\underset{\sim}{r}' \int_{-\infty}^{+\infty} dt'\ \overset{o}{a}_I(\underset{\sim}{r},t)\bar{\chi}_{ij}(\underset{\sim}{r},\underset{\sim}{r}',t-t')$$

$$a_J(\underset{\sim}{r}',t') + O(a^3) \tag{E.2}$$

This follows from (B.6).

Consider an external monochromatic field

$$a_I(\underset{\sim}{r},t) = \mathrm{Re}\{a_I(\underset{\sim}{r})\ e^{-i\omega t}\}$$

$$= \tfrac{1}{2}\{a_I(\underset{\sim}{r})\ e^{i\omega t} + a_I^*(\underset{\sim}{r})\ e^{i\omega t}\} \tag{E.3}$$

Then the time averaged rate of change of energy is given by

$$-\frac{d\bar{W}}{dt} = \sum_{I,J} \left(\frac{i\omega}{4} \int d\underset{\sim}{r} \int d\underset{\sim}{r}'\ \chi_{ij}(\underset{\sim}{r},\underset{\sim}{r}',\omega)\ a_j(\underset{\sim}{r}')\ a_I^*(\underset{\sim}{r})\right.$$

$$\left. \times -\frac{i\omega}{4} \int d\underset{\sim}{r} \int d\underset{\sim}{r}'\ a_I(\underset{\sim}{r})\ \chi_{IJ}(\underset{\sim}{r},\underset{\sim}{r}':-\omega)\ a_J^*(\underset{\sim}{r}')\right) \tag{E.4}$$

From symmetry consideration

$$\chi''_{ij}(\underset{\sim}{r},\underset{\sim}{r}',\omega) = -\chi''_{JI}(\underset{\sim}{r}',\underset{\sim}{r},-\omega)$$

$$\chi'_{IJ}(\underset{\sim}{r},\underset{\sim}{r}',\omega) = \chi_{JI}(\underset{\sim}{r}',\underset{\sim}{r},-\omega) \qquad \text{(E.5)}$$

Therefore

$$\frac{d\bar{W}}{dt} = \frac{1}{2}\sum_{IJ}\omega\int d\underset{\sim}{r}\int d\underset{\sim}{r}'\, a^{*}_{I}(\underset{\sim}{r})\,\chi''_{IJ}(\underset{\sim}{r},\underset{\sim}{r}',\omega)\,a_{J}(\underset{\sim}{r}') \quad . \qquad \text{(E.6)}$$

APPENDIX F

Scattering from a Bound System of Particles

Neutron Scattering

Consider an incident particle mass m_i and spin S_i. It is described by a plane wave and a spin function

$$\chi_{i\ \underset{\sim}{p},\nu} = \frac{1}{(2\pi)^3_2} e^{i\underset{\sim}{p}.\underset{\sim}{x}} U_{s_i,\nu(S_i)} \qquad (F.1)$$

p is the incident momentum.

Then

$$\hat{K}_i \chi_{i\ \underset{\sim}{p},\nu} = \epsilon_{\underset{\sim}{p}} \chi_{i\ \underset{\sim}{p},\nu} \qquad (F.2)$$

$$\epsilon_p = \frac{p^2}{2m_i}$$

is the incident kinetic energy and $K_i = \frac{1}{2m_i} v^2$.

The target particle is assumed to be composite, consisting of N bound particles of masses $M_1 \ldots M_n$ and spins $S_1 \ldots S_N$. The initial wave function of the scatterer is written $g_o(z_1,s_1 \ldots z_N S_N)$. A general state of the scatterer is written $g_\gamma(z_1,s_1 \ldots z_N S_N)$. Spin orientations are written as $O(\nu_t)$ and $\gamma(\nu_t)$.

Then the initial state eigenfunction is

$$\chi_{t:O(\nu_t),\underset{\sim}{p}} = \frac{1}{(2\pi)^{3}_2} e^{i\underset{\sim}{P}.\underset{\sim}{C}} g_o(z_1,s_1 \ldots Z_N,S_N) \qquad (F.3)$$

$\underset{\sim}{C}$ is the scattering centre of mass.

An arbitrary final state is

$$\chi^{\pm}_{t\ \gamma(\nu'_t)\ \underline{Q}} = \frac{1}{(2\pi)^{3}2}\, e^{i\underline{Q}.\underline{C}}\, g_{\gamma}(z_1,s_1 \ldots Z_N S_N) \quad \text{(F.4)}$$

The Hamiltonian of the scattering is of the form

$$\hat{h} = \sum_{\alpha=1}^{N} K_{\alpha} + U \quad \text{(F.5)}$$

U is the interaction energy.

Then

$$\hat{h}\ \chi_{t:0(\nu_t)\ \underline{P}} = W_o\ \chi_{t:0(\nu_t)\ \underline{P}} \quad \text{(F.6)}$$

$$\hat{h}\ \chi^{\pm}_{t:\gamma(\nu'_t)\ \underline{Q}} = W_{\gamma}\ \chi_{t:\gamma(\nu'_t)\ \underline{Q}} \quad \text{(F.7)}$$

$$W_o = w_o + \frac{P^2}{2M_t} \qquad W_{\gamma} = w_{\gamma} + \frac{Q^2}{2M_t}$$

The initial state of the entire system before scattering is

$$\chi_a = \chi_{i\underline{p}\nu}\ \chi_{t:0(\nu_t)\ \underline{P}} \quad \text{(F.8)}$$

Possible final states are then

$$\chi^{\pm}_b = \chi_{i\underline{k}\nu}\ \chi^{\pm}_{t\ \gamma(\nu'_t)\ \underline{Q}} \ . \quad \text{(F.9)}$$

Then, if

$$K = K_i + H$$

$$K\ \chi_a = E_a\ \chi_a = (\epsilon_p + W_o)\ \chi_a \quad \text{(F.10)}$$

$$K\ \chi^{\pm}_b = E_b\ \chi^{\pm}_b = (\epsilon_K + W_{\gamma})\ \chi^{\pm}_b \quad \text{(F.11)}$$

The Hamiltonian for the whole scattering system is

$$\hat{H} = K + V \tag{F.12}$$

$$V = \sum_{\alpha=1}^{N} V_\alpha \tag{F.13}$$

V_α represents the interaction between the incident particle and target particle α.

One now assumes that the incident particle is only scattered once, i.e. from one target particle.

The scattered wave from such a scattering is given by

$$\psi_{sc.\alpha} = \frac{1}{E_a + i\eta - K} \mathcal{T}_N \chi_a \qquad \alpha = 1 \ldots N \ . \tag{F.14}$$

Where $\tilde{\mathcal{T}}_a$ is the 'T' matrix.

One then assumes that $\mathcal{T}_N$ may be replaced by the scattering matrix with a free particle, i.e. one may neglect U.

Then

$$\psi_{sc} = \sum_{\alpha=1}^{N} \psi_{sc.\alpha} = \frac{¶}{(E_a + i\eta - K)} \tilde{\mathcal{T}}_N \chi_a \tag{F.15}$$

$$\tilde{\mathcal{T}}_N = \sum_{\alpha=1}^{N} \tilde{\mathcal{T}}_a \ . \tag{F.16}$$

For a final state $\underline{b}$ and incident state $\underline{a}$

$$\langle b|\tilde{\mathcal{T}}_N|a\rangle = \delta(\underline{k} + \underline{Q} - \underline{p} - \underline{P})\langle \underline{k},\nu',\underline{Q}\ \gamma(\nu_t')|T_N|\underline{p}\nu\ \underline{P}\ O(\nu_t)\rangle \tag{F.17}$$

T_N is the submatrix of $\tilde{\mathcal{T}}_N$ on the momentum shell.

Then the differential cross-section is

$$d\sigma = \frac{(2\pi)^4}{V_{rel}} \sum_{\gamma'} \int d^3\underset{\sim}{k}\ \delta(\varepsilon_K + W_\gamma - \varepsilon_p - W_o)|\langle b|T_N|a\rangle|^2 \tag{F.18}$$

a is the initial state $|\underset{\sim}{p}\ \nu\ \underset{\sim}{P}\ 0\ (\nu_t)\rangle$

$$= \frac{(2\pi)^4}{V_{rel}} \sum_{\gamma'} \int d^3\underset{\sim}{k}\ \delta(\varepsilon_K - \varepsilon_p + W_\gamma - W_o)|\langle \underset{\sim}{k}\ \nu'\ P\text{-}\rho\ \gamma|T_N|\underset{\sim}{p}\ \nu\ \underset{\sim}{P}\ 0\rangle|^2 \tag{F.19}$$

$$\underset{\sim}{\rho} = \underset{\sim}{K} - \underset{\sim}{p}$$

and

$$\frac{d\sigma}{d\Omega} = \frac{(2\pi)^4}{V_{rel}} \sum_{\gamma'} \int k^2\ dk\ \langle \underset{\sim}{p}\ \nu\ \underset{\sim}{P}\ 0|T_N|\delta(\varepsilon_K - \varepsilon_p + \hat{h} - W_o)|\underset{\sim}{k}\ \nu'\ P\text{-}\rho\ \gamma\rangle$$

$$\times\ \langle \underset{\sim}{k}\ \nu'\ P\text{-}\rho\ \gamma|T_N|\underset{\sim}{p}\ \nu\ \underset{\sim}{P}\ 0\rangle \tag{F.20}$$

Using

$$\mathcal{T}_\alpha|0\rangle = e^{-i\underset{\sim}{\rho}.\underset{\sim}{z}_\alpha}\ T_\alpha|Q\rangle \tag{F.21}$$

$$T_a = \langle \underset{\sim}{k}\ \nu',\ P\text{-}\rho|T_\alpha(\underset{\sim}{s}_\alpha)|\underset{\sim}{p}\ \nu\ P_\alpha\rangle \tag{F.22}$$

acting only on $\underset{\sim}{z}_\alpha$, s_α, and using $T_N = \sum_{\alpha=1}^{N} \mathcal{T}\alpha$ (F.23)

$$\frac{d\sigma}{d\Omega} = \frac{(2\pi)^4}{V_{rel}} \sum_{\gamma'} \sum_{\alpha\beta=1}^{N} \int k^2\ dk\ \langle \underset{\sim}{p}\ \nu\ \underset{\sim}{P}\ 0|T_\beta^+\ e^{-i\underset{\sim}{\rho}.\underset{\sim}{z}_\beta}\ \delta(\varepsilon_K - \varepsilon_p + h - W_o)$$

$$\times\ |\underset{\sim}{k}\ \nu'\ \underset{\sim}{P}\text{-}\rho\ \gamma\rangle\langle \underset{\sim}{k}\ \nu'\ \underset{\sim}{P}\text{-}\rho\ \gamma|\ e^{-i\underset{\sim}{\rho}.\underset{\sim}{z}_\alpha}\ T_\alpha|\underset{\sim}{p}\ \nu\ \underset{\sim}{P}\ 0\rangle \tag{F.24}$$

For a statistical ensemble

$$\frac{d\sigma}{d\Omega} = \frac{(2\pi)^4}{V_{rel}} \sum_{n_o} P_{n_o} \sum_{\gamma=n} \sum_{\alpha} \sum_{p=1} \int k^2 \, dk \, \langle \underset{\sim}{p} \; \nu \; \underset{\sim}{P} \; n_o | T_p^* \, e^{-i\rho \cdot z_\beta}$$

$$\times \; \delta(\varepsilon_K - \varepsilon_p + h - W_o) | \underset{\sim}{k} \; \nu' \; \underset{\sim}{P}-\rho \; n \rangle$$

$$\times \; \langle \underset{\sim}{k} \; \nu' \; \underset{\sim}{P}-\rho \; n | \; e^{+i\rho \cdot z_\alpha} \, T_\alpha | \underset{\sim}{p} \; \nu \; \underset{\sim}{P} \; n_o \rangle \qquad (F.25)$$

where one has not averaged over final spin states of the neutron nor considered an unpolarized neutron beam.

For neutrons one can take in the Born approximation

$$T_\alpha = V_\alpha \, , \qquad \text{and} \quad V_\alpha$$

for both nuclear and spin scattering is given by

$$V_\alpha = \hat{\eta}_\alpha \, V + F \left(\frac{2ge^2}{m_o c^2} \right)^{\frac{1}{2}} \{ \underset{\sim}{\rho} \cdot \underset{\sim}{S}_N \} \{ \underset{\sim}{\rho} \cdot \hat{\underset{\sim}{S}}_\alpha \} - (\underset{\sim}{S}_N \cdot \underset{\sim}{S}_\alpha) \qquad (F.26)$$

where $\hat{\eta}_\alpha$ is a projection operator onto the total spin states of nucleus and neutron, $\hat{\underset{\sim}{S}}_N$ is the spin of the neutron, $\hat{\underset{\sim}{S}}_\alpha$ is the spin of the atomic electrons, and F is a form factor.

If one considers unpolarized neutrons then the cross terms are zero and one can separate nuclear and magnetic scattering. Then, if

$$\langle k | F | \underset{\sim}{p} \rangle = F(\underset{\sim}{\rho}) \, ,$$

and averaging over final spin states one has to evaluate expressions of the form (Ref. (17))

$$\langle 0 | \{ (\underset{\sim}{\rho} \cdot \underset{\sim}{S}_N)(\underset{\sim}{\rho} \cdot \hat{\underset{\sim}{S}}_\beta) - (\underset{\sim}{S}_N \cdot \underset{\sim}{S}_\beta) \}^+ \{ (\underset{\sim}{\rho} \cdot \underset{\sim}{S}_N)(\underset{\sim}{\rho} \cdot \hat{\underset{\sim}{S}}_\alpha) - \underset{\sim}{S}_N \cdot \underset{\sim}{S}_\alpha \} | 0 \rangle_{av} \qquad (F.27)$$

av ≡ averaging over neutron spins.

Using

$$\langle 0|(\underline{e}.\underline{S}_N)^+(\underline{e}'.\underline{S}_N)|0\rangle_{av} = \frac{1}{4}\,\underline{e}.\underline{e}' \qquad (F.28)$$

one obtains equation (F.27) as

$$\langle 0|\sum_{ij}(\delta_{ij} - \frac{\rho_i\rho_j}{|\rho|^2})\,\hat{S}^i_\alpha\,\hat{S}^j_\beta|0\rangle_{av} \quad . \qquad (F.29)$$

For inelastic neutron scattering for an energy transfer of

$$\omega = \frac{k^2-p^2}{2m_N} \quad ,$$

one introduces a

$$\delta(\omega - \frac{(k^2-p^2)}{2m_N})$$

and find

$$\left.\frac{d\sigma}{d\Omega\,d\omega}\right|_{magn} = \left(\frac{2ge^2}{m_oc^2}\right)\frac{1}{h}\frac{|k|}{|p|}\,|F(\rho)|^2\sum_{n_o}p_{n_o}\sum_n\sum_{\alpha}\sum_{p=1}^{N}\sum_{ij}(\delta_{ij} - \frac{\rho_i\rho_j}{|\rho|^2})$$

$$\times\ \langle n_o|\hat{S}^i_\beta\,e^{-i\rho.z_\beta}\,\delta(\omega + h - W_o)|n\rangle\langle n|e^{+i\rho.z_\alpha}\,\hat{S}^j_\alpha|n_o\rangle \qquad (F.30)$$

Putting

$$\delta(\omega + h - W_o) = \int dt\; e^{-i(\omega + h - W_o)t} \qquad (F.31)$$

one can express the cross-section in terms of a time-dependent

correlation function. In fact, as it is the cross-section, it is expressed in terms of the spectral density of the spin-spin correlation function

$$S_{ij}(\rho,\omega) = \text{Im } K_{ij}(\underset{\sim}{\rho},\omega) \times \frac{I}{(1 - e^{-\beta\omega})}$$

(using theffluctuation dissipation theorem). (If $S_{ij} = S_{ji}$)

$$S_{ij}(\underset{\sim}{\rho},\omega) = \sum_N TH\langle \sum_{\alpha\beta}^N \hat{S}_\beta^i e^{-i\rho.z_\beta} \delta(\omega + h - W_o)|n\rangle\langle n| e^{+i\rho.z_\alpha} S_\alpha^j\rangle$$

$$= \int_{-\infty}^{+\infty} dt\, e^{-i\omega t} \sum_n \langle \sum_{\alpha\beta}^N S_\beta^i e^{-i\underset{\sim}{\rho}.\underset{\sim}{z}_\beta} e^{+i\omega_o t} e^{-i\hat{h}t}|n\rangle$$

$$\times \langle n| e^{i\rho.z_\alpha} S_\alpha^j\rangle_{TH} \qquad \text{(F.32)}$$

$$= \int_{-\infty}^{+\infty} dt\, e^{-i\omega t} \sum_{n_o} p_{n_o} \langle n_o| \sum_{\alpha\beta}^N \hat{S}_p^i e^{-i\rho.z_\beta} e^{-i\hat{h}t}$$

$$\times e^{i\rho.z_\alpha} S_\alpha^j e^{iht}|n_o\rangle$$

$$= \int dt\, e^{-i\omega t} S_{ij}(\rho,t)$$

$$S_{ij}(\rho,t) = \langle \sum_{\alpha\beta}^N \hat{S}_\beta^i e^{i\rho(z_\alpha - z_\beta(t))} S_\alpha^j(t)\rangle_{TH} \quad . \qquad \text{(F.33)}$$

If there is no thermal motion or it is neglected

$$z_\beta(t) = R_\beta \qquad z_\alpha(0) = \underset{\sim}{R}_\alpha$$

the lattice vector of the nuclei.

It can also be written as

$$S_{ij}(\underset{\sim}{\rho},t) = \int e^{i\rho.\underset{\sim}{r} - i\omega t}\, \Gamma_{ij}(\underset{\sim}{r},t)$$

$$\Gamma_{ij}(\underset{\sim}{r},t) = \sum_{\alpha\beta} \left\langle \int d\underset{\sim}{r}'\, \hat{S}^i_\beta(0)\, \delta(\underset{\sim}{r} + z_\alpha - \underset{\sim}{r}')\, \hat{S}^j_\beta(t)\, \delta(\underset{\sim}{r}' - z_\beta(t)) \right\rangle_{TH}.$$

(F.34)

Then finally

$$\left.\frac{d\sigma}{d\Omega\, dw}\right|_{magn} = \frac{2ge^2}{m_o c^2} \frac{1}{h} \frac{|k|}{|P|} |F(\rho)|^2$$

$$\times \sum_{n_o} p_{n_o} \sum_{\alpha} \sum_{\beta=1}^{N} \sum_{ij} \left(\delta_{ij} - \frac{\rho_i \rho_j}{|\rho|^2}\right) S_{ij}(\rho,\omega)$$

(F.34)

This is the prob/unit time of a neutron of wave vector $\underset{\sim}{k}$ being scattered in a unit solid angle around the direction $\underset{\sim}{k}$-$\underset{\sim}{\rho}$, with an energy change of $\hbar\omega$.

APPENDIX G

Calculation of Vertex Blocks

Let us first calculate the average of some operators $\hat{S}^{\alpha}(t)$. First consider the case when one has on the left the operator $\hat{S}^{+}$

$$\text{i.e.} \quad \langle \hat{S}^{+}\hat{S}^{z} \ldots \hat{S}^{-} \rangle = \text{Tr} \{\rho_{o} \hat{S}^{+}\hat{S}^{z} \ldots \hat{S}^{-}\} \qquad (G.1)$$

One has

$$\langle \hat{S}^{+}(\hat{S}^{z} \ldots \hat{S}^{-}) \rangle - \langle (\hat{S}^{z} \ldots \hat{S}^{-})\hat{S}^{+} \rangle$$

$$= \langle [\hat{S}^{+}, \hat{S}^{z}] \ldots \hat{S}^{-} \rangle + \ldots + \langle \hat{S}^{z} \ldots [\hat{S}^{+}, \hat{S}^{-}] \rangle \qquad (G.2)$$

since each intermediate term cancels.

The second term on the left can be rearranged by a cyclic transformation using

$$\hat{S}^{+}\hat{\rho}_{o} = e^{y} \hat{\rho}_{o}\hat{S}^{+} \qquad (G.3)$$

Therefore

$$(1 - e^{y})\langle \hat{S}^{+}\hat{S}^{z} \ldots \hat{S}^{-} \rangle = \langle \hat{S}^{+} \ldots \hat{S}^{-} \rangle + \ldots - \langle \hat{S}^{z} \ldots \hat{S}^{z} \rangle \qquad (G.4)$$

where one has used

$$[\hat{S}^{+}, \hat{S}^{z}] = -\hat{S}^{+} \qquad [\hat{S}^{+}, \hat{S}^{-}] = \hat{S}^{z} \; . \qquad (G.5)$$

The result is

$$\langle \hat{S}^{+}\hat{S}^{z} \ldots \hat{S}^{-} \rangle = n_{y}\{\langle \hat{S}^{+} \ldots \hat{S}^{-} \rangle + \ldots - \langle \hat{S}^{z} \ldots \hat{S}^{z} \rangle\} \qquad (G.6)$$

and the average of the product of a certain number of spin operators has been reduced to a sum of averages of products of a smaller number of operators. Further, the operator $\hat{S}^+$ has disappeared in each product, and one of the operators $\hat{S}^-$ and $\hat{S}$ has been replaced by $\hat{S}^z$ or $-\hat{S}^+$ respectively. Note that there are always the same number of $\hat{S}^-$ operators as there are $\hat{S}^+$ operators in any product (due to nature of $\hat{S}.\hat{S}$ interaction). This means that one does not have to consider strings of operators such as $\langle\hat{S}^-\hat{S}^-\ \hat{S}^z\ \hat{S}^-\hat{S}^z\rangle$. If there is no $\hat{S}^+$ operator in the product, then it is of the trivial form of a string of $\hat{S}_z$'s.

Then in order to complete the reduction of all operator products that one has to deal with, it remains only to consider the case when the operator $\hat{S}^+$ is not on the extreme left of the average in question. In this case one first transposes $\hat{S}^+$ to the left, commutations with $\hat{S}^z$ and $\hat{S}^+$ resulting in terms of the same form as in the right-hand-side of equation (G.4), but with a factor +1 or -1 for $\hat{S}^+$ and $\hat{S}^-$,

$$\text{e.g. } \langle S^z \ldots \hat{S}^+ \ldots \hat{S}^-\rangle = (n_y + 1)\langle\hat{S}^+ \ldots \hat{S}^-\rangle \ldots - n_y\langle\hat{S}^z \ldots \hat{S}^z\rangle \tag{G.7}$$

in the case of an $\hat{S}^-$ operator to the left one obtains a factor $-(n_y + 1)$.

Therefore terms obtained by contraction of $\hat{S}^+$ with operators on its left enter with a factor $\pm 1(n_y + 1)$ and those to the right with a factor $\pm n_y$. Taking into account that the time dependence of the operators is given by

$$\hat{S}^+(t) = e^{\hat{H}_o t}\, S^+(0)\, e^{-H_o t}$$

$$= e^{-ytT}\, \hat{S}^+(0) \tag{G.8}$$

$$\hat{S}^-(t) = e^{ytT}\, \hat{S}^-(0) \qquad \hat{S}^z(t) = S^z(0) \quad . \tag{G.9}$$

Then one can see (by writing out the product for each time ordering) that

$$\langle \hat{T}\{\hat{S}^+(t_1)\ \hat{S}^z(t_2)\ \ldots\ \hat{S}^-(t_n)\}\rangle$$

$$= G(t_1-t_2)\ \langle \hat{T}\{\hat{S}^+(t_2)\ \ldots\ \hat{S}^-(t_n)\}\rangle$$

$$+ \ \ldots\ - G(t_1-t_n)\ \langle \hat{T}\{\hat{S}^z(t_2)\ \ldots\ \hat{S}^z(t_n)\}\rangle$$

where

$$G(t) = e^{ytT} \begin{cases} n_y & t>0 \\ n_{y+1} & t<0 \end{cases} . \qquad (G.10)$$

One gets a + sign for a contraction with $\hat{S}^z$ and a -ve sign for a contraction with $\hat{S}^-$. If the process is continued one finally finds that one is always left with a string of one or several $\hat{S}_z$ operators.

Examples

1. $\Gamma_2^{zz}(t_1,t_2)$

$$\langle T\{\hat{S}^z(t_1)\ \hat{S}^z(t_2)\}\rangle = \langle T\{\hat{S}^z(0)\ S^z(0)\}\rangle$$

$$= \langle \hat{S}_z^2\rangle \ .$$

Then one must subtract the disconnected parts (equation (6-16), i.e. $\langle \hat{S}_z\rangle^2$. Therefore

$$\Gamma_2^{zz} = \langle \hat{S}_z^2\rangle - \langle S_z\rangle^2 = b'(y) \ .$$

Note that this is true only in the simple molecular field approximation. Therefore

$$\Gamma_2^{zz}(\omega_1,\omega_2) = b'\ \delta(\omega_1)\ \delta(\omega_2) \ .$$

2. $\Gamma_2^{+-}(t_1,t_2)$

$$\langle\hat{T}\{\hat{S}^+(t_1)\ \hat{S}^-(t_2)\}\rangle = \theta(t_1-t_2)\langle\hat{S}^+(t_1)\ \hat{S}^-(t_2)\rangle + \theta(t_2-t_1)\langle\hat{S}^-(t_2)\ \hat{S}^+(t_1)\rangle$$

$$= e^{y(t_2-t_1)T}\ \theta(t_1-t_2)\langle\hat{S}^+\hat{S}^-\rangle + \theta(t_2-t_1)\langle\hat{S}^-\hat{S}^+\rangle\ e^{y(t_2-t_1)T} \qquad (G-11)$$

$$\langle S^+S^-\rangle = n_y\langle S_z\rangle \qquad \langle S^-S^+\rangle = (n_y+1)\langle S_z\rangle \ ,$$

and

$$\langle S^+\rangle = \langle S^-\rangle = 0 \ . \qquad (G-12)$$

Therefore from equation (G-11)

$$\langle\hat{T}\{\hat{S}^+(t_1)\ \hat{S}^-(t_2)\}\rangle = \langle\hat{S}^z\rangle\ G(t_1-t_2) \ .$$

Because of equation (G-12) there are no disconnected diagrams to subtract. In general, the disconnected diagrams may be taken into account as stated in text.

3. $\Gamma_3^{+-z}(t_1,t_2,t_3) = \langle T\{S^+(t_1)\ S^-(t_2)\ S^z(t_3)\}\rangle - \langle T\{S^+(t_1)\ S^-(t_2)\}\rangle\langle S_z\rangle$

$$= -G(t_1-t_2)\langle T\{S^z(t_2)\ S^z(t_3)\}\rangle + G(t_1-t_3)\langle T\{\hat{S}^+(t_3)\ S^-(t_2)\}\rangle - \langle\hat{T}\{\hat{S}^+(t_1)\ S^-(t_2)\}\rangle\langle\hat{S}_z\rangle$$

$$= +G(t_1-t_2)\langle\hat{S}^z\hat{S}^z\rangle + G(t_1-t_2)\langle S^z\rangle^2 - G(t_1-t_3)\ G(t_3-t_2)\ b$$

$$= +b'\ G(t_1-t_2) - b\ G(t_1-t_3)\ G(t_3-t_2) \ .$$

4. $\Gamma^{+-zz}(t_1,t_2,t_3,t_4)$

We shall just calculate

$$<T\{S^+(t_1)\ S^-(t_2)\ S^z(t_3)\ S^z(t_4)\}>$$

and rely on the general theorem to take account of the disconnected diagrams

$$= - G(t_1-t_2)<\hat{T}\{\hat{S}^z(t_2)\ S^z(t_3)\ S^z(t_4)\}> + G(t_1-t_3)$$

$$<\hat{T}\{\hat{S}^+(t_3)\ S^-(t_2)\ S^z(t_4)\}> + G(t_1-t_4)$$

$$<T\{\hat{S}^+(t_4)\ S^-(t_2)\ S^z(t_3)\}>$$

$$= - b''\ G(t_1-t_2) + G(t_1-t_3)\{- G(t_3-t_2)<\hat{S}_z(t_2)\ S_z(t_4)\}>$$

$$+ G(t_3-t_4)\ G(t_4-t_2)b\} + G(t_1-t_4)$$

$$\{- G(t_4-t_2)\ b' + G(t_4-t_3)\ G(t_3-t_2)\ b\}$$

$$= b''\ G(t_1-t_4) - b'\ G(t_1-t_3)\ G(t_3-t_2) + b\ G(t_1-t_3)\ G(t_3-t_4)\ G(t_4-t_2)$$

$$- b'\ G(t_1-t_4)\ G(t_4-t_2) + b\ G(t_1-t_4)\ G(t_4-t_3)\ G(t_3-t_2)\ .$$

To obtain $\Gamma_4^{+-zz}(\omega_1 \ldots \omega_4)$ one has to fourier transform this expression (strictly speaking find the fourier coefficients).

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ACKNOWLEDGEMENTS

I would like to take this opportunity of acknowledging the help of my supervisor, Professor S. Doniach. I would like to thank the Science Research Council for the award of a research studentship held at Imperial College, and for the tenure of a Nato research studentship which allowed me to study at Harvard University for one year.