SPIN WAVES IN ITINERANT ELECTRON MAGNETS

A Thesis

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by

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ABSTRACT

This thesis is concerned with the development of a method for calculating spin wave energies in ferromagnets and antiferromagnets within the local exchange approximation. For a ferromagnetic metal the approach of Callaway and Wang (CW) is formulated in a new way which leads to an explicit formula for the spin wave stiffness constant D. It is found that the formula for D given by CW is incomplete since it neglects a term arising from local field effects. An explicit formula for the transverse dynamical susceptibility is obtained within the approximation of neglecting local field effects. It is shown that CW's method may be adopted to antiferromagnets and an equation for the spin wave energies is obtained for a general band structure. This is evaluated explicitly for the Hubbard model in the long wave length limit and the result agree with previous work by Skoloff. It is also shown how to calculate the dynamical susceptibility in the antiferromagnetic case.

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CHAPTER I

GENERAL INTRODUCTION

I.I Quantum Theories of Magnetism

Historically, Heisenberg[I] was the first to look for quantum mechanical origins of spontaneous magnetization - the phenomenon of ferromagnetism. The theory, which came to be known as the Heisenberg ferromagnetic theory, assumes electrons in a metal to be localised on atomic sites. They, in addition to having kinetic, potential and Coulomb repulsion energies, contribute an exchange energy term to the overall Hamiltonian of the system. The spins of electrons from each internal incomplete atomic shell, i.e. 3d shell in the iron group transition elements or 4f shell in the rare earths, are coupled together into a resultant spin moment S_j, which is localised at an ion situated at the lattice site j. The Heisenberg theory reduces the theory of a ferromagnet to that of a system of spin operators $S_j = (S_j^x, S_j^y, S_j^z)$ of magnitude S , belonging to each lattice point j of a crystal lattice.

The Heisenberg Model

To bring home the notion of how the exchange brings about spin alignment, thus giving rise to magnetism, we first consider the simplest case of two-atom molecule.

For two nuclei at positions a and b and two electrons at I and 2, the two energies E_a and $E_p - E_a$ is the antiparallel singlet energy and E_p the triplet energy belonging to the parallel orientation - were found as follows :

$$E_a = 2E_0 + (C + J)/(I + S^2)$$

$$E_p = 2E_0 + (C - J)/(I - S^2)$$

where E_0 is the energy of the isolated atom.

$C = \int |\psi_a(1)|^2 |\psi_b(2)|^2 V \, d\tau_1 d\tau_2$, is Coulomb Integral

$J = \int \psi_a^*(1) \psi_a(2) \psi_b(1) \psi_b^*(2) V \, d\tau_1 d\tau_2$, is exchange Integral

$S = \int \psi_a(1) \psi_b(1) \, d\tau_1$, the non-orthogonality Integral

$$V = e^2\left(\frac{1}{r_{ab}} - \frac{1}{r_{a2}} - \frac{1}{r_{b1}} + \frac{1}{r_{12}}\right)$$

The energy difference between the two spin alignments is

$$\begin{aligned} \Delta E &= E_a - E_p \\ &= 2(J - CS^2)/(1 - S^4) \\ &\simeq 2J \quad , \text{ if S is small.} \end{aligned}$$

So an important conclusion is that, for a spontaneous or stable ferromagnetic state to persist, $J > 0$. When $J < 0$, it gives antiferromagnetism.

In the Heisenberg model, as well as in the itinerant picture to be discussed later, the exchange interaction is the sole source of spontaneous magnetism in metals.

Working in the spin space only, which is adequate for dealing with magnetic phenomena, the effective spin Hamiltonian is written as

$$H = -\sum_{i \neq j} J_{ij} \underline{S}_i \cdot \underline{S}_j \qquad (I)$$

J_{ij} , known as the Exchange Integral, is equal in the case $S=\frac{1}{2}$ to the difference in energy between the configuration in which the spins on site i and site j are antiparallel and that in which they are parallel; and J_{ij} is a function of the distance $|R_i - R_j|$. This is known as the Heisenberg model and is in fact obtained by generalising the two-atom case to many atoms. It is rotationally symmetric in the spin space.

It is worth mentioning here that Dirac[2] too in 1929, in course of developing the vector model of the atom, arrived at the conclusion that the Coulomb interaction of electrons, together with the requirements imposed by the Pauli exclusion principle, gives rise to a peculiar quantum mechanical interaction - the exchange. However the notion that exchange causes spontaneous magnetism in solids is due to Heisenberg.

Exchange interactions are of more than one kind. The type of exchange we have referred to above is called the 'direct exchange'. Other kinds of exchanges viz. Rudermann-Kittel-Kasuya-Yosida and superexchange are known too. In the latter cases J_{ij} will have to be

appropriately redefined if the same form of Hamiltonian is to be retained.

The localised Heisenberg model was used by Bloch in the first theory of spin waves, as is described in chapter 2. Our principal interest is with the ferromagnetic and antiferromagnetic metals where the itinerant electron model is more appropriate.

The Itinerant Electron Model

In this model the electrons do not stay long enough at one atomic site for S_i to be defined as in the localised picture. Thus the Hamiltonian (I.I) is no longer acceptable. Electrons are now represented by the so-called Bloch waves $\psi(\underline{R},\underline{r})$ which are of the form

$$\psi(\underline{R},\underline{r}) = e^{i\underline{R}\cdot\underline{r}} u_{\underline{R}}(\underline{r})$$

where $u_k(r)$ has the periodicity of the lattice. These wave functions satisfy

$$H\psi(\underline{R},\underline{r}) = \mathcal{E}(\underline{R})\psi(\underline{R},\underline{r}) \qquad (I.2)$$

The wave vectors are labelled by k . If the one electron Hamiltonian H is derived using the H-F approximation, the potential energy includes Coulomb and exchange terms. The latter corresponds to a non-local interaction.

However, the simplest itinerant model was developed by Stoner[3] as a combination of the idea of energy bands in metals, replacement of the interaction by a molecular

field, and for finite temperature the use of Fermi-Dirac statistics for the electrons. Stoner assumed phenomenologically that exchange interactions led to a splitting of the energy bands of the two spins by an amount $2k_B\Theta'\zeta$ where ζ is the relative magnetisation, k_B is the Boltzmann constant, and Θ' is the exchange parameter.

There are two distinct microscopic approaches to the itinerant model. Both of these avoid the difficulty that use of the H-F approximation together with interactions of finite range leads to an exchange interaction which is non-local. The first approach, due to Hubbard[4], starts with a many body Hamiltonian, but with a screened Coulomb interaction so that electrons interact only on the same atomic site. The second approach, initially developed by Slater, introduces an effective exchange and correlation terms directly into the one electron equations.

To illustrate the first approach we may consider a metal such as Ni with a nearly filled d-band. A reasonable picture[5] of the top of the d-band in it is that of three independent tight-binding bands formed from xy, yz and zx orbitals with Bloch functions

$$\Psi_{m\underline{k}} = N^{-\frac{1}{2}} \sum_{R} \exp(i\underline{k}.R)\phi_m(r-R) \qquad (I.3)$$

$$m = 1, 2, 3$$

In the H-F approximation, with correlation neglected, there appears an exchange integral which is of the form

$$I^{HF}_{m\underline{k},n\underline{k}'} = N\iint \psi^{*}_{m\underline{k}}(\underline{r}_1)\,\psi_{n\underline{k}'}(\underline{r}_2)\,V(\underline{r}_1-\underline{r}_2) \times \psi_{m\underline{k}}(\underline{r}_2)\,\psi_{n\underline{k}'}(\underline{r}_1)\,d^3r_1\,d^3r_2 \qquad (I.4)$$

where $V(r_I - r_2)$ is the Coulomb interaction. This must be screened, and so it is considered to be acting only within a unit cell. On substituting (I.3) into (I.4), the exchange integral is found to be independent of $\underline{k}$ and $\underline{k}'$, and is given by the intra-atomic Coulomb integral

$$I_{mm} = \iint |\phi_m(\underline{r}_1)|^2 \left(\frac{e^2}{r_{12}}\right) |\phi_m(\underline{r}_2)|^2\, d^3r_1\, d^3r_2 \qquad (I.5)$$

for m = n, and by the Hund's rule exchange integral

$$I_{mn} = \iint \phi_m(\underline{r}_1)\,\phi_n(\underline{r}_2)\left(\frac{e^2}{r_{12}}\right)\phi_m(\underline{r}_2)\,\phi_n(\underline{r}_1) \times d^3r_1\, d^3r_2 \qquad (I.6)$$

for $m \neq n$.

For nickel $I_{mm} \approx 22$ ev and $I_{mn} \approx 0.8$ ev . But I_{mm} , which represents the interaction energy of two electrons - or two holes in the nearly-filled band case such as Nickel's - on the same atom, must certainly be modified due to correlation effects. This point was stressed by Wohlfarth[6]. Van Vleck's[7] method to estim-

ate I_{mm} is to consider the change in energy when two atoms change their configurations as follows :

$$d^9S + d^9S \longrightarrow d^{10}S + d^8S$$

From atomic spectroscopic data, this formula gives $I_{mm} \approx 8$ ev, which is very smaller than the value 22 ev calculated from the eqn (I.5) . Mott[8] and Herring[9], arguing that S electrons can follow the d-holes in the metal, suggested the change of configuration as

$$d^9S + d^9S \longrightarrow d^{10} + d^8S^2$$

which gives $I_{mm} \approx 2$ ev . For the lower value the screening must be assumed to be very good, and for the higher value 8 ev the vice versa. Thus, allowing for S screening, the integral I_{mm} should be replaced by an interaction parameter I, having a value within the range of 3 - 7 ev. This replacement done, the d-holes within a sub-band obey the Hamiltonian

$$H = \sum_{\underline{R}\sigma} \mathcal{E}(\underline{R}) n_{\underline{R}\sigma} + I \sum_i n_{i\uparrow} n_{i\downarrow} \qquad (I.7)$$

where i is the site index. This is the Hubbard [4] Hamiltonian within the first approach.

The interaction parameter I is crucially important in predicting spontaneous magnetism as it enters the criterion of ferro- or antiferromagnetism via the

susceptibility formula

$$\chi(q) = \frac{\chi^{\circ}(q)}{1 - I\chi^{\circ}(q)}$$

The criteria are

$$I\chi^{\circ}(0) > 1 \rightarrow \text{ferromagnetism}$$

$$I\chi^{\circ}(q) > 1 \rightarrow \text{antiferromagnetism}$$

But so far we have ignored the correlation effect in estimating I . If I_{mm} is small compared with the band-width, this non inclusion is justified since there is little correlation and two holes can and do often occupy the same site. But for I large, the d-band is correlated and we have to go beyond HF. Hubbard[4] and Kanamori[5] proposed theories which included correlation effects on I. Kanamori showed that the ground state properties of the hamiltonian (I.7) may be treated within the HF approximation if I is replaced by an effective interaction I_{eff},

$$I_{eff} = I(1+IG)^{-1},$$

$$G \simeq \frac{1}{2}\int_{E_F} \frac{N(\epsilon)}{\epsilon}\, d\epsilon \qquad \text{(I.8)}$$

and the hemiltonian of the eqn (I.7) is modified as

$$H = \sum_{\underline{R}\sigma} \varepsilon(\underline{R}) n_{\underline{R}\sigma} + I_{eff} \sum_{i} n_{i\uparrow} n_{i\downarrow} \qquad \text{(I.9)}$$

$N(\varepsilon)$ is the density of states per atom for holes and is measured from the bottom of the hole band, E_F being the hole Fermi energy. For Nickel Kanamori finds $I_{eff} \approx \frac{1}{2}$ ev which is less than the band width and depends more on the band structure.

The Hund's rule exchange integral is probably not important in Ni owing to fairly strong correlation. For Fe and Co this contribution must be significant.

The connection of this approach with the Stoner theory is found as follows : under the HF approximation the hamiltonian of (I.7) will be replaced by its diagonal part (q = 0) giving the total energy as

$$E = \sum_{\underline{R}\sigma} \varepsilon_{\sigma}(\underline{R}) n_{\underline{R}\sigma} + \frac{I_{eff}}{N} n_{\uparrow} n_{\downarrow} \qquad \text{(I.10)}$$

where $$n_{\sigma} = \sum_{\underline{R}} n_{\underline{R}\sigma} .$$

$$\frac{I_{eff}}{N} n_{\uparrow} n_{\downarrow} = \frac{1}{4} \frac{I_{eff}}{N} \left[(n_{\uparrow} + n_{\downarrow})^2 - (n_{\uparrow} - n_{\downarrow})^2 \right]$$

$$= \text{Constt} - \frac{I_{eff}}{4N} n^2 \zeta^2$$

where $\zeta = \frac{(n_{\uparrow} - n_{\downarrow})}{n}$ is the relative magnetization, n the total number of electrons. Thus it is established that the expression (I.10) is equivalent to the energy expression of the Stoner model

$$E_{\zeta} = \sum_{\underline{R}\sigma} \varepsilon_{\sigma}(\underline{R}) n_{\underline{R}\sigma} - \frac{I_{eff}}{4N} n^2 \zeta^2 \qquad \text{(I.11)}$$

There is now a splitting of band into $\uparrow$ and $\downarrow$ spin bands.

The energy of each spin band is given by

$$\epsilon_\sigma(\underline{R}) = \frac{\partial E}{\partial n_{\underline{R}\sigma}}$$

$$= \epsilon_\sigma(\underline{R}) - \frac{n I_{eff} \zeta}{2N} \frac{\partial}{\partial n_{\underline{R}\sigma}} (n_\uparrow - n_\downarrow)$$

$$= \epsilon_\sigma(\underline{R}) - \frac{n I_{eff} \zeta}{N} \sigma \qquad \text{(I.I2)}$$

$\sigma = \pm \frac{1}{2}$ for $\uparrow$ or $\downarrow$ spin.

The exchange splitting is

$$\Delta E = \frac{n I_{eff} \zeta}{N} \qquad \text{(I.I3)}$$

The original expression for the spin splitting in the Stoner model, $\Delta E = 2 R_B \theta' \zeta$, can be compared with (I.I3), i.e.

$$2 R_B \theta' \zeta = \frac{n I_{eff} \zeta}{N} \qquad \text{(I.I4)}$$

The eqn (I.I4) defines θ' in terms of the I_{eff} and thus connects the Stoner model with the present Hubbard approach.

The other approach is known as the local exchange approximation in which the non-local exchange potential is replaced by an averaged local potential. The first approximation was introduced by Slater[I0] who based it on the theory of free electron gas. The exchange potential in a paramagnetic gas of density ρ is given in the HF approximation by

$$V_{x\,gas} = -8F\left(\frac{|\underline{R}|}{k_F}\right)\left(\frac{3\rho}{8\pi}\right)^{\frac{1}{3}} \qquad \text{(I.I5)}$$

where

$$F(Y) = \frac{1}{2} + \frac{1-Y^2}{4Y} \ln\left|\frac{1+Y}{1-Y}\right| \qquad \text{(I.I6)}$$

Electrons occupy states within a sphere centered on

$\underline{k} = 0$ and of radius k_F for each spin. In the HF theory the density of state, which depends inversely on dE/dK, vanishes on the Fermi Surface. This is because the HF theory neglects electron correlation. This is avoided by considering an averaged local exchange potential. Because of this local exchange potential, band structure will be more important in determining the nature of magnetism of the metal. Kohn and Sham's work actually showed that there exists a local potential $V_\alpha(r)$ which leads to the exact particle and spin densities when these are calculated by summing amplitudes over occupied states. Treating ρ as the local charge density and replacing F(y) by its average value over all occupied states, $\frac{3}{4}$, the potential is

$$V_{xs\sigma} = -6\left[\frac{3}{\pi}\rho(r)\right]^{\frac{1}{3}} \qquad (I.17)$$

Kohn and Sham[II], following Gasper[I2], applied the variational method to an inhomogeneous system of interacting electrons and obtained

$$V_{x,KSG} = \frac{2}{3}V_{xs} \qquad (I.18)$$

In fact the current practice is to use an exchange potential $V_{x\alpha\sigma} = \alpha V_{xs\sigma}$ known as the $X\alpha$ method where α is treated as a parameter which is allowed to vary between I and $\frac{2}{3}$.

In calculating one electron Bloch wave functions in

this approach, one considers a single electron hamiltonian of the form

$$H = \frac{P^2}{2m} + \sum_{\ell} \frac{Ze^2}{|\underline{r}-\underline{R}_\ell|} + e^2 \int \frac{\rho(\underline{r}')}{|\underline{r}-\underline{r}'|} d^3r' - V_{xc,a}(\underline{r}) + V_f(\underline{r})\underline{\sigma}\cdot\underline{n} + H_{s.o.c} \qquad (I.19)$$

The 4th and 5th terms are defined by

$$V_{xc,a} = \tfrac{1}{2}\left[V_{xc\uparrow} + V_{xc\downarrow}\right]$$
$$V_f = \tfrac{1}{2}\left[V_{xc\uparrow} - V_{xc\downarrow}\right] \qquad (I.20)$$

Here $V_{xc\sigma}$ may be taken in the $X\alpha$ form $V_{x\alpha\sigma}$ or as a more complicated function of charge and spin density which may include additional correlation effects(von Barth and Hedin[I3]). In this approach self-consistent solutions of ferro and antiferromagnetic type of metals are possible.

The relation between Stoner theory and the spin density functional formalism has been discussed by Gunnarsson[I4].

In both the localised and itinerant models, a ferromagnetic system is composed of one lattice; but for antiferromagnetism an interpenetrating 2-sublattice picture must be assumed.

I.2 Spin Waves

The notion of a spin wave was first introduced by Bloch[I5] on the basis of the Heisenberg hamiltonian.

Field-theoretic methods were employed by Holstein and Primakoff[I6] and an improved treatment along this line was carried out by Dyson[I7], which enhanced the importance of spin wave phenomenon in the study of low temperature thermodynamic properties. The essence of the method lies in describing the low-lying energy levels of a system of a large number of strongly interacting spin moments in terms of a collective mode, whose quanta are known as spin waves or magnons. Nevertheless, it should be noted that spin waves are not the consequences of the particular microscopic model considered, rather phenomenologically too they were conjectured by Landau and Lifshitz and also by Herring and Kittel. First we discuss spin waves in the Heisenberg model.

The isotropic exchange hamiltonian of (I.I) receives quantisation direction by an external applied magnetic field $\mathcal{H}_A$, say in the Z-direction. A Zeeman term is therefore added and the hamiltonian takes the form

$$H = -g\mu_B \mathcal{H}_A \sum_j S_j^z - \sum_{i \neq j} J_{ij} \underline{S}_j \cdot \underline{S}_i \qquad (I.2I)$$

The ground state is $|0\rangle$ with all the spins aligned along the Z-direction, and with the property of S_j^+ operator acting upon it that

$$S_j^+ |0\rangle = 0$$

The total spin in the $|0\rangle$ is $NS = \sum_i S_i^z$ and the state

satisfies

$$H|0\rangle = E_0|0\rangle$$

where the eigenvalue is

$$E_0 = -g\mu_B NS\mathcal{H} - \sum_{i\neq j} S^2 J_{ij} \qquad \text{(I.22)}$$

An excited state, which is an exact eigenstate of the hamiltonian (I.2I) and in which the Z-component of the total spin has NS-I as the eigenvalue i.e. with one spin reversed, is constructed by superposing states with one reversed spin localised at a definite lattice site. Such a state is

$$|\underline{q}\rangle = \frac{1}{\sqrt{2S}} S^-_{\underline{q}}|0\rangle \qquad \text{(I.23)}$$

where $S^-_{\underline{q}} = \sum_i e^{i\underline{q}.\underline{R}_i} S^-_i$ i.e. the Fourier transform of S^-_i

The energy eigenvalue of this state is

$$E_1 = E_0 + g\mu_B\mathcal{H} + 2S[J(0) - J(\underline{q})]$$

where $J(\underline{q}) = \sum_{i\neq j} J_{ij} e^{-i\underline{q}.(\underline{R}_i - \underline{R}_j)}$ In this state there is said to propagate a spin wave having wave vector q with the energy

$$\mathcal{E}_{\underline{q}} = g\mu_B\mathcal{H} + 2S[J(0) - J(\underline{q})]$$

the excitation energy being

$$\hbar\omega_{\underline{q}} = 2S[J(0) - J(\underline{q})] \qquad \text{(I.24)}$$

For cubic crystals, with the condition that $aq \ll I$,

$$\tfrac{1}{\hbar}w_q = 2JSa^2q^2$$

$$= Dq^2$$

D is the so-called stiffness constant.

But it is not the unique property of the Heisenberg model which is responsible for spin waves. Herring and Kittel[I8] used a phenomenological approach which concentrated attention on the study of nonuniformity of magnetisation in ferromagnetics. By considering the production of a variation of magnetic moment with position, which is effected by a weak, spatially varying external field, they found that the energy change δE per unit volume of the crystal involved with the non-uniformity of the magnetisation M(r), is

$$\delta E = A\sum_{x,y,z}\left(\frac{\partial M}{\partial x}\right)^2 \Big/ M^2 \qquad \text{(I.25)}$$

where A is the Bloch-wall stiffness. 'A' can only be determined theoretically by quantum mechanical methods. And macroscopically, the spins in a small region experience a torque which press them to align parallel to an average of magnetisation in the neighbouring regions, thereby causing the spin density to precess gyroscopically. The normal modes are spin waves, whose quanta are the magnons. For small q, the frequency of precession is

$$\omega_q = \left(\frac{2A}{M_0}\right)\left(\frac{e}{mc}\right)q^2 \qquad \text{(I.26)}$$

M_o is the magnetisation per unit volume.

The phenomenon of spin waves within band model was first dealt with by Slater[I9] who obtained an expression for the spin wave energy for a half-filled band only. And Herring[20], Izuyama[2I], and Edwards[22] derived expression for spin wave energy for a more general case. The final breakthrough was however achieved by Izuyama, Kim and Kubo[23]. They were able to show, using Hubbard type hamiltonian and within RPA, that there are split off spin wave states below the Stoner continuum of single particle excitations. The operator $S^-_{\underline{q}} = \frac{1}{\sqrt{N}} \sum_{\underline{k}} C^+_{\underline{k}+\underline{q}\downarrow} C_{\underline{k}\uparrow}$ in the limit $q \to 0$ generates the spin waves which exist for $q < q_{max}$ below the Stoner continuum. This point is explained in detail in the next chapter.

Quantitatively the spin wave energy $\hbar\omega = Dq^2$ is measurable. And expressions for D under various approximate and exact schemes have been derived and compared with the measured values. In this thesis D will remain the topic of central concern and so a separate chapter is devoted to it.

CHAPTER II

SPIN WAVE ENERGY OF FERROMAGNETS

Spin wave energies are obtained by looking at the poles of the susceptibility function, which is expressible in the form of retarded Green's Function. And the imaginary part of the susceptibility is also involved in magnetic scattering of neutrons. Therefore a brief account of the method of Green's Function and susceptibility is given in this chapter. But before that, a variational approach, which in our case is equivalent to RPA at T = 0, gives an expression for D within the RPA and for the one as well as the many band case.

D within the RPA

Considering the wave function

$$|\underline{q}\rangle = \sum_{\underline{R}}^{*} f_{R} C^{+}_{\underline{R}+\underline{q}\downarrow} C_{\underline{R}\uparrow} |0\rangle \qquad (2.I)$$

$|0\rangle$ being the HF ground state and $\sum^{*}$ denoting the sum over k such that $\epsilon_{\underline{R}} < \epsilon_{f\uparrow}, \epsilon_{\underline{R}+\underline{q}} > \epsilon_{f\downarrow}$ and minimising

$$\langle \underline{q}|H|\underline{q}\rangle - \mathcal{E}\langle \underline{q}|\underline{q}\rangle,$$

where $\mathcal{E} = \mathcal{E}_0 + \hbar\omega$,

$\mathcal{E}_0$ is the ground state energy.

we obtain the secular equation

$$f_{\underline{R}}\left[\epsilon_{\underline{R}+\underline{q}}-\epsilon_{\underline{R}}+\Delta-\hbar\omega\right] = \frac{I_{eff}}{N}\sum_{\underline{R}}^{*} f_{\underline{R}'} \qquad (2.2)$$

The replacement of I by I_{eff} was shown by Lowde and Windsor[24] to successfully explain the neutron scattering data on nickel which is an itinerant ferromagnet. Solving (2.2) we get

$$f_{\underline{R}} = \frac{1}{\epsilon_{\underline{R}+\underline{q}}-\epsilon_{\underline{R}}+\Delta-\hbar\omega} \qquad (2.3)$$

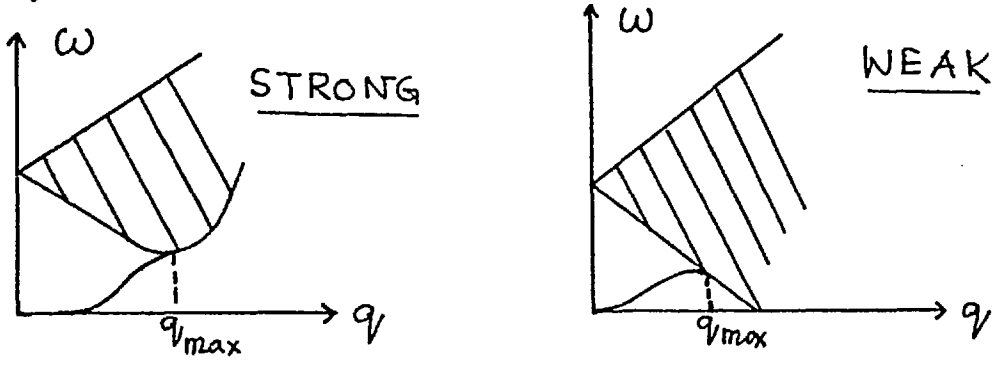
with ω satisfying

$$1 = \frac{I_{eff}}{N}\sum_{\underline{R}}^{*} \frac{1}{\epsilon_{\underline{R}+\underline{q}}-\epsilon_{\underline{R}}+\Delta-\hbar\omega} \qquad (2.4)$$

or

$$I_{eff}^{-1} = \frac{1}{N}\sum_{\underline{R}}^{*} \frac{1}{\epsilon_{\underline{R}+\underline{q}}-\epsilon_{\underline{R}}+\Delta-\hbar\omega} \qquad (2.5)$$

Eqn (2.5) has a continuum of roots which corresponds to the Stoner continuum of single particle excitations; and there will be a possible split off state below it. When $N \longrightarrow \infty$, the RHS of (2.5) goes to an integral which tends to a finite limit λ as ω approaches the continuum from below. Thus there will be a split off state for $I_{eff} > \frac{1}{\lambda}$; and λ depends on q. It is illustrated below



For $q < q_{max}$ there are spin waves as split off states from the stoner continuum and when $q \to 0$, $f_k \to I$. By expanding the RHS of (2.4) an expression for D for a cubic crystal and within one band is obtained as

$$D = \frac{1}{3(n_\uparrow - n_\downarrow)} \sum \left\{ \frac{n_{\underline{R}\uparrow} + n_{\underline{R}\downarrow}}{2} \nabla^2 \epsilon_{\underline{R}} - \frac{n_{\underline{R}\uparrow} - n_{\underline{R}\downarrow}}{\Delta} \left| \nabla \epsilon_{\underline{R}} \right|^2 \right\} \qquad (2.6)$$

$n_{\underline{k}\uparrow}$, $n_{\underline{k}\downarrow}$ are the ground state occupation numbers.

In principle the procedure can be extended to the many band case by summing eqn (2.I) over the bands. But to get to a managable form, Wakoh, Edwards and Wohlfarth[25] assumed exchange splitting in all the bands to be the same and used Green's theorem. The expression for D turned out to be

$$D = \frac{1}{3(n_\uparrow - n_\downarrow)} \left\{ \frac{1}{2} \left[M(\epsilon_{f\uparrow}) + M(\epsilon_{f\downarrow}) \right] - \frac{1}{\Delta} \int_{\epsilon_{f\downarrow}}^{\epsilon_{f\uparrow}} M(\epsilon)\, d\epsilon \right\} \qquad (2.7)$$

where

$$M(\epsilon) = \frac{\Omega}{8\pi^3} \sum_\lambda \int_{\epsilon_{\lambda \underline{R}} = \epsilon} \left| \nabla \epsilon_{\lambda \underline{R}} \right| dS$$

and λ the band index. This RPA expression for D compared well with the experimental value for Nickel. But for Co and Fe it remains unsuccessful. The same RPA

formula of (2.6) is obtained from the susceptibility formula of Kubo, which we will discuss later.

Green's Function, Susceptiblity and Neutron Scattering

The causal Green's Functions (henceforth to be called GF), which are used to determine the energy spectrum in the quantum field theory approach within the perturbation approximation, are defined as

$$G_1(t,t') = -\frac{i}{\hbar}\left\langle T\{A(t)\,B(t')\}\right\rangle \qquad (2.8)$$

where the ordering operator T is understood to act as

$$T\{A(t)B(t')\} = \theta(t-t')A(t)B(t') + \eta\theta(t'-t)B(t')A(t)$$

where $\eta = \begin{cases} +\,I \\ -\,I \end{cases}$ $\begin{matrix} \text{for A,B boson operators} \\ \text{for A,B fermion operators} \end{matrix}$

and $\theta(t'-t)$ is the wellknown step function,

$$\theta(t'-t) = \begin{matrix} I & , \text{ if } t' > t \\ 0 & , \text{ if otherwise} \end{matrix} \qquad (2.9)$$

To evaluate the causal GFs one must go via the imaginary time GF,

$$G_1(\tau) = \frac{-i}{\hbar}\left\langle T\{A(\tau)\,B(0)\}\right\rangle \qquad (2.10)$$

where $A(\tau) = e^{H\tau/\hbar} A\, e^{-H\tau/\hbar}$ with a hamiltonian $H = H_0 + H_I$, where H_I is treated as a perturbation. $G_1(\tau)$ can be written as a continuous product of imaginary time GFs involving H_0 only.

$$G_1(\tau) = -i/\hbar \left\langle T\left\{ \exp\left(-\int_0^{\hbar\beta} H_I(\tau')\, d\tau'/\hbar\right) A(\tau) B(0)\right\}\right\rangle_0$$

$$\Big/ \left\langle T\left\{ \exp\left(-\int_0^{\hbar\beta} H_I(\tau')\, d\tau'/\hbar\right)\right\rangle \qquad (2.II)$$

where

$$\langle X \rangle = Tr\left\{ e^{-\beta H_0} X\right\} \Big/ Tr\left\{ e^{-\beta H_0}\right\}$$

and $\quad 0 \leqslant \tau \leqslant \hbar\beta .$

The Fourier Transform of $G_1(\tau)$ is

$$G_1(\omega_n) = \frac{1}{2} \int_{-\hbar\beta}^{\hbar\beta} e^{i\omega_n \tau}\, G_1(\tau), \quad \omega_n = \frac{\pi n}{\beta\hbar} \qquad (2.I2)$$

and therefore

$$G_{Per}(\tau) = \frac{1}{\hbar\beta} \sum_{n=-\infty}^{\infty} e^{-i\omega_n \tau}\, G_1(\omega_n), \qquad (2.I3)$$

$$-\infty < \tau < \infty$$

But these $G_1(\omega_n)$s are not analytic and for application in magnetism and other fields, the socalled retarded and advanced GFs are introduced. They are analytic in the upper and lower energy half-plane. To describe propagation of electrons , retarded GFs were employed by Hubbard[26]. A fuller review of this technique is given by Zubarev[27]; that of the causal GFs are done by Martin and Schwinger[28] and Baym and Mermin[29]. The retarded (+)

and the advanced (-) GFs are defined by

$$\langle\langle A(t);B(t')\rangle\rangle^{\pm} = -i/\hbar\,\theta\left\{\pm(t-t')\right\}\left\langle\left[A(t),B(t')\right]_{\eta}\right\rangle \qquad (2.I4)$$

where $A(t)=e^{iHt/\hbar}A\,e^{-iHt/\hbar}$ and $B(t')$ are two operators and

$$\left[A,\,B\right]_{\eta} = \left.\begin{matrix} AB - BA \\ AB + BA \end{matrix}\right\} \quad \begin{matrix} \text{for bosons} \\ \text{for fermions} \end{matrix}$$

and $\theta\left\{\pm(t-t')\right\}$ is the step function. The thermal average is

$$\langle X\rangle = Tr\left\{e^{-\beta H}X\right\} / Tr\left\{e^{-\beta H}\right\}$$

$\langle\langle A(t);B(t')\rangle\rangle$ being a function of t - t', its Fourier Transform can be defined as

$$\langle\langle A,B\rangle\rangle^{\pm}_{\omega} = \int_{-\infty}^{\infty}\langle\langle A(t);B(0)\rangle\rangle\, e^{\pm i\omega t}\,dt \qquad (2.I5)$$

Of these, $\langle\langle A,B\rangle\rangle^{+}_{\omega}$ is analytic in the complex upper half-plane of ω, $\mathrm{Im}\,\omega>0$; and $\langle\langle A,B\rangle\rangle^{-}_{\omega}$ in the lower half-plane, $\mathrm{Im}\,\omega<0$ [27]. It can also be shown that[28]

$$G(\omega_n) = \langle\langle A;B\rangle\rangle^{+}_{i\omega_n}, \qquad \omega_n>0$$
$$G(\omega_n) = \langle\langle A;B\rangle\rangle^{-}_{i\omega_n}, \qquad \omega_n<0 \qquad (2.I6)$$

i.e. the causal GFs are derivable from the retarded and advanced GFs; and the analytic continuation of the causal GFs determines the retarded and advanced GFs.

But the solution of these Green's Functions and of their Fourier Transforms, by setting up their equation of motion and decoupling them by cutting after two terms, is more important for us. We therefore give here a brief sketch of that.

By noting that $i\hbar \frac{\partial A(t)}{\partial t} = [A(t), H]$

we obtain by differentiating retarded and advanced GFs

$$i\hbar \frac{\partial}{\partial t} \ll A(t); B(t') \gg^{\pm} = -\delta(t-t') \langle [A(t), B(t)]_{\eta} \rangle + \ll [A(t), H]; B(t') \gg^{\pm} \qquad (2.17)$$

and the second term has also an equation of motion with a higher order Green's Function on the right hand side,

$$i\hbar \frac{\partial}{\partial t} \ll [A(t), H]; B(t') \gg^{\pm} = -\delta(t-t') \langle [[A(t), H]; B(t)]_{\eta} \rangle + \ll [[A(t), H], H]; B(t') \gg^{\pm} \qquad (2.18)$$

The decoupling can be carried out at the second term in (2.17) by linearising , as for example in the case of χ within the RPA. Or, still higher order terms can be retained and other ingenious ways may be employed.

The other important point about these GFs is that the discontinuity across the real axis is related to the correlation function $\langle A(t)\, B(0)\rangle$ by the socalled spectral theorem,

$$\langle A(t)\, B(0)\rangle = \frac{i\hbar}{2\pi}\int_{-\infty}^{\infty} \lim_{\varepsilon\to 0}\frac{\left(\langle\langle A,B\rangle\rangle_{\omega+i\varepsilon} - \langle\langle A,B\rangle\rangle_{\omega-i\varepsilon}\right)}{1+\eta\, e^{-\beta\hbar\omega}} \times e^{-i\omega t}\, d\omega \qquad (2.19)$$

and $\langle\langle A;B\rangle\rangle_{\omega-i\varepsilon} = \langle\langle B;A\rangle\rangle^{*}_{\omega+i\varepsilon}$

The dynamic susceptibility, i.e. the response function of an oscillating magnetic field, involves the Fourier Transform of Green's Functions discussed above[23]. The interaction energy of the spin density $S_\alpha(r')$ of a metal and the oscillating magnetic field

$$\frac{1}{2} H_\alpha e^{-i(q.r' + \omega t')} e^{\varepsilon t'} + c.c.$$

is

$$\frac{1}{2} g\mu_B H_\alpha \int_V S_\alpha(r') e^{-i(q.r' + \omega t')} e^{\varepsilon t'} dr' + c.c. \qquad (2.20)$$

And the response of a point r of the spin density at a time t is

$$\delta S_\beta(r,t) = -(g\mu_B)^2 Re\left[\langle\langle S_\beta(r'); S_\alpha(-q)\rangle\rangle_{\omega+i\varepsilon} H_\alpha e^{-i\omega t} e^{\varepsilon t}\right]$$

$$= \frac{-(g\mu_B)^2}{V} Re\left[\sum_R \langle\langle S_\beta(R+q); S_\alpha(-q)\rangle\rangle_{\omega+i\varepsilon} \times H_\alpha e^{-i[(q+R).r + \omega t]} e^{\varepsilon t}\right] \qquad (2.21)$$

The summation is over reciprocal lattice vectors and

$$S_\alpha(\underline{q},\omega) = \int_{-\infty}^{\infty}\int_V S_\alpha(\underline{r})\, e^{i(\underline{q}\cdot\underline{r}+\omega t)}\, dr\, dt \qquad (2.22)$$

We have

$$S_\beta(\underline{R}+\underline{q},\omega) = \chi_{\beta\alpha}(\underline{R}+\underline{q},\underline{q},\omega)H_\alpha \qquad (2.23)$$

whence the dynamical susceptibility is

$$\chi_{\beta\alpha}(\underline{R}+\underline{q},\underline{q},\omega) = \frac{(g\mu_B)^2}{V}\langle\langle S_\beta(\underline{R}+\underline{q}); S_\alpha(-\underline{q})\rangle\rangle_{\omega+i\varepsilon} \qquad (2.24)$$

This is the Kubo formula. As mentioned earlier, the transverse susceptibility tensor $\chi_{+-}(\underline{q},\omega)$ has singularities which give the spectrum of single particle excitations as well as the spin wave energy.

The susceptibility

$$\chi_{-+}(\underline{q},\omega) = \lim_{\varepsilon\to 0}\int_\alpha^\infty \langle\langle S^-_{\underline{q}}(t); S^+_{-\underline{q}}\rangle\rangle e^{i(\omega-i\varepsilon)t}\, dt$$

is solved by the previously shown technique of equation of motion of Green's Function. Of the commutator

$$\sum_{\underline{R}}\left[\, c^+_{\underline{R}+\underline{q}\downarrow}c_{\underline{R}\uparrow}\,,\, H_0+H_I\,\right]$$

, which appears in the equation, the first part is evaluated exactly, but the $\left[c^+_{\underline{R}+\underline{q}\downarrow}c_{\underline{R}\uparrow}\,,\, H_I\right]$ is carried out within RPA which linearises the equation. Replacing number operators by the the thermally average occupation nos $f_{\underline{k}}$,

$\chi(q,\omega)$ is expressed by the following

$$\chi(\underline{q},\omega) = \frac{\Gamma(\underline{q},\omega)}{1 - \frac{I_{eff}}{N}\Gamma(\underline{q},\omega)} \qquad (2.25)$$

where

$$\Gamma(\underline{q},\omega) = \sum_{\underline{R}} \frac{f_{\underline{R}\uparrow} - f_{\underline{R}+\underline{q}\downarrow}}{\epsilon(\underline{R}+\underline{q}) - \epsilon(\underline{R}) + \Delta - \hbar\omega + i\varepsilon} \qquad (2.26)$$

By equating the denominator of (2.25) to zero, eqn (2.4) at T = 0 is obtained, which will give the single particle excitation spectrum and the spin wave pole including the expression for D derived previously. This indicates how an expression for D can be worked out by looking at the pole of χ .

The imaginary part is also important, since it enters into the cross-section of inelastic magnetic scattering of neutrons[23, 24]. The differential cross-section is

$$\frac{\partial^2\sigma}{\partial\Omega\partial\omega} = \left(\frac{e\gamma}{\hbar c}\right)\frac{\underline{k}'}{\underline{k}} \sum_{\alpha,\beta} \left(\delta_{\alpha\beta} - \hat{q}_\alpha \hat{q}_\beta\right) M^{\alpha\beta}(\underline{q},\omega) \qquad (2.27)$$

where $\underline{k}$ is the wave vector of the incident neutrons, $\underline{k}'$ that of the scattered neutrons, with $\underline{k}' = \underline{k} + \underline{q}$, q being the unit vector $\underline{q}/q$.

$$\hbar\omega = \frac{1}{2}\hbar^2 k^2/m - \frac{1}{2}\hbar^2 k'^2/m$$

and $M^{\alpha\beta}(\underline{q},\omega)$ is the correlation function which is equal to

$\left(\frac{e\hbar}{mc}\right)^2 S^{\alpha\beta}(\underline{q},\omega)$, when the scattering is principally due to spin magnetisation.

$$S^{\alpha\beta}(\underline{q},\omega) = \frac{1}{2\pi}\int_V d\underline{r}\int_V d\underline{r}'\int_{-\infty}^{\infty} dt\, e^{i(\underline{q}.\underline{r}+\omega t)} \left\langle S_\alpha(\underline{r}+\underline{r}',t) S_\beta(\underline{r}')\right\rangle \qquad (2.28)$$

$$= \frac{1}{2\pi}\int_{-\infty}^{\infty} dt\, e^{i\omega t}\left\langle S_\alpha(\underline{q},t)\, S_\beta(-\underline{q})\right\rangle \qquad (2.29)$$

The susceptibility function is involved in the expression for $S^{\alpha\beta}(\underline{q},\omega)$ via the following equation

$$S^{\alpha\beta}_{Symm}(\underline{q},\omega) = \frac{-\hbar}{\pi}\left(1-e^{-\beta\hbar\omega}\right)^{-1} Im\left\langle\!\left\langle S_\alpha(\underline{q})\,;\, S_\beta(-\underline{q})\right\rangle\!\right\rangle_\omega \qquad (2.30)$$

$$= \frac{\hbar}{\pi}\left(1-e^{-\beta\hbar\omega}\right)^{-1}\frac{V}{(g\mu_B)^2} Im\,\chi^{Symm}_{\alpha\beta}(\underline{q},\underline{q},\omega) \qquad (2.31)$$

'Symm' denotes the symmetric part of the function.

Thus it needs hardly any more emphasising the key role of the Green's Functions in the study of magnetism and magnetic response.

Exact Formula for D : Edwards-Fisher Formalism

Exact formulas for D, starting from first principles, were attempted by Abrikosov and Dzialoshinsky[30] by

extending to ferromagnetism Silin's[31] work in the paramagnetic case within Landau theory. But it was rejected on grounds of nonrigorousness, as discussed by Herring[9] .

Also, using the fact that $S_0^- |0\rangle$ is an exact eigenstate representing a spin wave of wave vector $\underline{q}$ in both the Heisenberg and the itinerant model, Edwards[32a,b] obtained an exact formula for D for a strong ferromagnet only. He used the first terms of an expansion in powers of q , the only condition being that the inverse life time of the spin wave will go to zero faster than q^2 , as $q \to 0$; the spin wave is then well defined and for very small values of q , the theory is exact. Still the restricted validity for strong ferromagnets only led to the search for a more general formula. Edwards and Fisher[33] derived such a formula by generalising Ma[34] et.al's work.

For a system having rotational symmetry in the spin space, and if spin-orbit and dipole-dipole interactions are ignored, the hamiltonian can be shown to commute with the total spin step down operator S_0^- . Because, if $|\psi\rangle$ is an eigenstate, so will be $S_0^- |\psi\rangle$ with the same total S but S^z less by one; energy eigenvalue remains unchanged.

$$\begin{aligned} [H, S_0^-]|\psi\rangle &= HS_0^-|\psi\rangle - S_0^- H|\psi\rangle \\ &= E S_0^-|\psi\rangle - S_0^- E|\psi\rangle \\ &= 0 \end{aligned} \qquad (2.32)$$

or $$[H, S_0^-] = 0$$

This property is exhibited by any isotropic ferromagnet along with the condition that the total magnetisation is aligned arbitrarily. In the ground state, however, an infinitesimally small magnetic field gives a preferred direction of magnetisation vector, so that we can assume almost all the spins are up.

We now set up the equation of motion for the generalised susceptibility,

$$\chi_{+-}(\underline{q},\omega) = \int dt \langle\langle S_{-\underline{q}}^+(t) ; S_{\underline{q}}^- \rangle\rangle e^{i\omega t}$$

S_q^+ S_q^- are the Fourier components of spin density defined by

$$S_{-\underline{q}}^+ = \int e^{-i\underline{q}.\underline{r}} S^+(r)\, dr$$
$$= \sum_i e^{-i\underline{q}.\underline{R}_i} S_i^+ = \sum_{\underline{R}} C_{\underline{R}-\underline{q}\uparrow}^+ C_{R\downarrow} \qquad (2.33)$$

The equation of motion for the Green's Function is

$$i\hbar \frac{\partial}{\partial t} \langle\langle S_{-\underline{q}}^+(t) ; S_{\underline{q}}^- \rangle\rangle$$
$$= \delta(t) \langle [S_{-\underline{q}}^+ , S_{\underline{q}}^-] \rangle + \hbar q \langle\langle J_{-\underline{q}}^+(t) ; S_{\underline{q}}^- \rangle\rangle \qquad (2.34)$$

where $$\hbar q J_{-\underline{q}}^+ = [S_{-\underline{q}}^+ , H] \qquad (2.35)$$

J^{+}_{-q} is also interpreted as a spin-current component in the $\underline{q}$-direction.

The commutator in the first term is well known,

$$[S^{+}_{-\underline{q}}, S^{-}_{\underline{q}}] = 2S^{z}_{o}$$

(2.34) is now multiplied by $e^{i\omega t}$ and integrated to give the Fourier Transform which gives

$$\hbar\omega\chi = 2\langle S^{z}_{o}\rangle + \hbar q v \chi_{I} \qquad (2.36)$$

where

$$\chi_{I} = \int e^{i\omega t} \langle\langle J^{+}_{-\underline{q}}(t) ; S^{-}_{\underline{q}} \rangle\rangle dt \qquad (2.37)$$

This χ_{I} too has an equation of motion involving on the right hand side Green's Functions of higher order i.e.

$$\hbar\omega\chi_{I} = \langle [J^{+}_{-\underline{q}}, S^{-}_{\underline{q}}] \rangle + \hbar q v \chi_{J} \qquad (2.38)$$

where

$$\hbar q v \chi_{J} = \int_{-\alpha}^{\alpha} \langle\langle [J^{+}_{-\underline{q}}(t), H] ; S^{-}_{\underline{q}} \rangle\rangle e^{i\omega t} dt \qquad (2.39)$$

Combining (2.36) and (2.38) we find

$$\chi = \frac{2\langle S^{z}\rangle}{\hbar\omega} + \frac{q^{2}}{\omega^{2}} \left\{ \chi_{J} + \frac{1}{\hbar q} \langle [J^{+}_{-\underline{q}}, S^{-}_{\underline{q}}] \rangle \right\} \qquad (2.40)$$

In arriving at the exact expression for D from this equation, a fundamental assumption is made that for small q the spin wave is the only low-lying mode near the ground state; i.e for small q and w , the susceptibility is dominated by the spin wave pole at $\omega = Dq^2$. Particularly for q = 0 , only the first term in (2.40) is left which is the spin wave pole for q = 0 . It satisfies the important sum rule,

$$\int_{\alpha}^{\infty} \mathrm{Im}\,\chi \, d\omega = \frac{2\pi}{\hbar}\langle S^z \rangle$$

χ is therefore written as

$$\chi_{+-}(\underline{q},\omega) = \frac{2\langle S^z\rangle(1+Aq^2)}{\omega - Dq^2} + O(q^2) \qquad (2.4\text{I})$$

$$= \frac{2\langle S^z\rangle}{\hbar\omega} + \frac{2\langle S^z\rangle Dq^2}{(\hbar\omega)^2}, \qquad (2.42)$$

$$\text{as } \omega \to 0,\ q/\omega \to 0$$

Therefore, from (2.40) and (2.42) we get

$$Dq^2 = \frac{1}{2\langle S^z\rangle}\left\{\hbar q\langle[J^+_{-\underline{q}}, S^-_{\underline{q}}]\rangle + \hbar^2 q^2 \lim_{\omega\to 0}\lim_{q\to 0}\chi_J\right\} \qquad (2.43)$$

(2.43) is an exact formula for D valid for any metallic and nonmetallic ferromagnet, or for any non-ferromagnetic material in a static magnetic field in which the

appropriate limiting condition is $\omega \to \omega_L$, $\omega_L = g\mu_B H$, the Larmor frequency[33]. In fact, the spin wave pole is contained by χ_J , which can easily be seen from (2.40); but the limit in eqn (2.43) is finite because the residue $|\langle 0|J^+_{\underline{q}}|0\rangle|^2$, tends to zero as $q \to 0$.

However, D in the above form is not of much help in application to real systems. χ_J in the limit is to be brought into a calculable form. Also, by working within different models $\lim_{q/\omega \to 0} \chi_J(\underline{q},\omega)$ was evaluated and the D value thus obtained has been compared with previous formulations by other authors. For a gas with short range interactions, it was shown [35] that

$$\lim_{q/\omega \to 0} \chi_J(\underline{q},\omega) = \chi'_J(0,\omega) \qquad (2.44)$$

where $\chi'_J(0,\omega)$ is the "irreducible" part of χ_J , consisting of all irreducible diagrams contributing to To this extent, the above formula is a generalisation of Ma et. al's [34] . More support to this formalism comes from the fact that the intensity of neutron scattering is always proportional to $\langle S^z \rangle$ in the long wavelength limit, which result was stressed by Marshal and Murrey [36] for the Heisenberg model and observed in metals by Stringfellow[37]. Also Fisher[35] showed in detail in his thesis how the exact formula (2.43) can for a Heisenberg model reproduce the first correction to the

magnon energy under Dyson-Born approximation[38] in a cubic lattice; and the spin wave life time of Akheiser et al[39], Boyd and Callaway[40], who used scattering amplitudes of two magnons.

For a general system with a hamiltonian

$$H=\sum_i\left(\frac{P_i^2}{2m}+V(r_i)\right)+\frac{1}{2}\sum_{i\neq j}\frac{e^2}{|r_i-r_j|} \qquad (2.45)$$

D becomes

$$D=\frac{\hbar^2}{n_\uparrow-n_\downarrow}\left\{\frac{n}{2m}+\lim_{\omega\to 0}\chi_J(0,\omega)\right\} \qquad (2.46)$$

In arriving at the above, it is to be noted that

$$\left[S_{-q}^{+},H_I\right]=0 \quad ; H_I=\sum_i V(r_i)+\sum_{i\neq j}\frac{e^2}{|r_i-r_j|}$$

and $\lim_{\omega\to 0}\chi_J(0,\omega)=\langle\langle J_o^{+}(t)\,;J_o^{-}\rangle\rangle_\omega$

In the one band itinerant electron model, with the hamiltonian

$$H=\sum_{\underline{R}\sigma}\varepsilon(\underline{R})n_{\underline{R}\sigma}+\frac{I}{N}\sum_{R_1,R_2,q}c^{+}_{\underline{R}_1+\underline{q}\uparrow}c_{\underline{R}_1\uparrow}c^{+}_{\underline{R}_2-\underline{q}\downarrow}c_{\underline{R}_2\downarrow}$$

and $S_{-q}^{+}=\sum_{\underline{R}}c^{+}_{\underline{R}-\underline{q}\uparrow}c_{\underline{R}\downarrow}$, $\hbar q J^{+}_{-q}=\sum_{\underline{R}}\left(\varepsilon(\underline{R}-\underline{q})-\varepsilon(\underline{R})\right)c^{+}_{\underline{R}-\underline{q}\uparrow}c_{\underline{R}\downarrow}$

this formula of D is the generalisation of Edwards' formula for a strong ferromagnet,

$$D q^2 = \frac{1}{n_\uparrow - n_\downarrow} \Bigg\{ \sum_{\underline{R},\sigma} \frac{1}{2} (\underline{q}.\nabla)^2 \varepsilon(\underline{R}) n_{\underline{R}\sigma} + \lim_{\omega \to 0} \sum_{\underline{R},\underline{R}'} (\underline{q}.\nabla \varepsilon(\underline{R}))(\underline{q}.\nabla \varepsilon(\underline{R}')) \times \langle\langle c^+_{\underline{R}\uparrow} c_{\underline{R}\downarrow} ; c^+_{\underline{R}'\downarrow} c_{\underline{R}'\uparrow} \rangle\rangle_\omega \tag{2.47}$$

But in practice itinerant ferromagnetic metals, for example Ni, Fe and Co, are many band cases. $\lim_{\omega \to 0} \chi_J(0,\omega)$ can also be expressed in terms of Bloch wave functions and energies belonging to different bands and the value of D can be calculated. This may be done using the HF approximation as follows :

$$\begin{aligned} J_0^- &= \lim_{q \to 0} J^-_{\underline{q}} \\ &= \lim -\frac{1}{2m} \sum_j e^{i \underline{q}.\underline{r}_j} \left[(2\underline{p}_j + \hbar \underline{q}) S_j^- \right] \\ &= -\frac{1}{m} \sum_j p_j S_j^- \\ &= -\sum_{\underline{R} n l} \langle \underline{R} n | \frac{p S^-}{m} | \underline{R} l \rangle a^+_n(\underline{R}) a_l(\underline{R}) \end{aligned} \tag{2.48}$$

Here the band index n refers to ↓ spin and the band index l to ↑ spin. Hence

$$\begin{aligned} &\lim_{\omega \to 0} \chi_J(0,\omega) \\ &= \lim_{\omega \to 0} \int_{-\infty}^{\infty} \langle\langle J_0^+ ; J_0^- \rangle\rangle e^{i\omega t} dt \\ &= \sum_{\underline{R} n l} |\langle \underline{R} n | \frac{p S^-}{m} | \underline{R} l \rangle|^2 \int_{-\infty}^{\infty} \langle\langle a^+_n(\underline{R},t) a_l(\underline{R},t) ; a^+_l(\underline{R}) a_n(\underline{R}) \rangle\rangle dt \end{aligned} \tag{2.49}$$

Other terms involving $\langle\langle a_{n'}^{\dagger} a_{l'}; a_l^{\dagger} a_n \rangle\rangle$ with $n' \neq n$ or $l' \neq l$ vanish. We know that in the HF approximation

$$a_n^{\dagger}(\underline{R},t) = e^{iE_n(\underline{R})t/\hbar} a_n^{\dagger}(\underline{R})$$

$$a_l(\underline{R},t) = e^{iE_l(\underline{R})t/\hbar} a_l(\underline{R})$$

and also

$$\langle\langle a_n^{\dagger}(\underline{R}) a_l(\underline{R}) ; a_l^{\dagger}(\underline{R}) a_n(\underline{R}) \rangle\rangle$$

$$= -i/\hbar \left\langle \left[a_n^{\dagger}(\underline{R}) a_l(\underline{R}) , a_l^{\dagger}(\underline{R}) a_n(\underline{R}) \right] \right\rangle$$

$$= -i/\hbar \left\langle (a_n^{\dagger} a_n - a_l^{\dagger} a_l) \right\rangle$$

$$= -i/\hbar \left[N_n(\underline{R}) - N_l(\underline{R}) \right]$$

Also

$$-i/\hbar \int_{-\infty}^{\infty} e^{i\left(E_n(\underline{R}) - E_l(\underline{R})\right)t/\hbar - \varepsilon|t|/\hbar} \, dt$$

$$= \frac{1}{E_n(\underline{R}) - E_l(\underline{R})} ,$$

if there is no singularity.

Therefore $\int_{-\infty}^{\infty} \langle\langle a_n^{\dagger} a_l ; a_l^{\dagger} a_n \rangle\rangle \, dt$ can be replaced by

$$\frac{N_n(\underline{R}) - N_l(\underline{R})}{E_n(\underline{R}) - E_l(\underline{R})}$$

in the HF approximation . Then

$$D = \frac{\hbar^2}{n_{\uparrow} - n_{\downarrow}} \left[\frac{n}{2m} + \frac{1}{m^2} \sum_{\underline{R} n l} \left| \langle \underline{R} l_{\downarrow} | P_x | \underline{R} n_{\uparrow} \rangle \right|^2 \times \frac{N_{n_{\uparrow}}(\underline{R}) - N_{l_{\downarrow}}(\underline{R})}{E_{n_{\uparrow}}(\underline{R}) - E_{l_{\downarrow}}(\underline{R})} \right]$$

(2.50)

Here $|\underline{R}n\sigma\rangle$ represents the spatial part of the wave function.

The formula (2.50) is reduced to a form suitable for numerical computation by using the 'f-sum' rule :

$$D = \frac{1}{6(n_\uparrow - n_\downarrow)} \left\{ \sum_{n\underline{R}} N_n(\underline{R}) \nabla^2 E_n(\underline{R}) \right.$$

$$+ 2 \sum_{n\ell\underline{R}} \frac{N_n(\underline{R}) - N_\ell(\underline{R})}{E_n(\underline{R}) - E_\ell(\underline{R})} \left| \langle n\underline{R} | S^+ \frac{P}{m} | \ell\underline{R} \rangle \right|^2$$

$$\left. - 2 \sum_{n\ell\underline{R}} \frac{N_n(\underline{R})[1 - N_\ell(\underline{R})]}{E_n(\underline{R}) - E_\ell(\underline{R})} \left| \langle n\underline{R} | \frac{P}{m} | \ell\underline{R} \rangle \right|^2 \right\} \qquad (2.5I)$$

Actual computation has been carried out by Callaway and Wang[4I] for Nickel and closer agreement with experimentally determined value was found.

The formula (2.47) has been adopted with success in ordered binary alloy cases[42]. However, recently Callaway and Wang[43] developed a perturbation approach to find the susceptibility $\chi(\underline{q},\omega)$ using the local exchange approximation within which they also computed band wave functions and energies for Ni, Fe etc. Although they derived $\chi(\underline{q},\omega)$ for a ferromagnetic system, the method is in fact general and is applicable to an antiferromagnetic or ordered binary alloy case.

Callaway and Wang[4I] derived a formula for D in the ferromagnetic case, which is identical with eqn. (2.50). However their derivation is in error and we shall show below that there is an additional term in D. In calcu-

calculating eqn. (2.50) we used the HF approximation and they neglected a vertex correction in the spin current -spin current response function. When this response is calculated in RPA, thus including a vertex correction, the additional term is obtained.

The CW Formulation

The method of Callaway and Wang, henceforth to be called CW's, starts with the hamiltonian for a single Bloch electron

$$H_o = -\frac{\hbar^2}{2m}\nabla^2 + V_o(\underline{r}) - V_{xc,\sigma}(\underline{r})$$

where $V_o(\underline{r})$ represents the Coulomb potential due to the ions and the average distribution of band electrons; and $V_{xc,\sigma}(\underline{r})$ is the exchange-correlation potential for an electron of spin σ . This may be written as

$$H_o = -\frac{\hbar^2}{2m}\nabla^2 + V_1(\underline{r}) - V_f(\underline{r})\,\bar{\sigma}\cdot\underline{n} \qquad (2.52)$$

where

$$V_1(\underline{r}) = V_o(\underline{r}) - \frac{1}{2}\left[V_{xc\uparrow} + V_{xc\downarrow}\right]$$

$$V_f(\underline{r}) = \frac{1}{2}\left[V_{xc\downarrow} - V_{xc\uparrow}\right]$$

The last term in (2.52) is the spin-dependent part of the potential in the local exchange approximation; and $\bar{n}$ is the unit vector in the direction of spin alignment and is assumed to be in the Z-direction. Using the $X\alpha$

method

$$V_f(\underline{r}) = \frac{3\alpha e^2}{2}\left(\frac{3}{4\pi}\right)^{\frac{1}{3}}\left(\rho_{\uparrow}^{\frac{1}{3}} - \rho_{\downarrow}^{\frac{1}{3}}\right),$$

α is the variable parameter. Under the impact of a time-dependent transverse rotating magnetic field

$$\underline{B}_{\perp} = B_0\left\{\hat{x}\cos[\underline{q}_s.\underline{r}-\omega t] + \hat{Y}\sin[\underline{q}_s.\underline{r} - \omega t]\right\}e^{-\eta|t|}$$

where $\underline{q}_s = \underline{q} + \underline{K}_s$, $\underline{q}$ is confined to the first Brillouin Zone and $\underline{K}_s$ is a reciprocal lattice vector; the interaction hamiltonian is

$$H_I = \frac{-1}{2} g\xi_B \underline{B}_{\perp}.\underline{\sigma}$$
$$= -\frac{1}{4} g\xi_B B_0\left[e^{i(\underline{q}_s.\underline{r}-\omega t)}\sigma_- + e^{-i(\underline{q}_s.\underline{r}-\omega t)}\sigma_+\right]e^{-\eta|t|} \qquad (2.53)$$

The perturbed wave function, which is found by using the standard time-dependent perturbation procedure, is found to be

$$\psi_n'(\underline{R},\underline{r},t) = e^{-iE_n(\underline{R})t/\hbar}\left\{\psi_n(\underline{R},\underline{r}) - \frac{g\xi_B}{4\hbar}B_0 e^{-\eta|t|} \times \right.$$
$$\left. \times \sum_{l\underline{q}'}\left(\frac{\langle l\underline{q}'|\, e^{i\underline{q}_s.\underline{r}}\sigma_-\,|n\underline{R}\rangle e^{-i\omega t}}{\omega_{n\underline{R},l\underline{q}'} + \omega + i\eta} + \frac{\langle l\underline{q}'|\, e^{-\underline{q}_s.\underline{r}}\sigma_+\,|n\underline{R}\rangle e^{i\omega t}}{\omega_{n\underline{R},l\underline{q}'} - \omega + i\eta}\right)\psi_l(\underline{q}',\underline{r})\right\}, \qquad (2.54)$$

$$\hbar\omega_{n\underline{R};l\underline{q}'} = E_n(\underline{R}) - E_l(\underline{q}')$$

$\psi_n(\underline{R},\underline{r},t)$ being the unperturbed wave function belonging to H_o. These are used to construct the transverse mag-

notisation

$$M_{\pm}(\underline{r},t) = \frac{g\xi_B}{\Omega}\sum_{n\underline{R}} N_n(\underline{R})\psi'^{*}(\underline{R},\underline{r},t)\sigma_{\pm}\psi'_n(\underline{R},\underline{r},t)$$

$$M_{\pm}(\underline{r},t) = M_x(\underline{r},t) \pm iM_y(\underline{r},t)$$

After some algebra we get

$$M_+(\underline{r},t) = \frac{-(g\xi_B)^2}{8\hbar}B_o\sum_{\ell n\underline{R}}\langle \ell\,\underline{R}+\underline{q}|e^{i\underline{q}_s\cdot\underline{r}}\sigma_-|n\,\underline{R}\rangle$$

$$\times\frac{[N_n(\underline{R}) - N_\ell(\underline{R}+\underline{q})]}{\omega_{n\underline{R},\ell\,\underline{R}+\underline{q}} + \omega + i\eta}\psi^{*}_n(\underline{R},\underline{r})\sigma_+\psi_\ell(\underline{R}+\underline{q},\underline{r})e^{-i\omega t} \qquad (2.55)$$

and a similar one for $M_-(\underline{r},t)$. In arriving at (2.55) use is made of the orthogonal property of the Bloch functions, i.e. $\langle \ell\underline{q}'|e^{\pm\underline{q}_s\cdot\underline{r}}\sigma_\pm|n\,\underline{R}\rangle = 0$,

unless $\underline{q}' = \underline{R}\pm\underline{q}_s$ and

also the fact that since the spin direction is included in the band index, the terms in $M_\pm$ which involve either σ_+ or σ_- twice vanish.

Writing the position-dependent terms of (2.55) in terms of a Fourier series i.e.

$$\psi^{*}_n(\underline{R},\underline{r})\sigma_\pm\psi_\ell(\underline{R}+\underline{q},\underline{r}) = \sum_j C_j \exp[\pm i(\underline{q}+\underline{k}_j).\underline{r}] \qquad (2.56)$$

with

$$C_j = (N\Omega)^{-1}\langle n\,\underline{R}|\sigma_\pm\exp[\mp i\,\underline{q}_j.\underline{r}]|\ell\,\underline{R}+\underline{q}\rangle \qquad (2.57)$$

where Ω is the volume of a unit cell and N the number

of atomic cells in the crystal volume, we can write (2.50) as

$$M_+(\underline{r},t) = \frac{1}{2} B_0 \sum_j \chi^{(o)}_{js+-} \exp[i(\underline{q}_j.\underline{r} - \omega t)] \qquad (2.58)$$

in which

$$\chi^{(o)}_{js+-}(\underline{q},\omega) = \frac{-(g\mu_B)^2}{4\hbar N\Omega} \sum_{\ell n \underline{k}} \frac{N_n(\underline{k}) - N_\ell(\underline{k}+\underline{q})}{\omega_{n\underline{k},\ell\underline{k}+\underline{q}} + \omega + i\eta}$$

$$\times \langle n\underline{k}|\sigma_+ \exp(-i\underline{q}_j.\underline{r})|\ell\underline{k}+\underline{q}\rangle\langle\ell\underline{k}+\underline{q}|\sigma_- \exp(i\underline{q}_s.\underline{r})|n\underline{k}\rangle \qquad (2.59)$$

$\chi^{(o)}_{js+-}(\underline{q},\omega)$ is the nonself-consistent susceptibility and was obtained in this form by Callaway and Wang. It reveals the important point that if an external field is applied with some definite vector, the induced magnetisation has components with wave vectors which can differ from that of the applied field by a reciprocal lattice vector.

But there is a change in the local exchange potential because of the rotation of n to n' by the applied magnetic field. This must be incorporated in the susceptibility of (2.59) by an iteration procedure to get the self-consistent susceptibility. The change in the exchange potential is

$$\Delta V_f(\underline{r}) = V_f(\underline{r})[\underline{\sigma}.(\hat{n}' - \hat{n})]$$

$$= V_f(\underline{r})(M_+\sigma_- + M_-\sigma_+)/2M_0 \qquad (2.60)$$

This is written in the Fourier-expanded form as

$$\Delta V_f(\underline{r},t) = \frac{g\mu_B}{4} B_o \sum_{tj} \lambda_{tj} \chi_{js+-}(\underline{q},\omega)\, \sigma_- e^{i(\underline{q}_t \cdot \underline{r} - \omega t)} + h.c. \qquad (2.6I)$$

where

$$\lambda_{tj} = \frac{3e^2\alpha}{(g\mu_B)^2\Omega}\left(\frac{3}{4\pi}\right)^{\frac{1}{3}} \int \frac{e^{i(\underline{K}_j - \underline{K}_t).\underline{r}}}{\rho_\uparrow^{2/3} + \rho_\uparrow^{1/3}\rho_\downarrow^{1/3} + \rho_\downarrow^{2/3}}\, d^3r \qquad (2.62)$$

When this change is included, the self-consistent susceptibility is given by the equation

$$\sum_t \chi^{(o)}_{mt+-}(\underline{q},\omega)\left[\delta_{ts} + \sum_j \lambda_{tj}\chi_{js+-}(\underline{q},\omega)\right] = \chi_{ms+-}(\underline{q},\omega) \qquad (2.63)$$

whose solution in the matrix form is $\chi(\underline{q},\omega) = \frac{\chi^{(o)}}{1-\lambda\chi^{(o)}}$ (2.64)

The spin wave energies are found by looking at the pole of (2.64) i.e. from the equation

$$\det\left[1 - \lambda\chi^{(o)}\right] = 0 \qquad (2.65)$$

CHAPTER III

A New Formulation of the Local Exchange Method for Calculating the Spin Wave Stiffness Constant and Dynamic Susceptibility

We made a departure from CW[44] by writing the self-consistency(refer to the one in CW above) in the form of an integral equation, instead of an infinite determinant. We note that in a transverse mode of wave vector $\underline{q}$ the local magnetisation $M_o(\underline{r})$ precesses about the equilibrium Z-direction with a small cone angle $m_q(\underline{r})$. We therefore define $M_{\pm}(\underline{r},t)$as

$$M_{\pm}(\underline{r},t) = 2M_o(\underline{r})m_q(\underline{r})e^{\pm i(\underline{q}.\underline{r}-\omega t)} \qquad (3.1)$$

With this definition, $\Delta V_f(\underline{r})$ of eqn. (2.60) becomes

$$\Delta V_f(\underline{r}) = V_f(\underline{r})\left\{e^{i(\underline{q}.\underline{r}-\omega t)}\sigma_- + e^{-i(\underline{q}.\underline{r}-\omega t)}\sigma_+\right\}m_q(\underline{r}) \qquad (3.2)$$

This shows that the local exchange field $V_f(\underline{r})$has a perturbing transverse component of amplitude $V_f(\underline{r})m_q(\underline{r})e^{i(\underline{q}.\underline{r}-\omega t)}$ We follow the previous procedure in obtaining the perturbed wave function with the perturbation $\Delta V_f(\underline{r})$and use them to construct $M_{\pm}(\underline{r},t)$. This leads to the self-con-

sistency equation

$$M_+(\underline{r},t) = -\frac{g\varepsilon_B}{4}\sum_{\ell n \underline{R}} \langle \ell \underline{R}+\underline{q}|\sigma_- e^{i\underline{q}.\underline{r}} V_f(\underline{r}) m_q(\underline{r})|n\underline{R}\rangle$$

$$\times \frac{N_n(\underline{R}) - N_\ell(\underline{R}+\underline{q})}{E_n(\underline{R}) - E_\ell(\underline{R}+\underline{q}) + \hbar\omega + i\eta} \psi^*_n(\underline{R},\underline{r})\sigma_+\psi_\ell(\underline{R}+\underline{q},\underline{r}) e^{-i\omega t}$$

$$= e^{i\underline{q}.\underline{r}} m_q(\underline{r}) M_0(\underline{r}) \qquad (3.3)$$

and a similar one for $M_-(\underline{r},t)$. Making the spin indices explicit the equation becomes

$$-g\varepsilon_B \sum_{\ell n \underline{R}} \langle \ell \underline{R}+\underline{q}\downarrow | e^{i\underline{q}.\underline{r}} V_f(\underline{r}) m_q(\underline{r}) | n\underline{R}\uparrow\rangle$$

$$\times \frac{N_{n\uparrow}(\underline{R}) - N_{\ell\downarrow}(\underline{R}+\underline{q})}{E_{n\uparrow}(\underline{R}) - E_{\ell\downarrow}(\underline{R}+\underline{q}) + \hbar\omega} \psi^*_{n\uparrow}(\underline{R},\underline{r})\psi_{\ell\downarrow}(\underline{R}+\underline{q},\underline{r}) e^{-i\underline{q}.\underline{r}}$$

$$= M_0(\underline{r}) m_q(\underline{r}) \qquad (3.4)$$

$\psi_{n\sigma}(\underline{R},\underline{r})$ or $|n\underline{R}\sigma\rangle$ is the spatial part of the electron wave function, n the band index. We solve for those values of ω for which (3.4) has a non-trivial solution $m_q(\underline{r}) \neq 0$. We shall first take up the case of a ferromagnet of cubic symmetry. The equation (3.4) could also be derived starting from M_- as well.

The Stiffness Constant D

In this section we shall first carry out the necessary algebra to arrive at an expression for D within the CW approach.

We first note that

$$V_f(\underline{r}) = \frac{1}{2}(H_\uparrow - H_\downarrow) \tag{3.5}$$

and

$$e^{-i\underline{q}\cdot\underline{r}}(H_\uparrow - H_\downarrow) = (H_\uparrow e^{-i\underline{q}\cdot\underline{r}} - e^{-i\underline{q}\cdot\underline{r}} H_\downarrow) + \left[e^{-i\underline{q}\cdot\underline{r}}, H_\uparrow\right]; \tag{3.6}$$

also similarly for $e^{i\underline{q}\cdot\underline{r}}(H_\uparrow - H_\downarrow)$. We assume $\underline{q}$ in the X-direction. The eqn. (3.4) is not solvable in its present form ; we therefore multiply both sides of it with $V_f(\underline{r})$ and integrate over space. We get

$$-g\mu_B \sum_{\ell n \underline{R}} \langle \ell_\downarrow \underline{k}+\underline{q} | e^{i\underline{q}\cdot\underline{r}} V_f(\underline{r}) m_{q'}(\underline{r}) | n_\uparrow \underline{k} \rangle \times \frac{N_{n\uparrow}(\underline{R}) - N_{\ell\downarrow}(\underline{R}+\underline{q})}{E_{n\uparrow}(\underline{R}) - E_{\ell\downarrow}(\underline{R}+\underline{q}) + \hbar\omega} \langle n_\uparrow R | e^{-i\underline{q}\cdot\underline{r}} V_f(\underline{r}) | \ell_\downarrow \underline{k}+\underline{q} \rangle = \int V_f(r) m_{q'}(\underline{r}) M_0(\underline{r}) dr \tag{3.7}$$

Using eqns. (3.5) and (3.6) we can write

$$\langle n_\uparrow \underline{R} | e^{-i\underline{q}\cdot\underline{r}} V_f(\underline{r}) | \ell_\downarrow \underline{R}+\underline{q} \rangle = \frac{1}{2} \langle n_\uparrow \underline{R} | e^{-i\underline{q}\cdot\underline{r}} | \ell_\downarrow \underline{R}+\underline{q} \rangle \left[E_{n\uparrow}(\underline{R}) - E_{\ell\downarrow}(\underline{R}+\underline{q})\right] + \frac{1}{2}\frac{\hbar q}{2m} \langle n_\uparrow \underline{R} | e^{-i\underline{q}\cdot\underline{r}} P_x + P_x e^{-i\underline{q}\cdot\underline{r}} | \ell_\downarrow \underline{R}+\underline{q} \rangle, \tag{3.8}$$

Since $\left[e^{-i\underline{q}\cdot\underline{r}}, H_\uparrow\right] = \left[e^{-i\underline{q}\cdot\underline{r}}, \frac{p^2}{2m}\right]$

$$= \frac{\hbar q}{2m}\left(e^{-i\underline{q}\cdot\underline{r}} P_x + P_x e^{-i\underline{q}\cdot\underline{r}}\right)$$

In the long wave length limit, $\hbar\omega = Dq^2$. Making this replacement and picking up the first part of eqn. (3.8), we get from (3.7)

$$-\frac{g\mu_B}{2}\sum_{\ell n \underline{k}}\langle \ell_\downarrow \underline{k}+\underline{q}|e^{i\underline{q}.\underline{r}}V_f(\underline{r})m_q(\underline{r})|n_\uparrow \underline{k}\rangle \times \frac{N_{n\uparrow}(\underline{k}) - N_{\ell\downarrow}(\underline{k}+\underline{q})}{E_{n\uparrow}(\underline{k}) - E_{\ell\downarrow}(\underline{k}+\underline{q}) + Dq^2} \times [E_{n\uparrow}(\underline{k}) - E'_{\ell\downarrow}(\underline{k}+\underline{q})]\langle n_\uparrow \underline{k}|e^{-i\underline{q}.\underline{r}}|\ell_\downarrow \underline{k}+\underline{q}\rangle$$

By adding and subtracting Dq^2 in the energy numerator, the term not involving D is :

$$-\frac{g\mu_B}{2}\sum_{\ell n \underline{k}}\langle \ell_\downarrow \underline{k}+\underline{q}|e^{i\underline{q}.\underline{r}}V_f(\underline{r})m_q(\underline{r})|n_\uparrow \underline{k}\rangle \times [N_{n\uparrow}(\underline{k}) - N_{\ell\downarrow}(\underline{k}+\underline{q})]\langle n_\uparrow \underline{k}|e^{-i\underline{q}.\underline{r}}|\ell_\downarrow \underline{k}+\underline{q}\rangle$$

$$= -\frac{g\mu_B}{2}\int V_f(\underline{r})m_q(\underline{r})\left[\sum_{n\underline{k}}|\psi_{n\uparrow}(\underline{k})|^2 N_{n\uparrow}(\underline{k}) - \sum_{\ell\underline{k}}|\psi_{\ell\downarrow}(\underline{k}+\underline{q})|^2 N_{\ell\downarrow}(\underline{k}+\underline{q})\right]d\underline{r},$$

$$= \int V_f(\underline{r})m_q(\underline{r})M_0(\underline{r})d\underline{r} \qquad (3.9)$$

using the closure relation $\sum_n |n\underline{k}\rangle\langle n\underline{k}| = 1$

This term cancels the RHS of (3.7). The term involving D and of $O(q^2)$ is :

$$\frac{g\mu_B}{2}Dq^2\sum_{\ell n \underline{k}}\langle \ell_\downarrow \underline{k}|V_f(\underline{r})|n_\uparrow \underline{k}\rangle \frac{N_{n\uparrow}(\underline{k}) - N_{\ell\downarrow}(\underline{k})}{E_{n\uparrow}(\underline{k}) - E_{\ell\downarrow}(\underline{k})} \times \langle n_\uparrow \underline{k}|\ell_\downarrow \underline{k}\rangle \quad ?$$

$$= \frac{g\mu_B}{2}\frac{Dq^2}{2}\left[\sum_{n\underline{k}} N_{n\uparrow}(\underline{k}) - \sum_{\ell\underline{k}} N_{\ell\downarrow}(\underline{k})\right] \quad)$$

, using the closure relation as above and $V_f(\underline{r}) = \frac{1}{2}(H_\uparrow - H_\downarrow)$

$$= \frac{1}{4}g\mu_B Dq^2[N_\uparrow - N_\downarrow] \qquad (3.10)$$

$$g\xi_B D q^2 [N_\uparrow - N_\downarrow]$$

In simplifying the remaining term we expand m_q as

$$m_q(\underline{r}) = 1 + q\, m_1(\underline{r}) \qquad (3.II)$$

The zeroth order contribution of m_q is :

$$-\frac{1}{2}\frac{g\xi_B}{4m}\hbar q \sum_{\ell n \underline{R}} \langle \ell_\downarrow \underline{R}+\underline{q} | e^{i\underline{q}\cdot\underline{r}} | n_\uparrow \underline{R} \rangle$$

$$\times \left[N_{n\uparrow}(\underline{R}) - N_{\ell\downarrow}(\underline{R}+\underline{q}) \right] \langle n_\uparrow \underline{R} | P_x e^{-i\underline{q}\cdot\underline{r}} + e^{-i\underline{q}\cdot\underline{r}} P_x | \ell_\downarrow \underline{R}+\underline{q} \rangle$$

$$= -\frac{1}{2}\frac{g\xi_B}{4m}\hbar q \left\{ \sum_{n\underline{R}} N_{n\uparrow}(\underline{R}) \langle n_\uparrow \underline{R} | P_x + e^{-i\underline{q}\cdot\underline{r}} P_x e^{i\underline{q}\cdot\underline{r}} | n_\uparrow \underline{R} \rangle \right.$$

$$\left. - \sum_{\ell \underline{R}} N_{\ell\downarrow}(\underline{R}) \langle \ell_\downarrow \underline{R} | e^{i\underline{q}\cdot\underline{r}} P_x e^{-i\underline{q}\cdot\underline{r}} + P_x | \ell_\downarrow \underline{R} \rangle \right\}$$

Noting that total momentum for ↑ and ↓ spins in equilibrium is zero, the above is further simplified to give :

$$= -\frac{1}{2}\frac{g\xi_B}{4m}\hbar q \left\{ \sum_{n\underline{R}} N_{n\uparrow}(\underline{R}) \langle n_\uparrow \underline{R} | \hbar q | n_\uparrow \underline{R} \rangle \right.$$

$$\left. - \sum_{\ell \underline{R}} N_{\ell\downarrow}(\underline{R}) \langle \ell_\downarrow \underline{R} | -\hbar q | \ell_\downarrow \underline{R} \rangle \right\}$$

$$= -\frac{1}{2}\frac{g\xi_B}{4m}\hbar^2 q^2 N, \quad N_\uparrow + N_\downarrow = N \qquad (3.I2)$$

and a term :

$$-\frac{1}{2}\frac{g\xi_B}{2}\hbar^2 q^2 \sum_{\ell n \underline{R}} \langle \ell_\downarrow \underline{R}+\underline{q} | \frac{e^{i\underline{q}\cdot\underline{r}} P_x + P_x e^{i\underline{q}\cdot\underline{r}}}{2m} | n_\uparrow \underline{R} \rangle$$

$$\times \frac{N_{n\uparrow}(\underline{R}) - N_{\ell\downarrow}(\underline{R}+\underline{q})}{E_{n\uparrow}(\underline{R}) - E_{\ell\downarrow}(\underline{R}+\underline{q})} \langle n_\uparrow \underline{R} | \frac{e^{-i\underline{q}\cdot\underline{r}} P_x + P_x e^{-i\underline{q}\cdot\underline{r}}}{2m} | \ell_\downarrow \underline{R}+\underline{q} \rangle ,$$

$$= -\frac{1}{2}\frac{g\xi_B}{2}\hbar q^2 \sum_{\ell n \underline{R}} \left| \langle \ell_\downarrow \underline{R} | \frac{P_x}{m} | n_\uparrow \underline{R} \rangle \right|^2$$

$$\times \frac{N_{n\uparrow}(\underline{R}) - N_{\ell\downarrow}(\underline{R})}{E_{n\uparrow}(\underline{R}) - E_{\ell\downarrow}(\underline{R})} , \qquad (3.I3)$$

in $O(q^2)$

The contribution from the Ist order term in q of m_q is :

$$-\frac{g\mu_B}{2}\left(\frac{\hbar q}{m}\right)^2 \sum_{\ell n \underline{k}} \langle \ell_\downarrow \underline{k} | V_f(\underline{r}) m_1(\underline{r}) | n_\uparrow \underline{k} \rangle \times \left[N_{n\uparrow}(\underline{k}) - N_{\ell\downarrow}(\underline{k})\right] \langle n_\uparrow \underline{k} | P_x | \ell_\downarrow \underline{k} \rangle \qquad (3.I4)$$

All the q^2-order terms have now been calculated. It is by equating the coefficients that we get the expression for D as follows :

$$\frac{1}{2}\frac{g\mu_B}{2} D q^2 (N_\uparrow - N_\downarrow) = \frac{1}{2}\frac{g\mu_B}{2} q^2 \left\{ \frac{\hbar^2 N}{2m} + \hbar^2 \sum_{\ell n \underline{k}} \left| \langle \ell_\downarrow \underline{k} | \frac{P_x}{m} | n_\uparrow \underline{k} \rangle \right|^2 \frac{N_{n\uparrow}(\underline{k}) - N_{\ell\downarrow}(\underline{k})}{E_{n\uparrow}(\underline{k}) - E_{\ell\downarrow}(\underline{k})} \right.$$

$$+ \frac{2\hbar}{m} \sum_{\ell n \underline{k}} \langle \ell_\downarrow \underline{k} | V_f(\underline{r}) m_1(\underline{r}) | n_\uparrow \underline{k} \rangle \times \left[N_{n\uparrow}(\underline{k}) - N_{\ell\downarrow}(\underline{k})\right] \langle n_\uparrow \underline{k} | \frac{P_x}{m} | \ell_\downarrow \underline{k} \rangle$$

Or,

$$D = \frac{\hbar^2}{N_\uparrow - N_\downarrow} \left\{ \frac{N}{2m} + \sum_{\ell n \underline{k}} \left| \langle \ell_\downarrow \underline{k} | \frac{P_x}{m} | n_\uparrow \underline{k} \rangle \right|^2 \frac{N_{n\uparrow}(\underline{k}) - N_{\ell\downarrow}(\underline{k})}{E_{n\uparrow}(\underline{k}) - E_{\ell\downarrow}(\underline{k})} \right.$$

$$\left. + \frac{2}{\hbar} \sum_{\ell n \underline{k}} \langle \ell_\downarrow \underline{k} | V_f(\underline{r}) m_1(\underline{r}) | n_\uparrow \underline{k} \rangle \frac{N_{n\uparrow}(\underline{k}) - N_{\ell\downarrow}(\underline{k})}{E_{n\uparrow}(\underline{k}) - E_{\ell\downarrow}(\underline{k})} \times \langle n_\uparrow \underline{k} | \frac{P_x}{m} | \ell_\downarrow \underline{k} \rangle \right\} \qquad (3.I5)$$

The first two terms yield just eqn. (2.50) and we now have a third term involving the function $m_I(\underline{r})$. This term was missed by Callaway and Wang in their incorrect derivation of D. However, this $m_I(\underline{r})$ cannot be obtained exactly but it satisfies an integral equation which we can deal with by an iteration process. The integral equation is obtained by starting from eqn. (3.4), and by putting $m_q(\underline{r}) = I + m_I(\underline{r})q$ viz.

$$-g\mathcal{E}_B \sum_{\ell n \underline{K}}' \left\langle \ell_\downarrow \underline{K}+\underline{q} \middle| e^{i\underline{q}.\underline{r}}(1+m_1(\underline{r})q)V_f(\underline{r}) \middle| n_\uparrow \underline{K} \right\rangle \times \frac{N_{n\uparrow}(\underline{K}) - N_{\ell\downarrow}(\underline{K}+\underline{q})}{E_{n\uparrow}(\underline{K}) - E_{\ell\downarrow}(\underline{K}+\underline{q}) + \hbar\omega} \psi^*_{n\uparrow}(\underline{K},\underline{r})\psi_{\ell\downarrow}(\underline{K}+\underline{q},\underline{r})$$
$$= e^{i\underline{q}.\underline{r}} M_0(\underline{r}) + q m_1(\underline{r}) e^{i\underline{q}.\underline{r}} M_0(\underline{r})$$

We proceed as before :

$$e^{i\underline{q}.\underline{r}} V_f(\underline{r})$$
$$= \frac{1}{2} e^{i\underline{q}.\underline{r}} (H_\uparrow - H_\downarrow)$$
$$= \frac{1}{2}\left(e^{i\underline{q}.\underline{r}} H_\uparrow - H_\downarrow e^{i\underline{q}.\underline{r}}\right) + \frac{1}{2}\left[H_\downarrow, e^{i\underline{q}.\underline{r}}\right]$$
$$= \frac{1}{2}\left(e^{i\underline{q}.\underline{r}} H_\uparrow + H_\downarrow e^{i\underline{q}.\underline{r}}\right) + \frac{1}{2}\frac{\hbar q}{2m}\left(e^{i\underline{q}.\underline{r}} P_x + P_x e^{i\underline{q}.\underline{r}}\right)$$

Therefore,

$$\left\langle \ell_\downarrow \underline{K}+\underline{q} \middle| e^{i\underline{q}.\underline{r}} V_f(\underline{r})(1+m_1(\underline{r})q) \middle| n_\uparrow \underline{K} \right\rangle$$
$$= \frac{1}{2}\left\langle \ell_\downarrow \underline{K}+\underline{q} \middle| e^{i\underline{q}.\underline{r}}(1+m_1(\underline{r})q) \middle| n_\uparrow \underline{K} \right\rangle \left[E_{n\uparrow}(\underline{K}) - E_{\ell\downarrow}(\underline{K}+\underline{q})\right]$$
$$+ \frac{1}{2}\frac{\hbar q}{2m}\left\langle \ell_\downarrow \underline{K}+\underline{q} \middle| \left(e^{i\underline{q}.\underline{r}} P_x + P_x e^{i\underline{q}.\underline{r}}\right) \times (1+m_1(\underline{r})q) \middle| n_\uparrow \underline{K} \right\rangle$$

The Ist order terms in q in this expression are :

$$\frac{1}{2}q\langle \ell_\downarrow \underline{R} \,|m_1(\underline{r})|\, n_\uparrow \underline{R}\rangle\left[E_{n\uparrow}(\underline{R}) - E_{\ell\downarrow}(\underline{R})\right]$$
$$+\frac{1}{2}\frac{\hbar q}{m}\langle \ell_\downarrow \underline{R}|\, P_x \,|n_\uparrow \underline{R}\rangle$$

Therefore, equating coefficients of q on both sides we get

$$-\frac{g\mu_B}{2}\Bigg\{\sum_{\ell n \underline{R}} \langle \ell_\downarrow \underline{R}|\, m_1(\underline{r})\,|n_\uparrow \underline{R}\rangle \times\left[N_{n\uparrow}(\underline{R}) - N_{\ell\downarrow}(\underline{R})\right]\psi^*_{n\uparrow}(\underline{R},\underline{r})\,\psi_{\ell\downarrow}(\underline{R},\underline{r})$$
$$+\frac{\hbar}{m}\sum_{\ell n \underline{R}}\langle \ell_\downarrow \underline{R}|\, P_x\,|n_\uparrow \underline{R}\rangle\,\frac{N_{n\uparrow}(\underline{R}) - N_{\ell\downarrow}(\underline{R})}{E_{n\uparrow}(\underline{R}) - E_{\ell\downarrow}(\underline{R})} \times \psi^*_{n\uparrow}(\underline{R},\underline{r})\,\psi_{\ell\downarrow}(\underline{R},\underline{r})\Bigg\}$$
$$= m_{\mathcal{Q}1}(\underline{r})\, M_0(\underline{r}) \qquad (3.16)$$

(3.16) is the desired integral equation for $m_I(\underline{r})$.

Equivalence of our Expression for D to that of EF's Exact Formula within the RPA

We commented earlier that in arriving at the formula (3.15) for D the spin current - spin current response function $\chi_J(\underline{q},\omega)$ was calculated in the HF approximation and thus the vertex term was missed. But in the random phase approximation it should appear. The message of the local exchange approximation is that an electron of spin σ

moves in a local potential $V_{xc,\sigma}$ in the ground state of the system. We may regard the ground state of the system as the HF ground state of the many-body hamiltonian

$$H = \sum_i \left[\frac{P_i^2}{2m} + V_o(\underline{r}_i) \right] + \sum_{i \neq j} \sum \int d\underline{r} f(\underline{r}) \delta(\underline{r} - \underline{r}_i) \delta(\underline{r} - \underline{r}_j)$$

$$= \sum_i \left[\frac{P_i^2}{2m} + V_o(\underline{r}_i) \right] + \int f(\underline{r}) \rho_\uparrow(\underline{r}) \rho_\downarrow(\underline{r}) \, d\underline{r} \qquad (3.I7)$$

where $\underline{P}_i$ and $\underline{r}_i$ are the momentum and position of electron i and

$$\begin{aligned} V_o(\underline{r}_i) &= (\rho_\uparrow V_\uparrow - \rho_\downarrow V_\downarrow)/(\rho_\uparrow - \rho_\downarrow) \\ f(\underline{r}) &= (V_\downarrow - V_\uparrow)/(\rho_\uparrow - \rho_\downarrow) \\ \rho_\uparrow(\underline{r}) &= \psi_\uparrow^*(\underline{r}) \psi_\uparrow(\underline{r}) \end{aligned} \qquad (3.I8)$$

Considered from this point of view, CW calculation of $\chi(\underline{q},\omega)$ corresponds to the time-dependent HF approximation which is equivalent to the random phase approximation. This fact is also revealed if $\lim_{\substack{\underline{q}\to 0 \\ \omega \to 0}} \chi_J(\underline{q},\omega)$ is calculated in the RPA whence a correction term in the formula for D , in addition to those found in the HF approximation, appears. It is proved below that this correction is the same as the vertex term in our formula for D , eqn (3.I5).

We have now to use the hamiltonian (3.I7). Writing the $J_{-\underline{q}}^\dagger$ and $J_{\underline{q}}^-$ in the second quantised form and carrying out some algebra, we arrive at

$$
\begin{aligned}
&\chi_J(\underline{q},\omega) \\
&= \sum_{\ell n \underline{R}} \langle \ell_\downarrow \underline{R} | e^{i\underline{q}\cdot\underline{r}} (2P_x + \hbar q) | n_\uparrow \underline{R} \rangle \\
&\quad \times \Bigg\{ \frac{\langle [J^+_{-q}, a^+_{\ell_\downarrow}(\underline{R}) a_{n_\uparrow}(\underline{R})] \rangle}{E_{n_\uparrow}(\underline{R}) - E_{\ell_\downarrow}(\underline{R}) + \hbar\omega} \\
&\qquad + \sum_{\ell' n' \underline{R}'} \Big(\int f(\underline{r}) \psi^*_{n_\uparrow}(\underline{R},\underline{r}) \psi_{n'_\uparrow}(\underline{R}',\underline{r}) \psi^*_{\ell'_\downarrow}(\underline{R}',\underline{r}) \psi_{\ell_\downarrow}(\underline{R},\underline{r}) \Big) \\
&\qquad \times \frac{N_{\ell_\downarrow}(\underline{R}) - N_{n_\uparrow}(\underline{R})}{E_{n_\uparrow}(\underline{R}) - E_{\ell_\downarrow}(\underline{R}) + \hbar\omega} \times \text{F.T.} \langle\langle J^+_{-q} ; a^+_{\ell'_\downarrow}(\underline{R}') a_{n'_\uparrow}(\underline{R}') \rangle\rangle \Bigg\} \qquad (3.19)
\end{aligned}
$$

In the limit $q \to 0$, $\omega \to 0$, the first term reduces to

$$
\sum_{\ell n \underline{R}} \left| \langle \ell_\downarrow \underline{R} | \frac{P_x}{m} | n_\uparrow \underline{R} \rangle \right|^2 \frac{N_{n_\uparrow}(\underline{R}) - N_{\ell_\downarrow}(\underline{R})}{E_{n_\uparrow}(\underline{R}) - E_{\ell_\downarrow}(\underline{R})} ,
$$

which is exactly what we found before. The remaining part prolongs into an infinite series of continuously multiplied terms. But, the m_I-involving term in our formula, too, gets into an infinite series if we try the iteration process. It is shown below that both the series are equal term by term, which establishes the desired equivalence. The first such term from the present RPA series is

$$\sum_{\ell n \underline{R}} \sum_{\ell' n' \underline{R}'} \left\langle \ell_{\downarrow} \underline{R} \left| \frac{P_x}{m} \right| n_{\uparrow} \underline{R} \right\rangle \left\langle n'_{\uparrow} \underline{R}' \left| \frac{P_x}{m} \right| \ell'_{\downarrow} \underline{R}' \right\rangle \left(\int f(\underline{r}) \psi^{*}_{n\uparrow}(\underline{R},\underline{r}) \psi_{n'\uparrow}(\underline{R}',\underline{r}) \psi^{*}_{\ell'\downarrow}(\underline{R}',\underline{r}) \psi_{\ell\downarrow}(\underline{R},\underline{r}) \, d\underline{r} \right) \times \frac{\left[N_{\ell\downarrow}(\underline{R}) - N_{n\uparrow}(\underline{R}) \right] \left[N_{\ell'\downarrow}(\underline{R}') - N_{n'\uparrow}(\underline{R}') \right]}{\left[E_{\ell\downarrow}(\underline{R}) - E_{n\uparrow}(\underline{R}) \right] \left[E_{\ell'\downarrow}(\underline{R}') - E_{n'\uparrow}(\underline{R}') \right]} \tag{3.20}$$

Also $V_f(\underline{r}) = \frac{1}{2}(\rho_{\downarrow} - \rho_{\uparrow}) f(\underline{r})$. And from the integral eqn. (3.I6) for $m_I(\underline{r})$, by replacing m_I with

$$\frac{1}{M_o} \times \frac{-g\mathcal{E}_B}{2} \times \frac{\hbar}{m} \sum_{\ell n \underline{R}} \left\langle \ell_{\downarrow} \underline{R} \left| P_x \right| n_{\uparrow} \underline{R} \right\rangle \frac{N_{n\uparrow}(\underline{R}) - N_{\ell\downarrow}(\underline{R})}{E_{n\uparrow}(\underline{R}) - E_{\ell\downarrow}(\underline{R})} \psi^{*}_{n\uparrow}(\underline{R},\underline{r}) \psi_{\ell\downarrow}(\underline{R},\underline{r})$$

as the first iteration, and integrating by parts we have a term

$$-\frac{g\mathcal{E}_B}{2} \frac{1}{M_o(\underline{r})} \sum_{\ell n \underline{R}} \sum_{\ell' n' \underline{R}'} \left\langle \ell_{\downarrow} \underline{R} \left| \frac{P_x}{m} \right| n_{\uparrow} \underline{R} \right\rangle \left\langle n'_{\uparrow} \underline{R}' \left| \frac{P_x}{m} \right| \ell'_{\downarrow} \underline{R}' \right\rangle \times \frac{\left[N_{n\uparrow}(\underline{R}) - N_{\ell\downarrow}(\underline{R}) \right] \left[N_{n'\uparrow}(\underline{R}') - N_{\ell'\downarrow}(\underline{R}') \right]}{\left[E_{n\uparrow}(\underline{R}) - E_{\ell\downarrow}(\underline{R}) \right] \left[E_{n'\uparrow}(\underline{R}') - E_{\ell'\downarrow}(\underline{R}') \right]} (\rho_{\downarrow} - \rho_{\uparrow}) \times \int f(\underline{r}) \psi^{*}_{\ell\downarrow}(\underline{R},\underline{r}) \psi_{\ell'\downarrow}(\underline{R}',\underline{r}) \psi^{*}_{n'\uparrow}(\underline{R}',\underline{r}) \psi_{n\uparrow}(\underline{R}) \, d\underline{r}, \tag{3.2I}$$

Noting that $M_o(\underline{r}) = -\frac{g\mathcal{E}_B}{2}(\rho_{\uparrow} - \rho_{\downarrow})$, (3.2I) is exactly the same as (3.20), and our proof is thus achieved.

The Behaviour of D in the Paramagnetic Limit.

In this section we have shown that $D \to 0$ as $N_\uparrow - N_\downarrow \to 0$ in the very weak ferromagnetic or paramagnetic limit, as should be.

From the expression for D in eqn. (3.15) we first we first deal with the first two terms viz.

$$\frac{\hbar^2}{N_\uparrow - N_\downarrow}\left\{\frac{N}{2m} + \sum_{\ell n \underline{R}} \left|\langle \ell_\downarrow \underline{R} \left| \frac{P_x}{m} \right| n_\uparrow \underline{k} \rangle\right|^2 \frac{N_{n\uparrow}(\underline{R}) - N_{\ell\downarrow}(\underline{R})}{E_{n\uparrow}(\underline{R}) - E_{\ell\downarrow}(\underline{R})}\right\}$$

From the f-sum rule

$$\begin{aligned}\frac{N}{2m} &= \frac{1}{2m}\sum_{n\underline{R}} N_n(\underline{R}) \\ &= \frac{1}{2}\sum_{n\underline{R}} N_n(\underline{R})\left(\frac{1}{m_n(\underline{R})}\right)_{\alpha\alpha} - \frac{1}{m^2}\sum_{(\ell\neq n}^{\ell} \frac{|\langle \underline{R}n | P_\alpha | \underline{R}\ell\rangle|^2 N_n(\underline{R})}{E_n(\underline{R}) - E_\ell(\underline{R})}\end{aligned} \tag{3.22}$$

and also

$$\begin{aligned}&\left(\frac{1}{m_n(\underline{R})}\right)_{\alpha\alpha} \\ &= \frac{1}{\hbar^2}\frac{\partial^2 E_n(\underline{R})}{\partial R_\alpha^2} \\ &= \frac{1}{3\hbar^2}\nabla^2 E_n(\underline{R}) \quad , \text{ assuming cubic symmetry.}\end{aligned} \tag{3.23}$$

Thus, assuming cubic symmetry,

$$\frac{N}{2m} = \frac{1}{6}\left\{\sum_{n\underline{R}}\left[\frac{N_n(\underline{R})}{\hbar^2}\nabla^2 E_n(\underline{R}) - \frac{1}{m^2}\sum_{(\ell\neq n)}^{\ell} |\langle n\underline{R}|\underline{P}|\ell\underline{R}\rangle|^2 \times \frac{N_n(\underline{R}) - N_\ell(\underline{R})}{E_n(\underline{R}) - E_\ell(\underline{R})}\right]\right\} \tag{3.24}$$

Also noting that

$$\lim_{\substack{l=n \\ q\to 0}} \frac{N_n(\underline{R}) - N_l(\underline{R}+\underline{q})}{E_n(\underline{R}) - E_l(\underline{R}+\underline{q})} = \frac{dN_n(\underline{R})}{dE_n(\underline{R})}$$

and
$$\nabla_{\underline{R}} E_n(\underline{R}) = \frac{\hbar}{m}\langle n\underline{R}|\underline{P}|n\underline{R}\rangle, \tag{3.25}$$

the first two terms of D reduces to

$$\frac{\hbar^2}{6(N_\uparrow - N_\downarrow)}\left\{\sum_{n\underline{R}}\left[N_n(\underline{R})\frac{\nabla^2 E_n(\underline{R})}{\hbar^2}\right.\right.$$
$$-\frac{1}{m^2}\sum_{\substack{l \\ (l\neq n)}}|\langle n\underline{R}|\underline{P}|l\underline{R}\rangle|^2\frac{N_n(\underline{R}) - N_l(\underline{R})}{E_n(\underline{R}) - E_l(\underline{R})}$$
$$\left.\left.+\frac{2}{m^2}\sum_{l(all)}|\langle n\underline{R}|\underline{P}S^-|l\underline{R}\rangle|^2\frac{N_n(\underline{R}) - N_l(\underline{R})}{E_n(\underline{R}) - E_l(\underline{R})}\right]\right\}$$
$$= \frac{\hbar^2}{6(N_\uparrow - N_\downarrow)}\sum_{n\underline{R}}\left\{\frac{1}{\hbar^2}\left[\nabla^2 E_n(\underline{R})N_n(\underline{R}) + |\nabla E_n(\underline{R})|^2\frac{dN_n(\underline{R})}{dE_n(\underline{R})}\right]\right.$$
$$+\frac{1}{m^2}\sum_{l(all)}\left[2|\langle n\underline{R}|\underline{P}S^-|l\underline{R}\rangle|^2 - |\langle n\underline{R}|\underline{P}|l\underline{R}\rangle|^2\right]\times$$
$$\left.\times\frac{N_n(\underline{R}) - N_l(\underline{R})}{E_n(\underline{R}) - E_l(\underline{R})}\right\}, \tag{3.26}$$

The right hand side is obtained by adding and subtracting the diagonal matrix (l = n) element.

Now

$$\nabla^2 E_n(\underline{R})N_n(\underline{R})$$
$$= \nabla\cdot\left(N_n(\underline{R})\nabla E_n(\underline{R})\right) - \nabla E_n(\underline{R})\nabla N_n(\underline{R})$$
$$= \nabla\cdot\left(N_n(\underline{R})\nabla E_n(\underline{R})\right) - |\nabla E_n(\underline{R})|^2\frac{dN_n(\underline{R})}{dE_n(\underline{R})}$$

since $\nabla_{\underline{R}} N_n(\underline{R}) = \frac{dN_n(\underline{R})}{dE_n(\underline{R})} \nabla_{\underline{R}} E_n(\underline{R})$, N being a function of energy only.

This reduces our expression for D to

$$\frac{1}{6(N_\uparrow - N_\downarrow)} \sum_{n\underline{R}} \Big\{ \nabla.(N_n(\underline{R}) \nabla E_n(\underline{R}) + \frac{1}{m^2} \sum_{\ell(all)} \Big[2 |\langle n\underline{R}|\underline{P}S^-|\ell\underline{R}\rangle|^2 - |\langle n\underline{R}|\underline{P}|\ell\underline{R}\rangle|^2 \Big] \times \frac{N_n(\underline{R}) - N_\ell(\underline{R})}{E_n(\underline{R}) - E_\ell(\underline{R})} \tag{3.27}$$

In the very weak ferromagnetic or paramagnetic limit, $N_\uparrow - N_\downarrow \to 0$ and also the exchange splitting $\Delta E \to 0$. The bands of and spins have the same energy. In this limit the matrix elements cancel, since there are twice as many matrix elements of $\underline{P}$ as of $\underline{P}S^-$ which connects only $\uparrow$ with $\downarrow$ spins and the numerical values will be equal. We are then left with

$$\begin{aligned} &\sum_{n\underline{R}} \nabla.(N_n(\underline{R}) \nabla E_n(\underline{R}) \\ &= \sum_n \int d^3R \, \nabla.(N_n(\underline{R}) \nabla E_n(\underline{R})) \\ &= \sum_n \int dS_R \, N_n(\underline{R}) \nabla E_n(\underline{R}) \end{aligned} \tag{3.28}$$

The normal derivative of energy vanishes on the surface of the Brillouin Zone and thus the integral of (3.28) is zero.

Thus $D \to 0$ as $N_\uparrow - N_\downarrow \to 0$, even when the vertex correction is neglected.

The Dynamic Susceptibility of a Ferromagnet

An explicit formula for $\chi(\underline{q},\omega)$ within the CW approach and with local field terms neglected is derived in the following way. The interaction hamiltonian is

$$H_I = -\frac{1}{2} g \mu_B \underline{B}_\perp \cdot \underline{\sigma}$$
$$= -\frac{1}{4} g \mu_B B_0 \left[e^{i(\underline{q}.\underline{r} - \omega t)} \sigma_- + e^{-i(\underline{q}.\underline{r} - \omega t)} \sigma_+ \right] e^{-\eta|t|}$$

and also $M_+(\underline{r},t)$

$$= \frac{1}{2} B_0 \chi_{+-}(\underline{q},\omega) e^{i(\underline{q}.\underline{r} - \omega t)} \underline{M_0(r)} / \bar{M}_0 \qquad (3.29)$$

where $\bar{M}_0 = \frac{1}{V} \int M_0(\underline{r}) dr$

When we include the effect of induced magnetisation viz. $\Delta V_f(\underline{r}) = V_f(\underline{r})(M_+ \sigma_- + M_- \sigma_+)/2M_0(\underline{r})$, the effective interaction hamiltonian is

$$H_I^{eff} = -\frac{g\mu_B}{4} B_0 \left\{ \left[1 + \frac{\chi_{+-}(\underline{q},\omega)}{\bar{M}_0} \frac{V_f(\underline{r})}{g\mu_B} \right] \sigma_- e^{i(\underline{q}.\underline{r} - \omega t)} + h.c \right\} e^{-\eta|t|} \qquad (3.30)$$

Using the expression for perturbed wave function as derived in eqn. (2.54)

$$M_+(\underline{r},t) = -\frac{g\mu_B}{2} \sum_{n\underline{R}} N_n(\underline{R}) \psi_n^*(\underline{R},\underline{r},t) \sigma_+ \psi_n(\underline{R},\underline{r},t)$$

$$= -\frac{(g\mu_B)^2}{2} B_0 \sum_{\ell n \underline{R}} \left\langle \ell_\downarrow \underline{R}+\underline{q} \left| \left[1 + \frac{\chi_{+-}(\underline{q},\omega)}{\bar{M}_0} V_f(\underline{r}) e^{i\underline{q}\cdot\underline{r}} \right| n_\uparrow \underline{R} \right\rangle \right.$$

$$\times \frac{N_{n\uparrow}(\underline{R}) - N_{\ell\downarrow}(\underline{R}+\underline{q})}{E_{n\uparrow}(\underline{R}) - E_{\ell\downarrow}(\underline{R}+\underline{q}) + \hbar\omega + i\eta} e^{-i\omega t} \psi^*_{n\uparrow}(\underline{R},\underline{r}) \psi_{\ell\downarrow}(\underline{R}+\underline{q},\underline{r}) \qquad (3.31)$$

Therefore,

$$\chi_{+-}(\underline{q},\omega) \frac{M_0(\underline{r})}{\bar{M}_0}$$

$$= -(g\mu_B)^2 \sum_{\ell n \underline{R}} \left\langle \ell_\downarrow \underline{R}+\underline{q} \left| \left[1 + \frac{\chi_{+-}(\underline{q},\omega)}{\bar{M}_0} \frac{V_f(\underline{r})}{g\mu_B}\right] e^{i\underline{q}\cdot\underline{r}} \right| n_\uparrow \underline{R} \right\rangle$$

$$\times \frac{N_{n\uparrow}(\underline{R}) - N_{\ell\downarrow}(\underline{R}+\underline{q})}{E_{n\uparrow}(\underline{R}) - E_{\ell\downarrow}(\underline{R}+\underline{q}) + \hbar\omega + i\eta} e^{-i\underline{q}\cdot\underline{r}} \psi^*_{n\uparrow}(\underline{R},\underline{r}) \psi_{\ell\downarrow}(\underline{R}+\underline{q},\underline{r})$$

Multiplying by $V_f(\underline{r})$ and integrating

$$\frac{\chi_{+-}(\underline{q},\omega)}{\bar{M}_0} \left\{ \int M_0(\underline{r}) V_f(\underline{r}) d\underline{r} + \right.$$

$$g\mu_B \sum_{\ell n \underline{R}} \left. \frac{N_{n\uparrow}(\underline{R}) - N_{\ell\downarrow}(\underline{R}+\underline{q})}{E_{n\uparrow}(\underline{R}) - E_{\ell\downarrow}(\underline{R}+\underline{q}) + \hbar\omega + i\eta} \left| \left\langle \ell_\downarrow \underline{R}+\underline{q} \left| V_f(\underline{r}) e^{i\underline{q}\cdot\underline{r}} \right| n_\uparrow \underline{R} \right\rangle \right|^2 \right\}$$

$$= -(g\mu_B)^2 \sum_{\ell n \underline{R}} \left\langle \ell_\downarrow \underline{R}+\underline{q} \left| e^{i\underline{q}\cdot\underline{r}} \right| n_\uparrow \underline{R} \right\rangle \left\langle n_\uparrow \underline{R} \left| e^{-i\underline{q}\cdot\underline{r}} V_f(\underline{r}) \right| \ell_\downarrow \underline{R}+\underline{q} \right\rangle$$

$$\times \frac{N_{n\uparrow}(\underline{R}) - N_{\ell\downarrow}(\underline{R}+\underline{q})}{E_{n\uparrow}(\underline{R}) - E_{\ell\downarrow}(\underline{R}+\underline{q}) + \hbar\omega + i\eta} \qquad (3.32)$$

whence

$$\chi_{+-}(\underline{q},\omega) = \frac{-\bar{M}_o(g\mathcal{E}_B)^2 \sum_{\ell n \underline{R}} \frac{\langle \ell_\downarrow \underline{R}+\underline{q}|e^{i\underline{q}\cdot\underline{r}}|n_\uparrow \underline{R}\rangle\langle n_\uparrow \underline{R}|e^{-i\underline{q}\cdot\underline{r}} V_f(\underline{r})|\ell_\downarrow \underline{R}+\underline{q}\rangle}{E_{n\uparrow}(\underline{R}) - E_{\ell\downarrow}(\underline{R}+\underline{q}) + \hbar\omega + i\eta}}{\int M_o(\underline{r}) V_f(\underline{r})\, d\underline{r} + g\mathcal{E}_B \sum_{\ell n \underline{R}} \left|\langle \ell_\downarrow \underline{R}+\underline{q}|V_f(\underline{r})e^{i\underline{q}\cdot\underline{r}}|n_\uparrow \underline{R}\rangle\right|^2 \times \frac{N_{n\uparrow}(\underline{R}) - N_{\ell\downarrow}(\underline{R}+\underline{q})}{E_{n\uparrow}(\underline{R}) - E_{\ell\downarrow}(\underline{R}+\underline{q}) + \hbar\omega + i\eta}} \qquad (3.33)$$

(3.33) is our desired formula for $\chi_{+-}(\underline{q},\omega)$

CHAPTER IV

Spin Wave Energy of Antiferromagnetism

In chapter I the Heisenberg hamiltonian defined by eqn. (I.I) produces ferromagnetism if J is positive. However, in antiferromagnetism the same hamiltonian may be retained with a fundamental redefinition of J i.e $J < 0$. As a consequence, from semiclassical or mean field arguments, the single lattice of the magnetic crystal is then to be conceived as composed of two interpenetrating sublattices, A and B, having magnetisation directions converse to each other. $J = |J|$ will now be the exchange interaction between the nearest neighbours, which will be on different sublattices; and the hamiltonian becomes, in the momentum space representation,

$$H = \frac{1}{N}\sum_{\underline{R}} J S_{A\underline{R}} S_{B-\underline{R}} \tag{4.I}$$

$$S_{A,Bq} = \sum_{i \in A,B} e^{i\underline{q}.\underline{R}_i} S_i \tag{4.2}$$

Anderson[45] and Kubo[46] were the first to propose a linear theory for antiferromagnetism, but the problem was with the ground state. With the hamiltonian (4.I), an exact

ground state is available only for a linear one-dimensional chain magnet, as discussed by des Cloizeaux and Pearson[47]. The ground state in this model is a non-degenerate singlet state which has the total spin operator

$$S = \sum_i S_i = 0$$

However, the ground state of the linear theory of Anderson is not the ground state of the isotropic antiferromagnet. Rather, an infinitesimal anisotropy field must be introduced into the hamiltonian (4.I) which will stabilise the sublattice magnetisation direction and prevent the theory from collapsing because of a divergence in the amplitude of the spin wave creation operators. However, the linear theory, whose ground state is not that of the classical one, is valid for a real 3-dimensional antiferromagnet[48].

The method of setting up equation of motion for the susceptibility function, with this hamiltonian and within the linear theory, can be applied here. It was done in good detail by Fisher[35], who also worked beyond the linear theory. But the work does not help the linear theory, rather strengthens confidence in the green function method. This fact reasonably prompts us to extend the EF method, which was employed in ferromagnetism, to antiferromagnetism. Real antiferromagnets, like Chromium etc, are band models; and, therefore, the itinerant antiferromagnetism would receive our consideration now.

In this model, the most general ground state is the spin density wave state in which the spin density oscillates with a wave vector $\underline{Q}$, which may or may not be commensurate with the lattice. First, considering the simple one band case, an interpenetrating sublattice structure is proposed. Essentially this was first proposed by Slater[49] and revised and refined by Matsubara[50] and des Cloizeaux[51]; and the incommensurate spin density wave was discussed by Overhauser[52] and Fedders and Martin[53]. Des Cloizeaux's model involved the notion of pairing of the same-spin electrons, while Fedders and Martin introduced the notion of coupling between opposite spin electrons. We shall be dealing with the two-sublattice scheme appropriate to the commensurate case.

The Two-Sublattice Scheme

Assuming that the original crystal lattice is the sum of two interpenetrating sublattices, A and B, we can define Bloch wave functions $\psi_A(\underline{R}), \psi_B(\underline{R})$ of a tight binding form on each sublattice separately. But now the symmetry of the magnetic lattice is reduced, and so we are to reorganise our calculations in terms of a reduced Brillouin Zone, which is half the original and reduced along the direction of $\underline{Q}$. Then $\psi_A(\underline{R})$ and $\psi_B(\underline{R})$ are related to the representation of bands in a paramagnet

by

$$\psi(\underline{k}) = \frac{1}{\sqrt{2}}\left(\psi_A(\underline{k}) + \psi_B(\underline{k})\right) \tag{4.3}$$

$$\psi(\underline{k}+\underline{Q}) = \frac{1}{\sqrt{2}}\left(\psi_A(\underline{k}) - \psi_B(\underline{k})\right) \tag{4.4}$$

and a Wannier representation of ψ_A's are

$$\left.\begin{matrix}\psi_A(\underline{k}) \\ \psi_B(\underline{k})\end{matrix}\right\} = \frac{1}{\sqrt{N}}\sum_i e^{i\underline{k}\cdot\underline{R}_i}\omega(\underline{r}-\underline{R}_i)\begin{cases} i\in A \text{ only} \\ i\in B \text{ only}\end{cases} \tag{4.5}$$

We restrict ourselves to the single band Hubbard type hamiltonian

$$H = \sum_{R\sigma}\varepsilon(\underline{R})n_{R\sigma} + I\sum_i n_{i\uparrow}n_{i\downarrow} \tag{4.6}$$

where I is the interaction energy between two electrons on the same Wannier site. Under our A and B sublattice scheme it is rewritten as

$$H = \sum_{R\sigma}\varepsilon_1(n_{A\underline{R}\sigma} + n_{B\underline{R}\sigma}) - \varepsilon_2(c^+_{B\underline{R}\sigma}c_{A\underline{R}\sigma} + c^+_{A\underline{R}\sigma}c_{B\underline{R}\sigma}) + I\sum_{i\in A,B} n_{i\uparrow}n_{i\downarrow} \tag{4.7}$$

where $\varepsilon_1(\underline{R})$ and $\varepsilon_2(\underline{R})$ are expressed as

$$\varepsilon_1(\underline{R}) = \frac{1}{2}\left(\varepsilon(\underline{R}+\underline{Q}) + \varepsilon(\underline{R})\right)$$
$$\varepsilon_2(\underline{R}) = \frac{1}{2}\left(\varepsilon(\underline{R}+\underline{Q}) - \varepsilon(\underline{R})\right) \tag{4.8}$$

The vector $\underline{Q}$ is important. As we mentioned earlier, because of reduced symmetry, the Brillouin Zone is divided into two zones, each containing the same number of states. If $\underline{k}$ lies in the first Brillouin Zone, then $\underline{k} + \underline{Q}$, where, as pointed out earlier, $\underline{Q}$ is one of the

magnetic reciprocal lattice vectors, is a vector in the new second Brillouin Zone modulo a vector in the paramagnetic reciprocal lattice. The vector $\underline{Q}$ has the property that $e^{i\underline{Q}\cdot\underline{R}_j}$ can be I on sublattice A and -I on sublattice B.

In the antiferromagnetic state, the single band breaks up into two bands for each spin, one with greater charge density on sublattice A than on sublattice B, and one with more charge density on sublattice B than on sublattice A . For the opposite spin, the sublattices are interchanged. Also, one band of each spin will lie lower in energy than the other and, therefore, will tend to contain more electrons than the other band of the same spin. In crystals of inversion symmetry, corresponding bands of opposite spins are degenerate. By carrying out the necessary algebra, we will see it clearly

Essentially, the method is to set up the equation of motion for the one electron Green Function which appears in the susceptibility function. But for the 2-sublattice structure, it will have a matrix form defined by

$$G^{\sigma}_{\alpha\beta}(\underline{R},\omega) = \langle\langle C_{\alpha\underline{R}\sigma} \,;\, C^{+}_{\beta\underline{R}\sigma} \rangle\rangle_{\omega} \qquad (4.9)$$

where $(\alpha,\beta) = (A,A),(A,B),(B,A)$ and (B,B) are the elements of the matrix. The equation of motion can be wri-

tten as

$$G^{\uparrow}_{\alpha\beta}(\underline{R},\omega) = \begin{pmatrix} \omega - \mathcal{E}_1(\underline{R}) - \frac{I n_{A\downarrow}}{N} & \mathcal{E}_2(\underline{R}) \\ \mathcal{E}_2(\underline{R}) & \omega - \mathcal{E}_1(\underline{R}) - \frac{I n_{B\downarrow}}{N} \end{pmatrix}^{-1} = W^{-1} \qquad (4.10)$$

Clearly (4.10) is in non-diagonal form. A canonical transformation of the original Bloch wave functions defined over the sublattices, which will generate quasi-particle wave functions in the form of linear combinations, will achieve this goal. Defining the quasi-particle creation operators for ↑ spin by $d_{\underline{R}_1\uparrow}$ and $d_{\underline{R}_2\uparrow}$, with the corresponding energies by $E_I(\underline{k})$, $E_2(\underline{k})$, the transformation will be

$$TWT^{+} = \begin{pmatrix} \omega - E_1(\underline{R}) & 0 \\ 0 & \omega - E_2(\underline{R}) \end{pmatrix} \qquad (4.11)$$

and $TT^{+} = T^{+}T = I$, the unitarity condition. The standard procedure of diagonalisation gives

$$E^{1}_{2}(\underline{R}) = \mathcal{E}_1(\underline{R}) \mp \sqrt{g^2 + \mathcal{E}_2^2(\underline{R})} \qquad (4.12)$$

with $\tan\theta_{\underline{R}} = \frac{\mathcal{E}_2(\underline{R})}{g}$, and $2g = \frac{I}{N}\langle n_{A\uparrow} - n_{A\downarrow}\rangle$.

is involved in the transforming matrix T such that

$$\begin{pmatrix} d^{+}_{\underline{R}_1\uparrow} \\ d^{+}_{\underline{R}_2\uparrow} \end{pmatrix} = T \begin{pmatrix} c^{+}_{A\underline{R}\uparrow} \\ c^{+}_{B\underline{R}\uparrow} \end{pmatrix} = \begin{pmatrix} \cos\frac{1}{2}\theta_{\underline{R}} & \sin\frac{1}{2}\theta_{\underline{R}} \\ -\sin\frac{1}{2}\theta_{\underline{R}} & \cos\frac{1}{2}\theta_{\underline{R}} \end{pmatrix} \begin{pmatrix} c^{+}_{A\underline{R}\uparrow} \\ c^{+}_{B\underline{R}\uparrow} \end{pmatrix} \qquad (4.13)$$

We can now write

$$\left\langle\!\!\left\langle \begin{pmatrix} d_{\underline{R}_1\uparrow} \\ d_{\underline{R}_2\uparrow} \end{pmatrix} ; \begin{pmatrix} d^{+}_{\underline{R}_1\uparrow} \\ d^{+}_{\underline{R}_2\uparrow} \end{pmatrix} \right\rangle\!\!\right\rangle = \begin{pmatrix} \frac{1}{\omega - E_1(\underline{R})} & 0 \\ 0 & \frac{1}{\omega - E_2(\underline{R})} \end{pmatrix} \tag{4.I4}$$

Similarly, for the down spin case, $d^{+}_{\underline{R}_1\downarrow}, d^{+}_{\underline{R}_2\downarrow}$ and the corresponding energies $E_I(\underline{k})$, $E_2(\underline{k})$ are defined by

$$\begin{pmatrix} d^{+}_{\underline{R}_1\downarrow} \\ d^{+}_{\underline{R}_2\downarrow} \end{pmatrix} = T^{+} \begin{pmatrix} c^{+}_{B\underline{R}\downarrow} \\ c^{+}_{A\underline{R}\downarrow} \end{pmatrix}, \tag{4.I5}$$

$$E^{1}_{2}(\underline{R}) = \varepsilon_1(\underline{R}) \mp \sqrt{g^2 + \varepsilon_2^2(\underline{R})}$$

with $2g = \frac{I}{N}\langle n_{B\downarrow} - n_{B\uparrow}\rangle$; but for the antiferromagnetic structure

$$\langle n_{A\uparrow}\rangle = \langle n_{B\downarrow}\rangle \tag{4.I6}$$

which shows that $g_\uparrow = g_\downarrow = g$, and hence $E^{I}_{2}(\underline{k})_\uparrow = E^{I}_{2}(\underline{k})_\downarrow$, i.e. spin-degenerate.

The linear combination giving the quasi-particle creation operators can be rewritten in a different set up using eqns. (4.3) and (4.4) viz.

$$\begin{pmatrix} d^{+}_{k_1\uparrow} \\ d^{+}_{k_2\uparrow} \end{pmatrix} = \begin{pmatrix} \cos\frac{1}{2}\left(\frac{\pi}{2} - \Theta_{\underline{R}}\right) & -\sin\frac{1}{2}\left(\frac{\pi}{2} - \Theta_{\underline{R}}\right) \\ \sin\frac{1}{2}\left(\frac{\pi}{2} - \Theta_{\underline{R}}\right) & \cos\frac{1}{2}\left(\frac{\pi}{2} - \Theta_{\underline{k}}\right) \end{pmatrix} \begin{pmatrix} c^{+}_{R\uparrow} \\ c^{+}_{\underline{k}+\underline{Q}\uparrow} \end{pmatrix} \tag{4.I7}$$

This corresponds to Sokoloff's[54] transformation , the only difference being the phase $\frac{\pi}{2}$. Actually, $\cos\frac{1}{2}\Theta_{\underline{R}}$ or $\sin\frac{1}{2}\Theta_{\underline{R}}$ is determined from the condition

$$i\hbar \frac{\partial}{\partial t} d_{\underline{R}\lambda\sigma} = E_{\lambda\sigma}(\underline{R})\, d_{\underline{R}\lambda\sigma} \tag{4.I8}$$

in the HF approximation. λ, σ denote band and spin

index.

The energy gap is $2(\varepsilon_2(\underline{k}) + g)$, whence the minimum energy gap value is $2g$. But in the absence of the antiferromagnetic ordering, g goes to zero. The eqn. from which g is to be calculated selfconsistently is obtained as follows. By using the transformation matrix we can express $n_{A\uparrow}$ and $n_{A\downarrow}$ in terms of the quasi-particle occupation numbers. Thus

$$\begin{aligned} &\langle n_{A\uparrow} - n_{A\downarrow} \rangle \\ &= \langle n_{A\uparrow} - n_{B\uparrow} \rangle \\ &= \sum_{\underline{k}} \cos\theta_{\underline{k}} (N_{\underline{k}1\uparrow} - N_{\underline{k}2\uparrow}) \end{aligned} \tag{4.19}$$

and therefore from the relation

$$2g = \frac{I}{N} \langle n_{A\uparrow} - n_{A\downarrow} \rangle ,$$ we derive

$$R = \frac{I}{2N} \sum_{\underline{k}} \frac{N_{\underline{k}1\sigma} - N_{\underline{k}2\sigma}}{\sqrt{\varepsilon_2^2(\underline{k}) + g^2}} \tag{4.20}$$

$N_{\underline{k}1\sigma}$, $N_{\underline{k}2\sigma}$ are the occupation numbers chosen so that the energy at $T = 0$, or the free energy at $T \neq 0$ is minimum. In our case of simple antiferromagnet, however, the occupation numbers are independent of spin, and hence the spin indices can be dropped henceforth.

Since we are interested in the excited spin wave spectrum, we shall not discuss some no less important points viz. choosing the appropriate Fermi Surface to minimise energy, predicting the criterion for antiferro-magnetism etc.

Susceptibility and Spin Waves

Proceeding along the Green Function approach, Fisher[35] introducing an ad hoc matrix form for the susceptibility function which we shall get to very shortly, arrived at an exact formula for the spin wave velocity C . But Sokoloff, too, worked in RPA and employed the Green Function scheme. Unfortunately Fisher's result for C, when simplified within HF, differed from Sokoloff's, which led Fisher to comment that his is the more general formula and Sokoloff's work suffered from being restricted to a subspace. We shall briefly point out the steps of both the works.

We start with the reduced susceptibility

$$\chi^{(\underline{q},\omega)}_{+-\,\xi\gamma} = \langle\langle S^{+}_{-q\xi} \,;\, S^{-}_{q\gamma} \rangle\rangle_{\omega} \qquad (4.2I)$$

where $(\xi,\gamma) = (A,A),(A,B),(B,A)$ and (B,B) The operators $S^{+}_{-q\xi}$, $S^{-}_{q\gamma}$ are expressed in terms of Bloch creation and destruction operators i.e.

$$S^{-}_{Aq} = \sum_{\underline{R}} C^{+}_{A\underline{R}+\underline{q}} C_{A\underline{R}\uparrow}$$
$$S^{+}_{A-q} = \sum_{\underline{R}} C^{+}_{A\underline{R}-q\uparrow} C_{A\underline{R}\downarrow} \qquad (4.22)$$

$S^{-}_{q} = \frac{1}{\sqrt{2}}(S^{-}_{Aq} + S^{-}_{Bq})$ commutes with when q = 0. At this stagewe can say that, if the Fermi level lies in the gap, so that the spin waves are the only low-lying modes, then because of the above commutation relation, we may assume that $\chi^{(\underline{q},\omega)}_{+-}$ will contain two spin wave poles. Once again, by canonical transformation $\chi^{(\underline{q},\omega)}_{+-}$

can be diagonalised so that the two spin wave branches are separated in the diagonal elements. Denoting by the similarity transformation,

$$\begin{aligned}\bar{\chi}(\underline{q},\omega) &= P\chi P^{+} \\ &= \begin{pmatrix} [\omega-\omega_s(\underline{q})]^{-1} & 0 \\ 0 & -[\omega+\omega_s(\underline{q})]^{-1} \end{pmatrix} \Delta n \end{aligned} \tag{4.23}$$

Or,

$$\left\langle\!\!\left\langle \begin{pmatrix} S^{+}_{A-\underline{q}} \\ S^{+}_{B-\underline{q}} \end{pmatrix} P^{+} ; P \begin{pmatrix} S^{-}_{A\underline{q}} \\ S^{-}_{B\underline{q}} \end{pmatrix} \right\rangle\!\!\right\rangle = \omega^{-1} \begin{pmatrix} 1+\frac{cq}{\omega} & 0 \\ 0 & -1+\frac{cq}{\omega} \end{pmatrix} \Delta n_0 \tag{4.24}$$

assuming that

$$\omega_s(\underline{q}) = cq + O(q^2), \quad \Delta n = \Delta n_0 + \Delta n_1 q$$

with $q/\omega \ll 1$. Eqn. (4.24) is Fisher's ad hoc assumption . In order to avoid the singularity of the transformation, a weak anisotropy field is required which will introduce a term $-h(S^z_A - S^z_B)$ into the hamiltonian and stabilise the system against rotations of the total spin. However, for h infinitesimal the assumption of ω_s linear

in q is still valid. Then, because of the oppositely directed spins on sublattices A and B , poles will occur at $\pm\omega_s$. Now the straightforward extension of the EF method in ferromagnetism is to set up the equation of motion for $\chi(\underline{q},\omega)$ and then compare, which gives

$$\chi^{(\underline{q},\omega)}_{+-} = \omega^{-2}\begin{pmatrix} a+(d+b)q^2 & -a \\ -a & a+(d-b)q^2 \end{pmatrix} + \omega^{-1}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\langle n_{A\uparrow} - n_{A\downarrow}\rangle \qquad (4.25)$$

a, b, d are given by

$$a = \lim_{\omega\to 0}\lim_{q\to 0} a_{AB} \qquad (4.26)$$

$$b = \lim_{\omega\to 0}\lim_{q\to 0}\frac{1}{2q^2}(a_{AA} - a_{BB}) \qquad (4.27)$$

$$d = \lim_{\omega\to 0}\lim_{q\to 0}\frac{1}{2q^2}(a_{AA} + 2a_{AB} + a_{BB}) \qquad (4.28)$$

with

$$a_{(r,s)} = \left\langle\left[\left[S^{+}_{r-q},H\right],S^{-}_{sq}\right]\right\rangle + \left\langle\!\!\left\langle\left[S^{+}_{r-q},H\right];\left[H,S^{-}_{sq}\right]\right\rangle\!\!\right\rangle_{\omega}$$

$$(r,s) = (A,A),(A,B),(B,A),(B,B) \qquad (4.29)$$

The eigenvalue of the matrix (4.25) will give the expression for C which is

$$C = \frac{\sqrt{2ad}}{\langle n_{A\uparrow} - n_{A\downarrow}\rangle}\,, \quad \Delta n_0 = \langle n_{A\uparrow} - n_{A\downarrow}\rangle \qquad (4.30)$$

This is an exact formula due to EF formalism. Fisher worked out a, d in the HF approximation (page 73 of ref.

35). Sokoloff started off with

$$\chi^{(q,\omega)}_{+-} = \begin{pmatrix} \chi_{q\,q} & \chi_{q\,q+Q} \\ \chi_{q+Q\,q} & \chi_{q+Q\,q+Q} \end{pmatrix} \qquad (4.3I)$$

which is equivalent to Fisher's matrix form within a similarity transformation. Sokoloff carried out his algebra in the random phase approximation and arrived at a result for C which was different from Fisher's. It appears to us that the disagreement is probably because Fisher evaluated the Green's Function in (4.29) using the HF approximation instead of the full RPA. We believe his ansatz (4.24) is correct.

CW Approach Applied to
Antiferromagnetism

The extension of CW approach to antiferromagnetism confirms Sokoloff's result. We carry it out in the following way. We first formulate the problem for a general band structure and then specialise to the Hubbard model.

The crucial argument is about the precessional cone angle $m_q(r)$, which was assumed to be constant within each unit cell for the ferromagnetic case when local field effects are neglected. The situation is altered in the antiferromagnetic case, m_q now having different values on the two sublattices. It is now defined as

$$m_q(r) = A_q + B_q e^{iQ\cdot r} \qquad (4.32)$$

so that its value is

$$\begin{aligned} &A_q + B_q && \text{on A sublattice} \\ &\text{and } A_q - B_q && \text{on B sublattice} \end{aligned} \tag{4.33}$$

Invoking equation (3.4) and inserting the new expression for $m_q(\underline{r})$, the corresponding fundamental equation for an antiferromagnet is obtained.

$$\begin{aligned} -g\mu_B \sum_{\ell n \underline{R}} &\left\langle \ell_\downarrow \underline{R}+\underline{q} \middle| e^{i\underline{q}.\underline{r}} V_f(\underline{r}) \left[A_q + B_q e^{i\underline{Q}.\underline{r}} \right] \middle| n_\uparrow \underline{R} \right\rangle \\ &\times \frac{N_{n\uparrow}(\underline{R}) - N_{\ell\downarrow}(\underline{R}+\underline{q})}{E_{n\uparrow}(\underline{R}) - E_{\ell\downarrow}(\underline{R}+\underline{q}) + \hbar\omega} \\ &\times \psi^*_{n\uparrow}(\underline{R},\underline{r}) \psi_{\ell\downarrow}(\underline{R}+\underline{q},\underline{r}) e^{-i\underline{q}.\underline{r}} \\ &= M_o(\underline{r}) \left(A_q + B_q e^{i\underline{Q}.\underline{r}} \right) \end{aligned} \tag{4.34}$$

Multiplying this eqn. with $V_f(\underline{r})$ and $V_f(\underline{r})e^{-iQ.r}$ two equations are obtained i.e.

$$\begin{aligned} &\left\{ A_q \times -g\mu_B \sum_{\ell n \underline{R}} \left\langle \ell_\downarrow \underline{R}+\underline{q} \middle| e^{i\underline{q}.\underline{r}} V_f(\underline{r}) \middle| n_\uparrow \underline{R} \right\rangle \right. \\ &\left. + B_q \times -g\mu_B \sum_{\ell n \underline{R}} \left\langle \ell_\downarrow \underline{R}+\underline{q} \middle| e^{i\underline{q}.\underline{r}} V_f(\underline{r}) e^{i\underline{Q}.\underline{r}} \middle| n_\uparrow \underline{R} \right\rangle \right\} \times \\ &\times \frac{N_{n\uparrow}(\underline{R}) - N_{\ell\downarrow}(\underline{R}+\underline{q})}{E_{n\uparrow}(\underline{R}) - E_{\ell\downarrow}(\underline{R}+\underline{q}) + \hbar\omega} \times \left\langle n_\uparrow \underline{R} \middle| V_f(\underline{r}) e^{-i\underline{q}.\underline{r}} \middle| \ell_\downarrow \underline{R}+\underline{q} \right\rangle \\ &= A_q \int M_o(\underline{r}) V_f(\underline{r}) \, d\underline{r} \end{aligned} \tag{4.35}$$

and

$$\begin{aligned} &\left\{ A_q \times -g\mu_B \sum_{\ell n \underline{R}} \left\langle \ell_\downarrow \underline{R}+\underline{q} \middle| e^{i\underline{q}.\underline{r}} V_f(\underline{r}) \middle| n_\uparrow \underline{R} \right\rangle \right. \\ &\left. + B_q \times -g\mu_B \sum_{\ell n \underline{R}} \left\langle \ell_\downarrow \underline{R}+\underline{q} \middle| e^{i\underline{q}.\underline{r}} V_f(\underline{r}) e^{i\underline{Q}.\underline{r}} \middle| n_\uparrow \underline{R} \right\rangle \right\} \\ &\times \frac{N_{n\uparrow}(\underline{R}) - N_{\ell\downarrow}(\underline{R}+\underline{q})}{E_{n\uparrow}(\underline{R}) - E_{\ell\downarrow}(\underline{R}+\underline{q}) + \hbar\omega} \times \left\langle n_\uparrow \underline{R} \middle| V_f(\underline{r}) e^{-i(\underline{q}+\underline{Q}).\underline{r}} \middle| \ell_\downarrow \underline{R}+\underline{q} \right\rangle \\ &= B_q \int M_o(\underline{r}) V_f(\underline{r}) \, d\underline{r} \end{aligned} \tag{4.36}$$

From (4.35) and (4.36), by eliminating A_q and B_q, a matrix will be obtained, whose determinant put equal to zero will yield the spin wave energy and hence the spin wave velocity. The matrix's determinant is

$$\begin{vmatrix} \frac{1}{\mathcal{E}_B}\int V_f(\underline{r})M_o(\underline{r})d\underline{r}+\Lambda(\underline{q},\underline{q}) & \Lambda(\underline{q},\underline{q}+\underline{a}) \\ \Lambda(\underline{q}+\underline{a},\underline{q}) & \frac{1}{\mathcal{E}_B}\int V_f(\underline{r})M_o(\underline{r})d\underline{r}+\Lambda(\underline{q}+\underline{a},\underline{q}+\underline{a}) \end{vmatrix} = 0 \qquad (4.37)$$

where

$$\Lambda(\underline{q},\underline{q}') = \sum_{\ell n \underline{k}} \langle \ell_\downarrow \underline{k}+\underline{q}|V_f(\underline{r})e^{i\underline{q}'.\underline{r}}|n_\uparrow \underline{k}\rangle\langle n_\uparrow \underline{k}|V_f(\underline{r})e^{-i\underline{q}.\underline{r}}|\ell_\downarrow \underline{k}+\underline{q}\rangle \times \frac{N_{n\uparrow}(\underline{k}) - N_{\ell\downarrow}(\underline{k}+\underline{q})}{E_{n\uparrow}(\underline{k}) - E_{\ell\downarrow}(\underline{k}+\underline{q})+\hbar\omega} \qquad (4.38)$$

with $\Lambda^*(\underline{q},\underline{q}') = \Lambda(\underline{q}',\underline{q})$

So far the work has been carried out for a general band structure. We now specialise to the case of the Hubbard model where there are two bands in the antiferromagnetic situation. The l,n are just summed over I and 2 so that

$$\Lambda(\underline{q},\underline{q}) = \sum_{\underline{k}} |\langle 1_\downarrow \underline{k}+\underline{q}|V_f(\underline{r})e^{i\underline{q}.\underline{r}}|2_\uparrow \underline{k}\rangle|^2 \frac{N_2(\underline{k}) - N_1(\underline{k}+\underline{q})}{E_2(\underline{k}) - E_1(\underline{k})+\hbar\omega} + \sum_{\underline{k}} |\langle 2_\downarrow \underline{k}+\underline{q}|V_f(\underline{r})e^{i\underline{q}.\underline{r}}|1_\uparrow \underline{k}\rangle|^2 \frac{N_1(\underline{k}) - N_2(\underline{k}+\underline{q})}{E_1(\underline{k}) - E_2(\underline{k}+\underline{q})+\hbar\omega} \qquad (4.39)$$

and also

$$\left.\begin{aligned} V_f(\underline{r}) &= 2\mathcal{G} \\ &= -2\mathcal{G} \end{aligned}\right\} \begin{aligned} &\text{on A sublattice} \\ &\text{on B sublattice} \end{aligned} \qquad (4.40)$$

??

Because the Fermi level is assumed to be in the gap, $N_1(\underline{k})=1$, $N_2(\underline{k})=0$. Using the relation $\tan\Theta_{\underline{k}}=\frac{\mathcal{E}_2(\underline{k})}{g}$ we find

$$E_2^1(\underline{k})=\mathcal{E}_1(\underline{k})\mp g\sec\Theta_{\underline{k}}\,;\quad E_2-E_1=2g\sec\Theta_{\underline{k}} \qquad (4.4I)$$

Putting in all these simplifications,

$$\Lambda(\underline{q},\underline{q},\omega)=4g^2\sum_{\underline{k}}\cos^2\tfrac{1}{2}(\Theta_{\underline{k}+\underline{q}}-\Theta_{\underline{k}})\times$$
$$\times\left\{\frac{1}{E_1(\underline{k})-E_2(\underline{k}+\underline{q})+\hbar\omega}-\frac{1}{E_2(\underline{k})-E_1(\underline{k}+\underline{q})+\hbar\omega}\right\}$$

$$\Lambda(0,0,0)=-4g\sum_{\underline{k}}\cos\Theta_{\underline{k}}=-\frac{8g^2}{N}I,$$

using the self-consistency equation for g. Also $\frac{1}{\mathcal{E}_B}\int V_f(\underline{r})M_0(\underline{r})\,d\underline{r}=\frac{8g^2I}{N}$ which checks that there is a solution $\omega=0$, for $q=0$, as should be the case. Proceeding in the same way

$$\Lambda(\underline{q},\underline{q}+\underline{Q})=\Lambda(\underline{q}+\underline{Q},\underline{q})$$
$$=2g^2\sum_{\underline{k}}(\cos\Theta_{\underline{k}}+\cos\Theta_{\underline{k}+\underline{q}})\times\left[\frac{1}{E_1(\underline{k})-E_2(\underline{k}+\underline{q})+\hbar\omega}+\frac{1}{E_2(\underline{k})-E_1(\underline{k}+\underline{q})+\hbar\omega}\right]$$

and

$$\Lambda(\underline{q}+\underline{Q},\underline{q}+\underline{Q})$$
$$=4g^2\sum_{\underline{k}}\cos^2\tfrac{1}{2}(\Theta_{\underline{k}+\underline{q}}+\Theta_{\underline{k}})\left[\frac{1}{E_1(\underline{k})-E_2(\underline{k}+\underline{q})+\hbar\omega}-\frac{1}{E_2(\underline{k})-E_1(\underline{k}+\underline{q})+\hbar\omega}\right]$$

We note that $\hbar\omega=Cq$ and $\Lambda(q,q+Q)$ is of order q. Also, because the zeroth order term in the first diagonal element is zero, but non-zero in the other diagonal one, we retain q^2-terms in the Ist diagonal and constant terms in the second diagonal element. Although it is possible

to go into further element by element simplification of the matrix, we would refrain from that, and instead will show that Sokoloff's matrix, whose determinant solves for C , is the same as that obtained here.

If we start from equation (I9) of Sokoloff's paper[54] and write it in matrix form, it becomes

$$\begin{pmatrix} IG^{\circ}_{11}-1 & IG^{\circ}_{13} \\ IG^{\circ}_{31} & IG^{\circ}_{33}-1 \end{pmatrix}\begin{pmatrix} G_{11}(\underline{q}) & G_{13}(\underline{q}) \\ G_{31}(\underline{q}) & G_{33}(\underline{q}) \end{pmatrix}=\begin{pmatrix} G^{\circ}_{11}(\underline{q}) & G^{\circ}_{13}(\underline{q}) \\ G^{\circ}_{31}(\underline{q}) & G^{\circ}_{33}(\underline{q}) \end{pmatrix} \qquad (4.42)$$

The matrix

$$\begin{pmatrix} IG^{\circ}_{11}-1 & IG^{\circ}_{13} \\ IG^{\circ}_{31} & IG^{\circ}_{33}-1 \end{pmatrix},$$ whose determinant set equal to zero will give the expression for C is the same as our matrix which was obtained by eliminating A_q and B_q .

To show the equivalence, we worked through as follows : We wrote out the expressions for G°_{11}, G°_{33} and G°_{13} from Sokoloff's equations (2Ia),(2Ib) and (2Ic); and made the phase adjustment by replacing θ by $\frac{\pi}{2}-\theta$ in them. Also we wrote out in full the expressions for $\Lambda(q,\underline{q})$, $\Lambda(q+\underline{a},q+\underline{a})$ and $\Lambda(\underline{q},q+\underline{a})$ from our equations (4.38) as shown earlier. By comparing these two set of expressions, we found that

$$\Lambda(q,q) = -8g^2 N G^{\circ}_{33} \; ; \Lambda(\underline{q}+\underline{a},\underline{q}+\underline{a}) = -8g^2 N G^{\circ}_{11}$$

and $\overset{*}{\Lambda}(\underline{q}+\underline{a},\underline{q}) = \Lambda(\underline{q},\underline{q}+\underline{a}) = -8g^2 N G^{\circ}_{13} = -8g^2 N G^{\circ}_{31}$

whereby we get that

$$\begin{pmatrix} \frac{1}{\mathcal{E}_B}\int V_f(\underline{r}) M_0(\underline{r})\,dr + \Lambda(\underline{q},\underline{q}) & \Lambda(\underline{q},\underline{q}+\underline{a}) \\ \Lambda(\underline{q}+\underline{a},\underline{q}) & \frac{1}{\mathcal{E}_B}\int V_f(\underline{r}) M_0(\underline{r})\,dr + \Lambda(\underline{q}+\underline{a},\underline{q}+\underline{a}) \end{pmatrix}$$

$$= -8g^2\frac{N}{I}\begin{pmatrix} IG^{\circ}_{33}-1 & IG^{\circ}_{31} \\ IG^{\circ}_{13} & IG^{\circ}_{11}-1 \end{pmatrix} \qquad (4.43)$$

This shows the complete equivalence of our results with those of Sokoloff, and confirms the equivalence of our approach to RPA. Expanding for small q and ω, following Sokoloff,

$$\left.\begin{aligned} G^{\circ}_{11}(\underline{q}) &= 2(2g)^2 D \\ G^{\circ}_{33}(\underline{q}) &\approx \frac{1}{I} + 2D(\hbar^2\omega^2 - v_2^2 q^2) \\ G^{\circ}_{13}(\underline{q}) &\approx 4g\hbar\omega D \end{aligned}\right\} \qquad (4.44)$$

where
$$D = \left(\frac{1}{2g}\right)^3 \frac{1}{N}\sum_{\underline{k}} (N_{\underline{k}1} - N_{\underline{k}2})\cos^3\theta_{\underline{k}} \qquad (4.45)$$

and
$$D v_2^2 = \left(\frac{1}{2g}\right)^3 \frac{1}{N}\sum_{\underline{k}} (N_{\underline{k}1} - N_{\underline{k}2}) \times \qquad (4.46)$$
$$\times \cos^2\theta_{\underline{k}}\left[g(\underline{q}\cdot\nabla_{\underline{k}})^2 E_2(\underline{k}) - \cos\theta_{\underline{k}}\,|\underline{q}\cdot\nabla_{\underline{k}} E_2(\underline{k})|^2\right]$$

The spin wave velocity C is given by

$$C = \left[1 - 2(2g)^2 I D\right]^{1/2} v_2 \qquad (4.47)$$

The Dynamic Susceptibility in the New Formulation

Following the procedure as in the previous chapter on ferromagnetism, a general matrix form for $\chi_{+-}(\underline{q},\omega)$ is also obtained for an antiferromagnet. In this case the applied external magnetic field is

$$B_{\perp} = \frac{B_0}{2}\left\{(\hat{x}-i\hat{y})\,e^{i(\underline{q}\cdot\underline{r}-\omega t)} + (\hat{x}+i\hat{y})\,e^{-i(\underline{q}\cdot\underline{r}-\omega t)}\right\}e^{-\eta|t|} \tag{4.48}$$

and

$$\begin{aligned} M_{+}(\underline{r},t) = {} & \frac{B_0}{2}\left\{\chi_{xx}(\underline{q},\underline{q},\omega) - i\chi_{xy}(\underline{q},\underline{q},\omega) + i\chi_{yx}(\underline{q},\underline{q},\omega) \right. \\ & \left. + \chi_{yy}(\underline{q},\underline{q},\omega)\right\} e^{i(\underline{q}\cdot\underline{r}-\omega t)} e^{-\eta|t|} \\ & + \frac{B_0}{2}\left\{\chi_{xx}(\underline{q}+\underline{Q},\underline{q},\omega) - i\chi_{xy}(\underline{q}+\underline{Q},\underline{q},\omega) + i\chi_{yx}(\underline{q}+\underline{Q},\underline{q},\omega) \right. \\ & \left. + \chi_{yy}(\underline{q}+\underline{Q},\underline{q},\omega)\right\} e^{i[(\underline{q}+\underline{Q})\cdot\underline{r}-\omega t]} e^{-\eta|t|} \\ = {} & \frac{B_0}{2}\chi_{+-}(\underline{q},\underline{q},\omega)\, e^{i(\underline{q}\cdot\underline{r}-\omega t)} e^{-\eta|t|} \\ & + \frac{B_0}{2}\chi_{+-}(\underline{q}+\underline{Q},\underline{q},\omega)\, e^{i[(\underline{q}+\underline{Q})\cdot\underline{r}-\omega t]} e^{-\eta|t|} \end{aligned} \tag{4.49}$$

Also

$$B_{eff} = \frac{M_+(\underline{r},t)}{|\bar{M}_0|} \frac{V_f(\underline{r}) e^{i\underline{Q}\cdot\underline{r}}}{g\mu_B} \tag{4.50}$$

where $$|\bar{M}_0| = \frac{1}{V}\int e^{i\underline{Q}\cdot\underline{r}} M_0(\underline{r}) d\underline{r}$$

With these,

$$\begin{aligned} H_I^{eff} &= -\frac{g\mu_B}{2} \underline{B}_{eff}\cdot\underline{\sigma} \\ &= -\frac{g\mu_B}{4}\left\{B_{eff}^x \sigma_x + B_{eff}^y \sigma_y\right\} \\ &= -\frac{g\mu_B}{4}\left(B_{eff}^+ \sigma_- + h.c\right) \\ &= -\frac{g\mu_B}{4}\frac{1}{|\bar{M}_0|}\frac{V_f(\underline{r})}{g\mu_B}(M_+\sigma_- + h.c) \end{aligned} \tag{4.51}$$

h.c means the hermitian conjugate. When we include the Zeeman term, the perturbing hamiltonian becomes

$$\begin{aligned} H_I^{eff} = -\frac{g\mu_B B_0}{4}\Bigg\{ &\left[1 + \frac{\chi_{+-}(\underline{q},\underline{q},\omega)}{2|\bar{M}_0|}\frac{V_f(\underline{r})}{g\mu_B} e^{i\underline{Q}\cdot\underline{r}}\right]\sigma_- e^{i(\underline{q}\cdot\underline{r}-\omega t)} \\ &+ \left[\frac{\chi_{+-}(\underline{q}+\underline{Q},\underline{q},\omega)}{2|\bar{M}_0|}\frac{V_f(\underline{r}) e^{i\underline{Q}\cdot\underline{r}}}{g\mu_B}\right]\sigma_- e^{i[(\underline{q}+\underline{Q})\cdot\underline{r}-\omega t]} \\ &+ h.c\Bigg\} e^{-\eta|t|} \end{aligned} \tag{4.52}$$

Similar to ferromagnetic case,

$$\begin{aligned} M_+(\underline{r},t) = -\frac{(g\mu_B)^2}{2} B_0 \sum_{\ell_2 \underline{k}} \Bigg\langle \ell_\downarrow \underline{k}+\underline{q} \Bigg| &\left[1 + \chi_{+-}(\underline{q},\underline{q},\omega) e^{i\underline{Q}\cdot\underline{r}} + \chi_{+-}(\underline{q}+\underline{Q},\underline{q},\omega)\frac{V_f(\underline{r})}{g\mu_B}\right] \times \\ &\times e^{i\underline{q}\cdot\underline{r}} e^{-\eta|t|} \Big| n_\uparrow \underline{k}\Bigg\rangle \\ &\times \frac{N_{n\uparrow}(\underline{k}) - N_{\ell\downarrow}(\underline{k}+\underline{q})}{E_{n\uparrow}(\underline{k}) - E_{\ell\downarrow}(\underline{k}+\underline{q}) + \hbar\omega + i\eta} \\ &\times e^{i\omega t} \psi^*_{n\uparrow}(\underline{k},\underline{r}) \psi_{\ell\downarrow}(\underline{k}+\underline{q},\underline{r}) \end{aligned} \tag{4.53}$$

and also

$$M_+(\underline{r},t) = \frac{1}{2} B_0 \chi_{+-}(\underline{q},\underline{q},\omega) e^{i(\underline{q}\cdot\underline{r}-\omega t)} \frac{M_0(\underline{r})}{|\bar{M}_0|} e^{i\underline{Q}\cdot\underline{r}}$$
$$+ \frac{1}{2} B_0 \chi_{+-}(\underline{q}+\underline{Q},\underline{q},\omega) e^{i(\underline{q}\cdot\underline{r}-\omega t)} \frac{M_0(\underline{r})}{|\bar{M}_0|} \qquad (4.54)$$

Hence

$$\chi_{+-}(\underline{q},\underline{q},\omega) e^{i\underline{Q}\cdot\underline{r}} \frac{M_0(\underline{r})}{|\bar{M}_0|} + \chi_{+-}(\underline{q}+\underline{Q},\underline{q},\omega) \frac{M_0(\underline{r})}{|\bar{M}_0|}$$
$$= -(g\mu_B)^2 \sum_{\ell n \underline{k}} \langle \ell_\downarrow \underline{k}+\underline{q} | \left[1 + \frac{\chi_{+-}(\underline{q},\underline{q},\omega) e^{i\underline{Q}\cdot\underline{r}} + \chi_{+-}(\underline{q}+\underline{Q},\underline{q},\omega)}{g\mu_B} V_f(\underline{r}) \right]$$
$$\times e^{i\underline{q}\cdot\underline{r}} | n_\uparrow \underline{k} \rangle \times \frac{N_{n\uparrow}(\underline{k}) - N_{\ell\downarrow}(\underline{k}+\underline{q})}{E_{n\uparrow}(\underline{k}) - E_{\ell\downarrow}(\underline{k}+\underline{q}) + \hbar\omega + i\eta}$$
$$\times e^{-i\omega t} \psi^*_{n\uparrow}(\underline{k},\underline{r}) \psi_{\ell\downarrow}(\underline{k}+\underline{q},\underline{r}) \qquad (4.55)$$

Multiplying (4.55) by $V_f(\underline{r}) e^{-i\underline{Q}\cdot\underline{r}}$ and integrating we get

$$\frac{\chi_{+-}(\underline{q},\underline{q},\omega)}{|\bar{M}_0|} \left\{ \int M_0(\underline{r}) V_f(\underline{r}) d\underline{r} \right.$$
$$\left. + \frac{g\mu_B}{2} \sum_{\ell n \underline{k}} \left| \langle \ell_\downarrow \underline{k}+\underline{q} | V_f(\underline{r}) e^{i(\underline{q}+\underline{Q})\cdot\underline{r}} | n_\uparrow \underline{k} \rangle \right|^2 \times \frac{N_{n\uparrow}(\underline{k}) - N_{\ell\downarrow}(\underline{k}+\underline{q})}{E_{n\uparrow}(\underline{k}) - E_{\ell\downarrow}(\underline{k}+\underline{q}) + \hbar\omega + i\eta} \right\}$$

$$+ \frac{\chi_{+-}(\underline{q}+\underline{Q},\underline{q},\omega)}{|\bar{M}_0|} \frac{g\mu_B}{2} \sum_{\ell n \underline{k}} \langle \ell_\downarrow \underline{k}+\underline{q} | V_f(\underline{r}) e^{i\underline{q}\cdot\underline{r}} | n_\uparrow \underline{k} \rangle \langle n_\uparrow \underline{k} | V_f(\underline{r}) e^{-i(\underline{q}+\underline{Q})\cdot\underline{r}} | \ell_\downarrow \underline{k}+\underline{q} \rangle$$
$$\times \frac{N_{n\uparrow}(\underline{k}) - N_{\ell\downarrow}(\underline{k}+\underline{q})}{E_{n\uparrow}(\underline{k}) - E_{\ell\downarrow}(\underline{k}+\underline{q}) + \hbar\omega + i\eta}$$

$$= -(g\mu_B)^2 \sum_{\ell n \underline{k}} \langle \ell_\downarrow \underline{k}+\underline{q} | e^{i\underline{q}\cdot\underline{r}} | n_\uparrow \underline{k} \rangle \langle n_\uparrow \underline{k} | V_f(\underline{r}) e^{-i(\underline{q}+\underline{Q})\cdot\underline{r}} | \ell_\downarrow \underline{k}+\underline{q} \rangle$$

$$= \frac{I(\underline{q},\underline{q}+\underline{Q})}{|\bar{M}_0|} \quad , \text{ let us say.} \qquad (4.56)$$

And again multiplying by $V_f(\underline{r})$ and integrating we get

$$\frac{\chi_{+-}(\underline{q},\underline{q},\omega)}{|\bar{M}_0|}\frac{g\mathcal{E}_B}{2}\sum_{\ell n\underline{k}}\langle \ell_\downarrow \underline{k}+\underline{q}|V_f(\underline{r})e^{i(\underline{q}+\underline{Q})\cdot\underline{r}}|n_\uparrow\underline{k}\rangle\langle n_\uparrow\underline{k}|V_f(\underline{r})e^{-i\underline{q}\cdot\underline{r}}|\ell_\downarrow\underline{k}+\underline{q}\rangle \times \frac{N_{n\uparrow}(\underline{k})-N_{\ell\downarrow}(\underline{k}+\underline{q})}{E_{n\uparrow}(\underline{k})-E_{\ell\downarrow}(\underline{k}+\underline{q})+\hbar\omega+i\eta}$$

$$+\frac{\chi_{+-}(\underline{q}+\underline{Q},\underline{q},\omega)}{|\bar{M}_0|}\left\{\int M_0(\underline{r})V_f(\underline{r})\,d\underline{r}+\frac{g\mathcal{E}_B}{2}\sum_{\ell n\underline{k}}|\langle \ell_\downarrow\underline{k}+\underline{q}|V_f(\underline{r})e^{i\underline{q}\cdot\underline{r}}|n_\uparrow\underline{k}\rangle|^2 \times \frac{N_{n\uparrow}(\underline{k})-N_{\ell\downarrow}(\underline{k}+\underline{q})}{E_{n\uparrow}(\underline{k})-E_{\ell\downarrow}(\underline{k}+\underline{q})+\hbar\omega+i\eta}\right\}$$

$$=-\left(\frac{g\mathcal{E}_B}{2}\right)\sum_{\ell n\underline{k}}\langle \ell_\downarrow\underline{k}+\underline{q}|V_f(\underline{r})e^{i(\underline{q}+\underline{Q})\cdot\underline{r}}|n_\uparrow\underline{k}\rangle\langle n_\uparrow\underline{k}|V_f(\underline{r})e^{-i\underline{q}\cdot\underline{r}}|\ell_\downarrow\underline{k}+\underline{q}\rangle \times \frac{N_{n\uparrow}(\underline{k})-N_{\ell\downarrow}(\underline{k}+\underline{q})}{E_{n\uparrow}(\underline{k})-E_{\ell\downarrow}(\underline{k}+\underline{q})+\hbar\omega+i\eta}$$

$$=\frac{I(\underline{q},\underline{q})}{|\bar{M}_0|}\quad\text{, let us say.}\qquad(4.57)$$

Using our previous notations, (4.56) and (4.57) can be written as

$$\left\{M_0(\underline{r})V_f(\underline{r})\,d\underline{r}+\frac{g\mathcal{E}_B}{2}\Lambda(\underline{q}+\underline{Q},\underline{q}+\underline{Q})\right\}\chi_{+-}(\underline{q},\underline{q},\omega)+\frac{g\mathcal{E}_B}{2}\Lambda(\underline{q},\underline{q}+\underline{Q})\chi_{+-}(\underline{q}+\underline{Q},\underline{q},\omega)=I(\underline{q},\underline{q}+\underline{Q})$$

$$\frac{g\mathcal{E}_B}{2}\Lambda(\underline{q}+\underline{Q},\underline{q})\chi_{+-}(\underline{q},\underline{q})+\left\{\int M_0(\underline{r})V_f(\underline{r})\,d\underline{r}+\frac{g\mathcal{E}_B}{2}\Lambda(\underline{q},\underline{q})\right\}\chi_{+-}(\underline{q}+\underline{Q},\underline{q},\omega)=I(\underline{q},\underline{q})\qquad(4.58)$$

In the matrix form the pair of equations (4.58) can be written as

$$\begin{pmatrix} \lambda + \Lambda(\underline{q}+\underline{G},\underline{q}+\underline{G}) & \Lambda(\underline{q},\underline{q}+\underline{G}) \\ \Lambda(\underline{q}+\underline{G},\underline{q}) & \lambda + \Lambda(\underline{q},\underline{q}) \end{pmatrix} \begin{pmatrix} \chi_{+-}(\underline{q},\underline{q},\omega) \\ \chi_{+-}(\underline{q}+\underline{G},\underline{q},\omega) \end{pmatrix} = \frac{2}{g\mu_B} \begin{pmatrix} I(\underline{q},\underline{q}+\underline{G}) \\ I(\underline{q},\underline{q}) \end{pmatrix}$$

$$\lambda = \frac{2}{g\mu_B} \int M_0(\underline{r}) V_f(\underline{r})\, d\underline{r} \qquad (4.59)$$

If we start with an external field $\underline{B}_\perp \alpha\, e^{i(\underline{q}+\underline{G})\cdot\underline{r}}$ we will arrive at a similar equation

$$\begin{pmatrix} \lambda + \Lambda(\underline{q}+\underline{G},\underline{q}+\underline{G}) & \Lambda(\underline{q},\underline{q}+\underline{G}) \\ \Lambda(\underline{q}+\underline{G},\underline{q}) & \lambda + \Lambda(\underline{q},\underline{q}) \end{pmatrix} \begin{pmatrix} \chi_{+-}(\underline{q},\underline{q}+\underline{G},\omega) \\ \chi_{+-}(\underline{q}+\underline{G},\underline{q}+\underline{G},\omega) \end{pmatrix} = \frac{2}{g\mu_B} \begin{pmatrix} I(\underline{q}+\underline{G},\underline{q}+\underline{G}) \\ I(\underline{q}+\underline{G},\underline{q}) \end{pmatrix} \qquad (4.60)$$

Combining (4.59) and (4.60) we get the general equation for the χ_{+-} matrix for an antiferromagnet

$$\begin{pmatrix} \lambda + \Lambda(\underline{q}+\underline{G},\underline{q}+\underline{G}) & \Lambda(\underline{q},\underline{q}+\underline{G}) \\ \Lambda(\underline{q}+\underline{G},\underline{q}) & \lambda + \Lambda(\underline{q},\underline{q}) \end{pmatrix} \begin{pmatrix} \chi_{+-}(\underline{q},\underline{q},\omega) & \chi_{+-}(\underline{q},\underline{q}+\underline{G},\omega) \\ \chi_{+-}(\underline{q}+\underline{G},\underline{q},\omega) & \chi_{+-}(\underline{q}+\underline{G},\underline{q}+\underline{G},\omega) \end{pmatrix}$$

$$= \frac{2}{g\mu_B} \begin{pmatrix} I(\underline{q},\underline{q}+\underline{G}) & I(\underline{q}+\underline{G},\underline{q}+\underline{G}) \\ I(\underline{q},\underline{q}) & I(\underline{q}+\underline{G},\underline{q}) \end{pmatrix} \qquad (4.6I)$$

The solution of the matrix equation (4.6I) will give the transverse susceptibility χ_{+-} for an antiferromagnet when local field corrections are neglected.

This result, when combined with a band calculation, could be used as the basis for a numerical calculation of $\chi_{+-}(\underline{q},\omega)$ for a real antiferromagnetic metal such as Mn. It would be of considerable interest to compare such a calculation, which would not involve any adjustable parameters, with the calculations of Young and Cade[56] using a many-band Hubbard hamiltonian approach.

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