A thesis entitled,

" MANY - BODY PROBLEMS "

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ABSTRACT.

This thesis includes the generalization to all spin magnitudes of two fermion representations which were previously known only for the spin - half case. The resulting "2S" fermion representation is found to be useful for converting electronic exchange Hamiltonians into Hamiltonians which involve only spin operators. This is used to exhibit the general correspondence between the Anderson and Kondo model Hamiltonians. The generalized drone - fermion representation is used to establish two new Wick's theorems for spin half andspin one operators. These results are both simple and easy to use. They extend the use of standard diagrammatic Quantum Field Theory techniques to those proble-ms involving such spin operators.

The properties of a metal which contains a single localized paramagnetic impurity (the Kondo model) are then investigated with these new methods. The results include a derivation of a log T term in the impurity g - shift, close agreement with previous low - order perturbation treatments, and a high - order equation for the resistivity, which is obtained by a selective resummation of a complete sub - series of self - energy diagrams. The resistivity derived using this approximation, is shown to exhibit a resonance - like behaviour (rather than a divergence) for both ferro - and anti - ferromagnetic coupling (although at different temperatures) in passing from the high to

low temperature regions, through the Nagaoka - Suhl instability temperature T_k.

At higher concentrations , the disappearance of the first - order Yosida g - shift is shown in a microscopic theory. The narrowing of the local - moment resonance line, which has recently been measured for such dilute paramagnetic alloys, is similarly demonstrated.

An examination of the rare - earth ferromagnetic model results in equations which explicitly demonstrate the coupled spin - wave behaviour of both local - moments, and of the conduction electrons. This is a more general result than previously demonstrated.

Finally these methods are applied in an extensive investigation of the Heisenberg model in high and low temperature domains, where the expansion criteria of Stinchcombe et al are closely followed. Renormalization is now quite simple and straight-forward. At low temperatures, Dyson's T^4 contribution to the free energy is obtained in the first Born approximation to spin wave scattering. Higher order spin -wave contributions give a damping term, which , upon evaluation in the lowest approximation, is identical to that found by ter Haar and Tahir-Kheli.

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* - The work covered in these sections has been submitted for publication.

** - Some of the results in these sections have been published, with Dr. S. Doniach, in "Physical Review Letters", 18 , 994 (1967).

Chapter 1.

INTRODUCTION.

The principal perturbation techniques of Quantum Field Theory were originally devised by Feynman, Dyson and others 1.) to investigate the central problems of quantum electrodynamics. In essence these are zero temperature formulations. It was not until Matsubara 2.) extended them to finite temperatures, that they could be used to solve any of the problems in Solid - State Physics. Since that date, many problems in so - called many - body theory, have been dealt with, successfully, using these powerful techniques. Unfortunately, these methods could only be used to analyse systems containing bose or fermion particles (see Appendix A for a brief summary) and one class of problems has stubbornly refused to be accomodated. This is that group of many - body systems described by a Hamiltonian, which contains explicit spin operators whose commutators are no longer c- numbers. Even the addition of only one localized spin, as in the "Kondo" problem (see later), can prevent these new techniques from being successfully employed. The crux of these difficulties is the absence of a simple analogue of Wick's theorem. 3.) This is the important step which reduces multiple products of operators, in a thermal average over the free eigenstates of the Hamiltonian, to products of pairs of operators. The simplest example of this result is presented in Appendix B for the usual case of fermion or bose operators. The present thesis is an attempt to solve this problem when spin operators are present. Simple methods for spins of one -half and one (in units of ħ) will be established here and will then be applied to several model Hamiltonians. Since 1960 many earlier attempts at this problem have been made, and it continues to attract fresh solutions. Davis 4.) used Schwinger's coupled - boson representation 5.) of the spin - operators, (valid for all spin magnitudes, S) to derive a useful Linked - Cluster theorem, although this was not given a diagrammatic representation. This theorem usually follows from Wick's theorem and eliminates much of the resulting calculation. As Davis' method involved bosons, great care had to be taken so that only the finite number of spin states in the boson - space of infinite states were considered. Indeed, this is the major problem in almost all representational attempts at a spin - Wick theorem. A bose method usually has the advantage of a simple representation of the spin operators , in contrast to a fermion representation, but a fermion space has only a finite set of states, although these are not always all spin states.

Mills et al, 6.) in their treatment of the spin half anti - ferromagnet,introduced operators which had fermion properties on the same site, but behaved like bosons with respect to different sites. This involved the use of diagrams with additional , partially overlapping lines, and therefore produced rather unconvential structures. In fact, Wang et al 7.) have re - derived these results (using the coupled - fermion representation) 8.) in establishing a Wick -

like theorem at zero temperature; this resulted in retarded propagators with special "locked" diagrams.

In 1965 Yolin[9.] established a finite temperature spin-Wick theorem for $S = \frac{1}{2}$, again using the coupled - fermion representation to investigate the spin - phonon interactions in paramagnets - this method is reviewed in section (3.5) where the complications of a normalization co-efficient are discussed. Abrikosov[10.] generalized this method to spins greater than one half, by introducing the 2S + 1 coupled - fermion representation. This is also reviewed in section (3.5), where his method of handling the difficulty of the extra states is summarized. Doniach[11.] has introduced a new Wick theorem for general spin operators at zero temperature, again concentrating on a single spin. This was a generalization of the usual (zero temperature) Wick approach involving normal - ordering, and resulted in special multi - linked diagrams corresponding to commutators of more than one pair of operators. However, important techniques, like the Linked - Cluster theorem are not readily available. A form of Wick's theorem for spin operators has also been introduced in the work of Giovannini et al.[12.] This involves "remembering" all the previous commutations which have been carried out, and appears to be a finite temperature method, related to the zero temperature theory of Doniach.
Although a Linked - Cluster theorem was established, their diagrams lack the elegance of the Feynman graphical technique.
Very recently, Lewis and Stinchcombe[13.] have generalized the work of Wang et al to finite temperatures for the case of

$S = \frac{1}{2}$, treating the Pauli matrices directly. Again this resulted in a somewhat unconventional diagrammatic formulation. As final evidence for the continuing interest in this subject a recent letter by Jäger and Kühnel[14.)] indicated a low-order perturbation method, using an analogous method to that of Tyablikov and Moskalenkow.[15.)] Mention should also be made here of the very early work of Holstein and Primakoff[16.)] who introduced a square-root boson correspondence with the spin operators. This is used in the large S limit in section (3.4).

The present work uses the drone-fermion representation, which is generalized here to all spin values from the previously known case of spin-half.[17.)] An analysis of the resulting eigenstates then shows that very simple Wick's theorems can be established for spin half and spin one. The advantage of these methods (especially $S = \frac{1}{2}$) is that <u>ALL</u> the standard techniques of Quantum Field Theory[18.)] for handling fermion operators at finite temperature, can be used, including the use of conventional diagrammatic display.

These new methods are then used to investigate two general types of Hamiltonian, namely localized-moments interacting with the conduction electrons in Chapter 5, and the Heisenberg model in Chapter 6.

The interesting problem of how the local moment appears will not be pursued here, except to mention some of the investigations stemming from the two seminal models of Anderson[19.)] and of Clogston[20.)] and Wolff.[21.)] In brief,[22.)]

the Anderson model assumes the impurity to be represented by an extra well - localized orbital, (preferably of different symmetry to the conduction band) on which electronic interactions only occur when it is doubly occupied. This model also contains a mixing term which exchanges s and d - electrons; this has the effect of broadening the local level and allowing the d - electrons to escape (a virtual level).

In the Wolff model, the impurity is assumed to affect only the lattice potential. This then scatters the conduction electrons, which are also in the Hartree potential of all the other electrons. These are combined to form a single self - consistent potential. Finally a Fock potential is taken between electrons with parallel pairs of spins, but now with a different value between the two spin sub - bands.

Kim[23.] extended this model beyond the Hartree - Fock approximation originally used by Anderson to a higher order in the decoupling - hierarchy, and he found that the non - magnetic localized state became unstable below a certain temperature with consequent resistivity anomalies. Earlier, Moriya[24.] had investigated the spin polarization in dilute magnetic alloys of iron in palledium, but only in the Hartree - Fock approximation. Scalapino[25.] applied simple perturbation theory, and found a logarithmic temperature dependence in the Curie law for the static susceptibility of the Anderson model, while Kjöllerström et al[26.] have also investigated the ground - state energy and specific heat of this model in the ladder - approximation. Schrieffer and Wolff[27.] replaced the mixing term in Anderson's model by an equivalent Hamiltonian term, which scatters a conduction electron, and possibly changes the quantum number of the electron on the impurity, but now no longer mixes the two types of electrons. This is generalized in section (3.3) for the case of several impurities, each of which has more than one degenerate d -orbital. This uses the 2S fermion representation which has been generalized here. In a later paper, Schrieffer[28] showed that, for an S - state ion like Mn, only the l = 2 conduction electrons, constructed from spherical harmonics about the impurity, are scattered - not the l = 0 electrons. This is used to explain the variation of resistivities of Al based 3-d alloys across the 3-d series.[29.]

The s - d exchange Hamiltonian has been derived by several authors, namely Kasuya,[30.] Mitchell,[31.] and Liu,[32.] among others. However, Zener[33.] originally proposed , on phenomenological grounds, a longitudinal s - d type interaction, in 1951, although Kasuya's treatment of the s - f model (for rare - earths) in 1956 is usually considered the first rigorous analysis for the exchange interaction between 6s conduction electrons and the 4f electrons.

Korringa[34.], as early as 1950, applied the point - contact model to the problem of nuclear magnetic relaxation, and the shift of the resonance line in metals. Straightforward perturbation theory leads to second order results which are recovered by the present Green's function methods.

The advantage of any Green's function method is that, not only is their use more systematic, but the complete line shape is usually found, with the relaxation time given as a special case on the energy shell. Yosida[35.)] found the first order polarization of the electron band, when an s - d model is assumed for Cu - Mn alloys, and showed that this is concentrated around the magnetic Mn ions (so only small hyperfine shifts result for the Cu nuclei[36.)]). The equivalent R.K.Y. interaction[37.)] was also found for this system. These alloys continued to interest theorists[38.)] but it was not until Kondo[39.)] evaluated the conduction electron scattering cross - section, by standard perturbation theory, to second Born approximation, that the phenomenon of the resistance minimum was given a satisfactory theoretical explanation. It was found that the sharpness of the Fermi surface led to a log. T term for anti - ferro - magnetic coupling. This was fitted to the results for Fe in Cu alloys by assuming a T^5 dependence of the non - spin resistivity. The interaction parameter J was also found to be approximately 2% of the Fermi energy of the conduction electrons for this alloy. A further series of papers lead to the conclusion that a divergence at low temperatures was introduced by these higher order terms. Liu[40.)] also found this log T term in third order, when he evaluated the Green's functions directly - without the aid of a Wick theorem, (as did Doniach with his Wick - type theorem) Nagaoka[41.)], by a decoupling procedure, pointed out that even in third order, the life - times of the conduction electrons would also go negative at the Fermi surface, below a critical temperature T_k, while Suhl[42.)] also found complex poles in his earlier papers. In Chapter 5 it is found that these life - times remain positive if the self - energies are suitably defined by an effective potential, following Doniach[11.)]. A diagrammatic resummation of higher order propagators results in a closed - form expression for the effective potential, which does diverge at Tk for anti - ferromagnetic coupling; but as the denominator is now evaluated to $O(J^2)$ (in contrast to Abrikosov's results, which were to O(J)) it also introduces a new divergence at a much lower temperature for ferromagnetic coupling. However, the one electron damping term does not diverge, but passes through a broad resonance at Tk, of width about 3Tk, and finally vanishes at absulute zero like $\log^{-2} T$, which agrees with a very recent decoupling procedure of Fischer[43.)].

Takano and Ogawa[44.)] have also found this second ferromagnetic resonance peak, by using Gor'kov's[45.)] decoupling method, in contrast to that of Zubarev[46.)], used by Nagaoka[41.)]. Unfortunately, they used the coupled - fermion representation for spin - half operators, and did not account for the two anomalous states, which occur in this representation (see section (3.5). Moreover, their temperature parameters differ from all other theories, as is shown in Chapter 7, and their results indicate a sharp phase - transition to a possible low - temperature "bound - state" at Tk. These two - types of singular points have also been found by

Kurata[47], who used a simple solvable model of just one electron above the Fermi surface at zero temperature, scattering off the single impurity. Yosida[48] has also analyzed this new "bound - state" at 0°k by imposing Cooper - like restrictions on the electrons, and adopting possible trial wave - functions. This is not found however by Ishikawa and Mizuno[49] who used Wigner - Brillouin perturbation theory. The magnetic properties of this model have not been studied so thoroughly[50-1] although Yosida and Okiji[52] suggest that a similar log T divergence appears, on the basis of their fourth order calculations. The present static result for the magnetization is compared with their result, and with those of Nagaoka[41]. This result is shown here to arise from a $J^2 \log T$ correction to the impurity g - shift. All of these magnetic properties can be derived directly from the transverse susceptibility function (introduced in Chapter 2), which, in this model, is found to have a Lorentzian form with a Korringa - like damping term proportional to J^2T. This part is concluded with a new manipulation of Nagaoka's second approximation to his high temperature result, into a form which is quite similar to the present treatment.

The recent measurements of Gossard et al.[53] of a "bottle - neck" effect in the local - moment relaxation process of s - d type alloys, (resulting in a narrowing of the measured line - width) are here given a microscopical explanation, as opposed to the phenomenological Bloch equations, originally proposed by Hasegawa.[54] The gyromagnetic anomalies occuring in ferromagnetic metals, discussed by Kittel and Mitchell[31.) 55.)] are now given an explicit microscopic formulation, based on an expression originally proposed by Giovannini et al[12.)] The ferromagnetic rare - earth model[56.-8)] is investigated in the last section of this Chapter, and the coupling of the two spin wave systems of the localized and conduction spins is exhibited. This is a more general proof than originally given by Doniach and Wohlfarth[59.)], where only the long - wavelength limitis strictly valid (section (5.5)) due to the averaging procedure adopted for alloys.

The equivalence of the electronic exchange term in insulators with the Heisenberg model of a ferromagnet, is demonstrated for general spin , in Chapter 6; again using the 2S fermion representation. Linear spin - wave theory, founded by Bloch[60.)], is not discussed here, as extensive reviews are well - known[5.)61.-2)], however the basic equations of this theory are rapidly recovered by use of the present formalism, in Chapter 6. Dyson[63.)] first gave a rigorous theory of the low temperature behaviour of this model, when, (inter alia) he showed that long wave - length spin-waves interact very weakly at low temperatures. The introduction of a restrictive cut - off condition for his equivalent Hamiltonian in the bose space, leads to a gap of order J (the interaction strength) in the eigenvalue spectrum. This meant that the anomalous (or improper) states gave a contribution $e^{-\beta J}$ to the free energy, and this vanishes at low temperature. This new form of the Hamiltonian <u>cannot</u>[61.)] be obtained directly from the simple

Maleev substitution of the spin operators, (as is often supposed,) for the cut - off property is not included[64.)]. This cut - off property can be included , (and hence, the so - called kinematic terms) by the introduction of a metric operator F in the bose - space. Mills and Kenan[65.)] have shown that Dyson's boson Hamiltonian is the correct generator for time displacements in the boson space, and has real eigenvalues. The new metric operator indicates that the non-Hermiticity of this Hamiltonian is irrelevant, and in fact, if calculations were carried out with F explicitly, no problems would arise. Unfortunately, any known form of F[66.)] is too complicated.

Later theories, which relied on Dyson's treatment,[67-8.)] to justify their own low temperature results, included Oguchi,[69.)] M.Bloch,[70.)] Szaniecki among others. Tahir - Kheli and ter Haar[71.)] analysed this model in a Green's function formalism, by the decoupling procedure of Bogolyubov and Tyablikov.[72.)] In a second paper, starting with Dyson's boson Hamiltonian, they found the spin - wave renormalization obtained by Brout and Englert[73.)] . A further decoupling resulted in a damping coefficient in the spin - wave energies. These results are recovered here, exhibiting their approximations. Further decoupling methods were introduced in the papers of Haas and Jarrett[74.)] and Callen[75.)] (who found a spurious T^3 error for $S = \frac{1}{2}$, but not for higher S), and of Morita and Tanaka[76.)] who successfully obtained the famous Dyson T^4 contribution to the magnetization at low temperatures.

This is also obtained in Chapter 6.

These low - temperature theories have been supplemented in the Curie temperature (Tc) region by the cluster method of Strieb et al 77.) and by the work of Rushbrooke 78.) and co - workers, who attempt to find Tc by evaluating the partition function directly at high temperatures.

Finally the work of Englert 79.), Brout 80), Stinchcombe et 81.) al, Lewis and Stinchcombe 13.), presented theories which are applicable in both the high and low temperature domains. The present fermion Green's function theory fits into this category. In fact, it bears a very close similarity to the quantum - mechanical semi - invariants, introduced by Stinchcombe et al 81.) and effectively gives dynamical sub-structure, to their semi - invariant averages. However, due to the Feynman diagram nature of this present work, renormalization of the propagators and vertices is greatly siplified, compared with their analysis - although, in general, their treatment is closely followed.

In order to introduce the concept of spin propagators (or Green's functions) the next Chapter begins with the Kubo response formalism 82.) for paramagnetic spins. This leads naturally to the idea of temperature - ordered, temperature dependent Green's functions, which then become the focus of interest in subsequent Chapters of this thesis.

Chapter 2.

SPIN GREEN'S FUNCTIONS

(2.1) Introduction.

In this chapter the Kubo response formalism 82) is presented for the case of thermal averages reacting to a small adiabatic perturbation. In this work the particular example of paramagnetic resonance 83) is chosen to introduce both the properties of spin operators and retarded propagators for spin operators. These are the general functions which describe the dynamical behaviour of any spin system 84) and are the natural extension of the usual static susceptibilities of paramagnetic theory. A more detailed discussion of the properties of these Green's functions (in a general form) is given in Appendix C. The simple example of free spins is chosen to illustrate analytic behaviour of these functions in an explicit form. Finally the concept of electronic spin density is introduced in a second quantized formulation, and its properties investigated. It is also shown that the Kondo-type interaction term leaves the dynamics of the total spin unaffected.

(2.2) The Kubo Response Formula.

The dynamics of a complex system can be analysed in terms of the response of such a system to a small, adiabatic, external perturbation. The Kubo formalism determines the linear change in the system in response to an (non-quantized) external driving force. The fully interacting system can be described by the Hamiltonian H, then at $t = 0$ the additional perturbation $H_{ext.}$ is applied - the total Hamiltonian is then $H' = H + H_{ext.}$ The time - dependent eigenstates of H' are denoted by $\Psi'(t)$ and satisfy the following Schrödinger equation

$$i \frac{\partial}{\partial t} |\Psi'(t)> = H' |\Psi'(t)> \tag{2.1}$$

These states are related to the states in the Heisenberg picture $\Phi'(t)$ by the unitary transformation,

$$|\Psi'(t)> = e^{-iHt} |\Phi'(t)> \tag{2.2}$$

and the operators in the Heisenberg picture are described by

$$A(t) = e^{iHt} A e^{-iHt} \tag{2.3}$$

The Schrödinger equation of the transformed states is

$$i \frac{\partial}{\partial t} |\Phi'(t)> = H_{ext.}(t) |\Phi'(t)> \tag{2.4}$$

This equation cannot be solved in general, so the usual perturbation approach of expanding in powers of the perturbation is adopted, that is

$$|\Phi'(t)> = |\Phi(t)> + \sum_{j=1}^{\infty} |\Phi^{(j)}(t)> \tag{2.5}$$

If this is substituted in (2.4) and powers of $H_{ext.}$ equated, then a series of equations results, the lowest order equation involving no powers of $H_{ext.}$ is,

$$i \frac{\partial}{\partial t} |\Phi(t)> \;=\; 0 \quad \text{so} \quad |\Phi(t)> = |\Phi> \qquad (2.6)$$

where Φ is a time - independent eigenstate of H in the Heisenberg picture. The next equation is the one linear in $H_{ext.}$

$$i \frac{\partial}{\partial t} |\Phi^{(1)}(t)> \;=\; H_{ext.}(t)|\Phi> \qquad (2.7)$$

This can be converted to an integral form, remembering that the perturbation only begins at t = 0, so

$$|\Phi^{(1)}(t)> = -i \int_0^t dt' \; H_{ext.}(t')|\Phi> \qquad (2.8)$$

So, to first order, the states Φ' are given by,

$$|\Phi'(t)> \;=\; (1 - i\int_0^t dt' \, H_{ext.}(t')|\Phi> \qquad (2.9)$$

This is true for all states Φ_α which have eigenvalues E_α, that is,

$$H|\Phi_\alpha> \;=\; E_\alpha|\Phi_\alpha> \qquad (2.10)$$

A statistical average, as in (A.5), over the new orthonormal eigenstates $\Psi'_\alpha(t)$ for any operator A, is weighted by the original Boltzmann factor $e^{-\beta E_\alpha}$ as an adiabatic perturbation does not change the population distribution of the original states. The exact averages are defined by,

$$<A(t)>_{ext.} \;=\; \frac{\sum_\alpha e^{-\beta E_\alpha} <\Psi'_\alpha(t)|A|\Psi'_\alpha(t)>}{\sum_\alpha e^{-\beta E_\alpha}} \qquad (2.11)$$

These averages will be related to those inthe Heisenberg picture of the fully interacting system (without the external perturbation); in this case, defined by,

$$\langle A\ (t) \rangle = \frac{\sum_{\alpha} e^{-\beta E_{\alpha}} \langle \Phi_{\alpha} \,|\, A(t) \,|\, \Phi_{\alpha} \rangle}{\sum_{\alpha} e^{-\beta E_{\alpha}}} \tag{2.12}$$

So, using Eq.s (2.2) and (2.9). one has, to first order in the perturbation,

$$\langle \Delta A(t) \rangle_{\text{ext.}} = i \int_{0}^{t} dt' \langle [H_{\text{ext.}}(t'), A(t)] \rangle \tag{2.13}$$

where the change in the average must be used if $\langle A(t) \rangle \neq 0$, that is,

$$\langle \Delta A(t) \rangle_{\text{ext.}} = \langle A(t) \rangle_{\text{ext.}} - \langle A(t) \rangle \tag{2.14}$$

Equation (2.13) is the general form for the linear change in any system produced by any external, adiabatic perturbation.

(2.3) Spin Susceptibility Functions.

In the case of paramagnetic resonance experiments on magnetic systems the perturbation is a small radio - frequency (r.f.) magnetic field $\underline{h}_{\text{rf}}$ of constant magnitude h_1 , which rotates with frequency ω around a large static magnetic field h^z , defining the z - axis.

$$\underline{h}_{\text{r.f.}} = \underline{i}\, h_1 \cos \omega t + \underline{j}\, h_1 \sin \omega t \tag{2.15}$$

If this field is coupled to a well - localized spin vector, described by the operator $\underline{S}$, then the perturbation is

$$H_{ext.} = \underline{S} \cdot \underline{h}_{r.f.} \tag{2.16}$$

In all future work (exept when stated explicitly) the gyromagnetic ratio γ will be defined to be unity, moreover the r.f. field is <u>not</u> quantized and so can be taken outside any trace.

The components of the spin operators (at any one site) denoted S^i (i = x,yzor 1,2,3) obey the commutation rules 85)

$$[S^i, S^j] = i\sum_k \varepsilon_{ijk} S^k \tag{2.17}$$

where ε_{ijk} is the usual third - order anti - symmetric tensor which is zero if two indices are equal, 1 if it is an even permutation of 123, and -1 if it is an odd permutation of 123.

A more useful form of Eq. (2.17) occurs in terms of the " raising or lowering" spin operators S^+ and S^- , defined by

$$S^\pm = S^x \pm i S^y \tag{2.18}$$

In this case, direct substitution leads to

$$[S^z, S^\pm] = \pm S^\pm ; [S^+, S^-] = 2S^z \tag{2.19}$$

If Eq. (2.16) is used in Eq. (2.13) for the components S^i then,

$$< \Delta S^i (t) >_{ext.} = -i \sum_j \int_0^t dt' < [S^i(t), S^j(t')]> h^j_{r.f.} (t') \tag{2.20}$$

Remembering that $h_{r.f.}(t')$ vanishes for $t' < 0$, this integral can be extended to minus infinity and to plus infinity by the introduction of an explicit Θ-function (see A.16).

This also enables the generalized (retarded) susceptibility function $\chi_{ret.}$ to be introduced, with a sign convention chosen as for C.2, thus

$$\langle \Delta S^{i}(t)\rangle_{ext.} = -\sum_{j} \int_{-\infty}^{\infty} dt' \; \chi^{ij}_{ret.}(t-t')\, h^{j}_{r.f.}(t'). \qquad (2.21)$$

So, the retarded susceptibility tensor is defined by

$$\chi^{ij}_{ret.}(t-t') = i\,\Theta(t-t')\langle [S^{i}(t),S^{j}(t')] \rangle \qquad (2.22)$$

The Fourier transforms of these expressions may readily be written down, if the notation of (C.6) is used. Thus, Eq. (2.21) transforms to the following, if the δ-function, identity (C.17) is used;

$$\langle \Delta S^{i}(\omega) \rangle_{ext.} = -\sum_{j} \chi^{ij}_{ret.}(\omega)\, h^{j}_{r.f.}(\omega) \qquad (2.23)$$

Following Appendix C, the retarded susceptibility leads to its generalization in the temperature dependent susceptibility (or spin - operator Green's functions) defined by

$$\chi^{ij}(\tau-\tau') = \langle P(S^{i}(\tau), S^{j}(\tau')) \rangle \qquad (2.24)$$

where the spin - operators are written in the thermal Heisenberg picture,

$$S^{i}(\tau) = e^{H\tau} S^{i} e^{-H\tau} \qquad (2.25)$$

As in (C.7) this can be even - Fourier transformed (for the spins obey commutation rules)

$$\chi^{ij}(\tau) = \beta^{-1} \sum_{\alpha} e^{-i\bar{\alpha}\tau} \chi^{ij}(\bar{\alpha}) \qquad (2.26)$$

In terms of its analytically continued form $i\bar{\alpha} = \omega + is$ one has, (c.10)

$$\chi^{ij}(\omega + is) = \chi^{ij}_{ret.}(\omega) \qquad (2.27)$$

Instead of the Cartesian components of χ^{ij}, the transverse propagator will be used as it has several simpler features, it is defined by,

$$\chi^{T}_{ret.}(t - t') = i\,\Theta(t - t') < [S^{-}(t), S^{+}(t')] > (2.28)$$

The x - y components of the susceptibility can be found in terms of χ^{T} and its conjugate χ^{T*}, thus,

$$\chi^{xx}_{ret.}(t) = \chi^{yy}_{ret.}(t) = \tfrac{1}{4}(\chi^{T}_{ret.}(t) + \chi^{T*}_{ret.}(t)) \qquad (2.29)$$

similarly for the off - diagonal components

$$\chi^{xy}_{ret.}(t) = \chi^{yx}_{ret.}(t) = \tfrac{1}{4}i(\chi^{T}_{ret.}(t) - \chi^{T*}_{ret.}(t)) \qquad (2.30)$$

The Fourier transforms are similarly defined if one notes that the transform of $\chi^{T*}_{ret.}(t)$ is $-\chi^{T}_{ret.}(-\omega - is)$.

The transverse temperature dependent susceptibility will be used in all future discussions, and so a simplified notation for it is used; it is defined by

$$F(\tau - \tau') = < P(S^{-}(\tau), S^{+}(\tau')) > \qquad (2.31)$$

Its Fourier transform is defined as in Eq. (2.26), so

$$F(\tau) = \beta^{-1} \sum_{\alpha} e^{-i\bar{\alpha}\tau} F(\bar{\alpha}) \qquad (2.32)$$

So, finally in terms of its analytically continued form

$$4\chi^{xx}_{ret.}(\omega) = F(\omega + is) - F(-\omega - is) \qquad (2.33)$$

and $$4i\,\chi^{xy}_{ret.}(\omega) = F(\omega + is) + F(-\omega - is) \qquad (2.34)$$

The simplest example of this formalism is the case of free spins when there exists no interaction between the individual spins, so only one spin need be considered. The Hamiltonian for this system is just the Zeeman term 85)

$$H_0 = \omega_0 S^z \qquad (2.35)$$

This is just the interaction picture; one finds in a similar method to that used in evaluating (A.11), that

$$S^{\pm}(t) = e^{iH_0t} S^{\pm} e^{-iH_0t} = e^{\pm i\omega_0 t} S^{\pm} \qquad (2.36)$$

so $$\chi^{T}_{ret.}(t)_0 = -2i < S^z >_0 e^{-i\omega_0 t} \Theta(t) \qquad (2.37)$$

or $$\chi^{T}_{ret.}(\omega)_0 = \frac{2 < S^z >_0}{\omega + is - \omega_0} \qquad (2.38)$$

Moreover, as its commutator vanishes, so does $\chi^{zz}_{ret.}$ as does χ^{xz} or χ^{yz} because S^z cannot be diagonalized simultaneously with S^x or S^y. Thus using (2.29), (2.30), the real, symmetric retarded susceptibility matrix is given by,

(2.39)

$$\chi^{ij}_{ret.}(t)_o = - < S^z >_o \Theta(t) \begin{vmatrix} \sin \omega_o t & \cos \omega_o t & 0 \\ \cos \omega t & \sin \omega_o t & 0 \\ 0 & 0 & 0 \end{vmatrix}$$

If this result is used in Eq. (2.21) with $h_1 = \omega_1$ ($\gamma = 1$) then

$$< S^x (t) >_{r.f.} = . \frac{\omega_1 < S^z >_o}{(\omega - \omega_o)} (\cos \omega_o t - \cos \omega t) \quad (2.40)$$

this is a maximum when $\omega = \omega_o$ when

$$< S^x(t) >_{resonance} = \omega_1 t < S^z >_o \sin \omega_o t \quad (2.41)$$

similarly

(2.42)

$$< S^y(t) >_{r.f.} = \frac{\omega_1 < S^z >_o}{(\omega + \omega_o)} (\sin \omega_o t + \sin \omega t)$$

and this is a maximum when $\omega = - \omega_o$, when

$$< S^y(t) >_{resonance} = \omega_1 t < S^z > \cos \omega_o t. \quad (2.43)$$

(2.4) Magnetic Interactions of the Electrons.

Each electron has a spin one - half or $\frac{1}{2}\underline{\sigma}$ where $\sigma^i_{\lambda\lambda'}$ is one of the 2 -dimensional Pauli spin matrices, with matrix elements $\lambda\lambda'$ ($\lambda = \pm 1$). These obey the product rule,[85]

$$\sum_\mu \sigma^i_{\lambda\mu} \sigma^j_{\mu\lambda'} = 2i \sum_k \epsilon_{ijk} \sigma^k_{\lambda\lambda'} + \delta_{ij} \delta_{\lambda\lambda'} \qquad (2.44)$$

If the electron is described by the spinor field $\psi_\lambda(\underline{x})$, then the spin density at the point $\underline{x}$ is given by

$$\underline{S}_e(\underline{x}) = \frac{1}{2} \sum_{\lambda\lambda'} \psi^+_\lambda(\underline{x}) \, \underline{\sigma}_{\lambda\lambda'} \psi_{\lambda'}(\underline{x}) \qquad (2.45)$$

In the second quantized representation

$$\psi_\lambda(\underline{x}) = (V)^{-\frac{1}{2}} \sum_p e^{i\underline{p}.\underline{x}} a_{p\lambda}$$

the total spin of the electronic system is given by the integral of (2.45) over the whole volume, so that

$$S^i_e = \frac{1}{2} \sum_{p\lambda\lambda'} a^+_{p\lambda} \sigma^i_{\lambda\lambda'} a_{p\lambda'} \qquad (2.46)$$

where the electrons obey the anti - commutation rules (A.6):

$$[a_{p\lambda}, a^+_{p'\lambda'}]_+ = \delta_{pp'} \delta_{\lambda\lambda'} \qquad (2.47)$$

The use of Eq. (2.47) shows that the total electronic spin obeys the spin commutation rules (c.f. 2.17)

$$[S^i_e , S^j_e] = i \sum_k \epsilon_{ijk} S^k_e \qquad (2.48)$$

The generalized form of the electronic - Pauli operators (2.46) will be useful,[57)]

$$\sigma_q^i = \sum_{p\lambda\lambda'} a^+_{p+q,\lambda} \, \sigma^i_{\lambda\lambda'} \, a_{p,\lambda'} \qquad (2.49)$$

with $(\sigma^i_q)^+ = \sigma^i_{-q}$ and the generalized commutation rules

$$[\sigma^i_q , \sigma^j_{q'}] = 2_i \sum_k \varepsilon_{ijk} \, \sigma^k_{q+q'} \qquad (2.50)$$

The commutation rules of these operators with the electron operators are,

$$[\sigma^i_q , a^+_{p,\lambda}] = \sum_{\lambda'} a^+_{p+q,\lambda'} \, \sigma^i_{\lambda'\lambda} \qquad (2.51)$$

The total electronic spin can be written in this representation as

$$S^i_e = \tfrac{1}{2} \sigma^i_c \qquad (2.52)$$

The magnetic behaviour of the electrons in an external field h^z is described by their own Zeeman term,

$$H^m_e = \tfrac{1}{2}\omega_e \sum_{\lambda p} a^+_{p\lambda} a_{p\lambda} = \omega_e S^z_e \qquad (2.53)$$

where the Zeeman splitting ω_e is given in terms of the Bohr magneton β and the electronic g- factor g_e, so

$$\omega_e = g_e \beta h^z \qquad (2.54)$$

So

$$S^{\pm}_e (t) = e^{iH_e^m t} S^{\pm}_e e^{-iH_e^m t} = e^{\pm i\omega_e t} S^{\pm}_e \qquad (2.55)$$

The combined Hamiltonian of the system of electrons and localized spin (A.2) is given by

$$K_o = K_e^o + H_e^m + H_s^m \qquad (2.56)$$

where H_s^m is the Hamiltonian of the localized spin (2.35) and K_e^o is the kinetic energy term for the electrons (see Chapter 5).

Thus, the total spin of the whole system (electrons plus localized spin) is $\underline{S}_T$ where,

$$\underline{S}_T = \underline{S} + \underline{S}_e. \qquad (2.57)$$

$$\begin{aligned} \text{Now } [\, K_o \,,\, S_T^z \,] &= 0 \\ \text{while } [\, K_o \,,\, \underline{S}_T^2 \,] &= 0 \end{aligned} \qquad (2.58)$$

only if $\omega_e = \omega_o$ or $g_e = g_s$

If the electrons interact with the single localized spin through an interaction term (see Chapter 5, Eq. (5.5)),

$$H_1 = N^{-1} \sum_q J_q \, \underline{S} \cdot \underline{\sigma}_q \qquad (2.59)$$

then

$$[\, H_1 \,,\, S_T^j \,] = 0 \quad \text{so} \quad [\, H_1 \,,\, \underline{S}_T^2 \,] = 0 \qquad (2.60)$$

Thus, this type of interaction term does not affect the dynamics of the <u>total</u> spin operator Eq. (2.57), which are determined only by K_o , so,

$$-[\, S_T^{\pm} \,,\, K_o \,] = \pm \omega_o \, S^{\pm} \pm \omega_e \, S_e^{\pm} \qquad (2.61)$$

Hence for the special case, $g_e = g_s$

$$S_T^{\pm}(t) = e^{iK_o t} \; S_T^{\pm} \, e^{-iK_o t} = e^{\pm i \omega_o t} \; S_T^{\pm} \qquad (2.62)$$

If this is used in Eq. (2.28) for the total spin susceptibility, then its transform is,

$$\chi^{T}_{\text{ret.}}(\omega)_{\text{total}} = \frac{2 < S_T^z >}{\omega + is - \omega_o} \qquad (2.63)$$

As the r.f. field couples to both the electrons and the localized spin, then by Eq.s (2.38) and (2.21) , one has,

$$\chi^{T}_{\text{ret.}}(\omega)_{\text{total}} = \frac{< S_T^z >_o}{< S^z >_o} \; \chi^{T}_{\text{ret}}(\omega)_o \qquad (2.64)$$

Equation(2.64) implies that dynamical information about the interacting electron - moment system can be found from examining $F(\tau)$ for the localized spin or the electrons or for the coupled spin propagator $F_{es}(\tau)$, but not from the total spin propagator. The coupled - spin propagator $F_{es}(\tau)$ is defined, for completeness, by

$$F_{es}(\tau - \tau') = < T_W (S^-(\tau), \; S_e^+(\tau')) > \qquad (2.65)$$

The purpose of the following chapters is to arrive at a perturbation method for evaluating such propagators, which contain all the information about the system when expressed in the Heisenberg picture of the fully interacting system.

Chapter 3.

PERTURBATION AND OTHER METHODS.

(3.1) Introduction.

The fermion representation[8)] for S = ½ is generalized to all S values and the resulting eigenstates investigated in the next section for the case of S = ½ and S = 1. Those with no equivalent spin states are called "anomalous" and are at the root of all the difficulties associated with spin representations. This generalized representation is then used in section (3.3) to exhibit the relationship between the Anderson[19)] and Kondo[30)] Hamiltonians for the case of several d-orbitals per atom. This is an extension of the work of Schrieffer and Wolff,[27)] who showed the correspondence for the single d-orbital, single impurity model (S = ½). Their general approach will be followed here but in much more detail, to exhibit the approximations used in their equivalence. This is followed by section (3.4) where low - order perturbation methods are used to exhibit the first order Knight shifts of the Kondo model[35)] using the Holstein-Primakoff[16)] approximation for the spin operators (i.e. large S limit) and by an equations-of-motion method for decoupling the Green's functions.[86)] Finally in section (3.5), the proof of a Wick's theorem for S = ½ using the coupled-fermion representation first given by Yolin,[9)] is repeated here and it is shown that it is not possible to use this simple approach for S = 1 with this representation. The (2S + 1) fermion representation for spin S, given by Abrikosov,[10)] (which was also derived independently by the present author), is presented, and Abrikosov's method of establishing a successful Wick's theorem for the s - d model is outlined.

(3.2) The 2S Fermion Spin Representation.

The general 2S fermion representation is an obvious extension of the simple case for $S=\frac{1}{2}$.8) If a set of spin half operators $\underline{S}i$ are associated with a set of well localized positions (e.g. atomic sites), then their operator properties can be reproduced by introducing a set of fermion operators $a_{i,\lambda}$ and their Hermitian conjugates $a^+_{i,\lambda}$ so that one pair ($\lambda= \pm 1$) is associated with each site through the equivalence relations

$$S_i^z = \tfrac{1}{2}\Sigma_\lambda \lambda N_{i,\lambda} \qquad \text{and} \qquad S_i^+ = a^+_{i,+}\, a_{i,-} \qquad (3.1)$$

where $N_{i,\lambda} = a^+_{i,\lambda}\, a_{i,\lambda}$ and $[\, a_{i,\lambda}\, ,\, a^+_{j,\lambda'}]_+ = \delta_{ij}\,\delta_{\lambda\lambda}$ (3.2).

It is then quite straight forward to show that Eq.s (3.1) satisfy the spin commutation rules. This can be imagined in a pictorial way as each site having one electron level, which can be accupied by a spin up and/or a spin down electron. In the light of this fact it may be termed the "electronic representation". However certain difficulties are automatically introduced in this representation which can be seen by considering the state vectors associated with these "particles". If the empty level is represented by the vacuum state $|0,0>$ with

$$a_{i,\lambda}|0,0> \;=\; 0\;. \qquad (3.3)$$

then the two singly occupied states $|1,0> = a^+_+|0,0>$ and $|0,1> = a^+_-|0,0>$ correspond to the two spin eigenstates for $S=\frac{1}{2}$ i.e. $|\frac{1}{2},m>$ (the site labels have been dropped for the moment.) One further state $|1,1> = a^+_+ a^+_-\, |0,0>$ completes the closure property of these fermion operators and corresponds to the doubly occupied level. The zero and two particle states do not correspond to spin states but fortunately they are null eigenvectors of the spin operators.

$$\underline{S} | 0,0 \rangle = \underline{S} |1,1\rangle = 0. \tag{3.4}$$

This latter property was used by Yolin 9) in establishing a Wick theorem for $S=\frac{1}{2}$ operators. The details of this method will be given in section (3.5) of this chapter. The representation is generalized by taking 2S equivalent sets of operators for each site, labelled by an additional index α . This corresponds to the splitting of the original level into a set of α levels. The corresponding equations are,

$$\begin{aligned} S_i^z(\alpha) &= \tfrac{1}{2}\Sigma_\lambda \, \lambda \, a^+_{i,\alpha,\lambda} \, a_{i,\alpha,\lambda} \quad ; \\ S_i^+(\alpha) &= a^+_{i,\alpha,+} \, a_{i,\alpha,-} \end{aligned} \tag{3.5}$$

while the corresponding anti-commutation rules are,

$$[a_{i,\alpha,\lambda} \, , \, a^+_{j,\beta,\lambda'}]_+ = \delta_{ij} \, \delta_{\lambda\lambda'} \delta_{\alpha\beta} \tag{3.6}$$

The following operators are then constructed by summing over the index α from 1 to 2S for each site.

$$\begin{aligned} S^z{}_i &= \tfrac{1}{2}\Sigma_{\alpha\lambda} \lambda \, a^+_{i,\alpha,\lambda} \, a_{i,\alpha,\lambda} \\ S_i^\lambda &= \sum_\alpha a^+_{i,\alpha,\lambda} \, a_{i,\alpha,-\lambda} \end{aligned} \tag{3.7}$$

The use of Eq.(3.6) readily shows that these new operators still obey spin-commutation rules. It is always possible to find a sub-set of the fermion states which correspond to eigenstates of $\underline{S}^2$ and S^z, while the remaining states can be grouped in eigenstates of smaller S values. This can be seen by considering the case $S=1$. There are now 5 operators which span this space (for every site), acting on the general vacuum state $|0\rangle$; they are,

$$1 \ , \quad a^{+}_{1,+1} \ , \quad a^{+}_{1,-1} \ , \quad a^{+}_{2,+1} \quad a^{+}_{2,-1}$$

The corresponding set of 16 eigenvectors can be assigned to the following simultaneous eigenvectors of $\underline{S}^2$ and S^z denoted as usual by $| s,m >$. There is only one set of states corresponding to $|1,m>$ and this is bounded by the operators $\underline{S}$; they are,

$$|1,-1> = a^{+}_{1,-} a^{+}_{2-}|0> \ ; \qquad |1,+1> = a^{+}_{1+} a^{+}_{2+}|0>$$

$$|1,0> = 2^{-\frac{1}{2}} (a^{+}_{1+} a^{+}_{2-} + a^{+}_{1-} a^{+}_{2+}) |0> \tag{3.8}$$

There are 4 independent series corresponding to $|\frac{1}{2},m>$, they are, (with α=1 or 2),

$$| \tfrac{1}{2},-\tfrac{1}{2} > = a^{+}_{\alpha-}|0> \quad \text{and} \quad a^{+}_{\alpha+}a^{+}_{\alpha-}a^{+}_{\beta-} |0>$$

and $$| \tfrac{1}{2},+\tfrac{1}{2} > = a^{+}_{\alpha+} |0> \quad \text{and} \quad a^{+}_{\alpha+}a^{+}_{\alpha-}a^{+}_{\beta+}|0>$$

Finally there are 4 independent solutions corresponding to $|0,0>$ they are,

$$|0> \quad a^{+}_{\alpha+} a^{+}_{\alpha-} |0> \quad \text{and} \quad a^{+}_{1+}a^{+}_{1-}a^{+}_{2+}a^{+}_{2-} |0>$$

This process can be extended to larger spin values with a corresponding increase in complexity.

(3.3) The Relation Between The Anderson and Kondo Hamiltonians for General Spin.

The Anderson model 19) for several d- orbitals (in this case taken to be 2S) can be written in terms of a generalized Coulomb repulsion between electrons on the same atom. In general this Coulomb repulsion can be writtan as $U^{\lambda\lambda'}_{\alpha\beta}$ between an electron of spin λ occupying the α-orbital and one of spin λ' occupying the β -orbital. So for Nd atoms in the lattice, the diagonal part of the Hamiltonian can be written as,

$$H_0 = \sum_{p\lambda} \xi_p N_{p\lambda} + \sum_{i\alpha\lambda} \xi_\alpha N_{i\alpha\lambda} + \frac{1}{2} \sum_{\substack{i\alpha\beta \\ \lambda\lambda'}} U^{\lambda\lambda'}_{\alpha\beta} N_{i\alpha\lambda} N_{i\beta\lambda'} \qquad (3.11)$$

where ξ_p and ξ_α are the one - electron energies of the conduction and localized orbitals, measured reoative to the Fermi energy. The conduction and the localized states are mixed by the small s - d mixing potentialV leading to an interaction term in the Hamiltonian.

$$H_1 = \sum_{\substack{ip \\ \alpha\lambda}} (V_{ip\alpha} a^+_{p\lambda} a_{i\alpha\lambda} + V^*_{ip\alpha} a^+_{i\alpha\lambda} a_{p\lambda}) \qquad (3.12)$$

The mixing terms, linear in V can be eliminated by performing a canonical transformation on the Hamiltonian

$$\bar{H} = e^{T} H e^{-T} \qquad (3.13)$$

If the exponentials are expanded the following series of commutators results,

$$\bar{H} = H + [T,H] + \frac{1}{2} [T,[T,H]] + \frac{1}{3}[T,[T,[T,H]]] + .. \qquad (3.14)$$

By choosing T to be first order in V, the transformed Hamiltonian will only involve terms at least quadratic in Vif,

$$[H_o , T] = H_1 \tag{3.15}$$

In terms of the orthonormal eigenstates E and E' of H_o this equation becomes,

$$< E | H_1 | E'> = (E - E') < E | T | E'> \tag{3.16}$$

This has a solution (for $E \neq E'$) of the form,

$$T = \sum_{EE'} \frac{|E >< E | H_1 | E' > < E'|}{(E - E')} \tag{3.17}$$

Thus H_1 only connects an occupied d-orbital with an empty conduction orbital (or vice-versa). These states can be generated from $|E'>$ in the form,

$$| E_1 > = a^+_{p\lambda} a_{i\alpha\lambda} | E' > \quad \text{and} \quad | E_2 > = a^+_{i\alpha\lambda} a_{p\lambda} | E' > \tag{3.18}$$

So

$$T = \sum_{\alpha E'} \left(\frac{| E_1 > V_{ip\alpha} < E' |}{E_1 - E'} + \frac{| E_2 > V^*_{ip\alpha} < E' |}{E_2 - E'} \right) \tag{3.19}$$

This can be solved in the following manner, using the two alternatives for manipulating the commutator,

$$[H_o , a^+_{p\lambda} a_{i\alpha\lambda}] | E' > = (E_1 - E') | E_1 > \tag{3.20}$$

or

$$[H_o , a^+_{p\lambda} a_{i\alpha\lambda}] | E' > = (\xi_p - \xi_\alpha - \sum_{\beta\lambda'} N_{i\beta\lambda'} U^{\lambda'\lambda}_{\beta\alpha}) | E_1 > \tag{3.21}$$

where the symmetry properties of the Coulomb term have been used i.e. symmetric with respect to interchange of thespin labels or the orbital labels and also use of the Pauli principle for the same orbital i.e. $U^{\lambda\lambda}_{\alpha\alpha} = 0$; using Eq.s (3.20 and 3.21) to obtain the eigenvalue equation gives,

$$(E_1 - E')| E_1 > = (\xi_p - \xi_\alpha - \sum_{\beta\lambda'} N_{i\beta\lambda'} U^{\lambda'\lambda}_{\beta\alpha})| E_1 > \tag{3.22}$$

Similarly for the eigenstates $|E_2>$, with the result,

$$(E_2 - E')| E_2 > = -(\xi_p - \xi_\alpha - \sum_{\beta\lambda'} N_{i\beta\lambda'} U^{\lambda'\lambda}_{\beta\alpha})| E_2 > \tag{3.23}$$

Using Eq.s (3.21 and 3.23) in Eq.(3.19), T can be written down using the appropriate inverse operator,

$$T = \sum_{\substack{\alpha\lambda \\ ipEE'}} | E >< E |(\xi_p - \xi_\alpha - \sum_{\beta\lambda'} N_{\beta\lambda'} U^{\lambda\lambda}_{\beta\alpha})^{-1} (V_{ip}\, a^{+}_{\alpha\lambda}\, a_{\alpha\lambda} - V^{*}_{ip\alpha}\, a^{+}_{\alpha\lambda}\, a_{\lambda})| E' >< E'| \tag{3.24}$$

This can now be linearized in the inverse operator by approximating the Coulomb repulsion matrix by its largest contributions, that is, only considering the diagonal parts between the same orbitals.

$$U^{\lambda\lambda'}_{\beta\alpha} = \delta_{\alpha\beta}\ \delta_{\lambda'-\lambda}\, U_\alpha \tag{3.25}$$

Moreover as $| E'>$ is diagonal with respect to $N_{i\alpha\lambda}$ then it can be only either occupied or unoccupied with number eig values 1 or 0, so in this space,

$$T = \sum_{\substack{ip \\ \alpha\lambda}} \left(\frac{N_{i\alpha-\lambda}}{\varepsilon_p - \varepsilon_\alpha - U_\alpha} + \frac{(1 - N_{i\alpha-\lambda})}{\varepsilon_p - \varepsilon_\alpha} \right)(V_{ip\alpha}\, a^{+}_{p\lambda}\, a_{i\alpha\lambda} - V^{*}_{ip\alpha}\, a^{+}_{i\alpha\lambda}\, a_{p\lambda}) \tag{3.26}$$

This can be rewritten in a more compact form by defining the following d-level energies in terms of $\gamma = \pm 1$. .

$$\varepsilon_\alpha^\gamma = \varepsilon_\alpha + \tfrac{1}{2}(1 + \gamma) U_\alpha \quad \& \quad N_{i\alpha\lambda}^\gamma = \tfrac{1}{2}(1 - \gamma) + \gamma N_{i\alpha\lambda} \tag{3.27}$$

So finally the generalized form of the canonical generator T is,

$$T = \sum_{\substack{ip \\ \alpha\lambda\gamma}} \frac{N_{i\alpha,-\lambda}^\gamma}{\varepsilon_p - \varepsilon_\alpha^\gamma} \left(V_{ip\alpha} a_{p\lambda}^+ a_{i\alpha\lambda} - V_{ip\alpha}^* a_{i\alpha\lambda}^+ a_{p\lambda} \right) \tag{3.28}$$

Now higher order commutators will involve higher order terms in the dimensionless ratio $r_{\alpha\gamma}$,

$$r_{\alpha\gamma} = \frac{\langle |V_{ip\alpha}|^2 \rangle}{\varepsilon_\alpha^\gamma} \rho(\xi_\alpha^\gamma) \tag{3.29}$$

where $\rho(\xi_\alpha^\gamma)$ is the density of conduction band states in the perfect metal at energy ξ_α^γ , while the matrix elements are averaged over the conduction states p of this energy. So in the limit $r_{\alpha\gamma} \ll 1$ the Hamiltonian $\bar{H}$ is well approximated by $H_0 + H_2$, where,

$$H_2 = \tfrac{1}{2} [T, H_1] \tag{3.30}$$

Evaluation of this commutator, using the anti-commutation rules for the electron operators, results in a series of terms,

$$H_2 = H_0' + H_{ch} + H_{rest} \tag{3.31}$$

with

$$H_0' = -\tfrac{1}{2} \sum_{\substack{ijp \\ \alpha\beta\lambda}} \left(W_{ip\alpha}^{jp\beta} + \tfrac{1}{2} J_{ip\alpha}^{jp\beta} \left(N_{i\alpha,-\lambda} + N_{j\beta,-\lambda} \right) \right) a_{j\beta\lambda}^+ a_{i\alpha\lambda} \tag{3.32}$$

and

$$H_{ch} = \tfrac{1}{4} . \sum_{\substack{ipp' \\ \alpha\lambda}} J^{ip'\alpha}_{ip\alpha} a^{+}_{i\alpha\lambda} a^{+}_{i\alpha-\lambda} a_{p\lambda} a_{p'-\lambda} + \text{h.c.} \tag{3.33}$$

where the matrix elements are defined by,

$$J^{jp'\beta}_{ip\alpha} = \sum_{\gamma} \gamma V_{ip\alpha} V^{*}_{jp'\beta} \left(\frac{1}{\varepsilon_p - \varepsilon^{\gamma}_{\alpha}} + \frac{1}{\varepsilon_{p'} - \varepsilon^{\gamma}_{\alpha}} \right) \tag{3.34}$$

and

$$W^{jp'\beta}_{ip\alpha} = V_{ip\alpha} V^{*}_{jp'\beta} \left(\frac{1}{\varepsilon_p - \varepsilon^{-}_{\alpha}} + \frac{1}{\varepsilon_{p'} - \varepsilon^{-}_{\alpha}} \right) \tag{3.35}$$

The remaining terms in Eq. (3.31) are given by

$$H_{rest} = \tfrac{1}{2} . \sum_{\substack{ipp' \\ \alpha\lambda\lambda'}} \lambda\lambda' U^{ip'\alpha}_{ip\alpha} a^{+}_{p\lambda} a_{p'\lambda'} a^{+}_{i\alpha-\lambda} a_{i\alpha-\lambda} + \tfrac{1}{2} . \sum_{\substack{ipp' \\ \alpha\lambda}} W^{ip'\alpha}_{ip\alpha} a^{+}_{p\lambda} a_{p'\lambda} \tag{3.36}$$

The first term can now be manipulated into an s-d exchange form using the 2S - fermion representation of section (3.2), and the notation,

$$\underline{\sigma}_{pp'} = \sum_{\lambda\lambda'} a^{+}_{p\lambda} \underline{\sigma}_{\lambda\lambda'} a_{p'\lambda'} \tag{2.37}$$

so

$$\sum_{\lambda\lambda'} \lambda\lambda' a^{+}_{p\lambda} a_{p'\lambda'} a^{+}_{i\alpha-\lambda} a_{i\alpha-\lambda'} = \tfrac{1}{2} . \sum_{\lambda} \Big(a^{+}_{p\lambda} a_{p'\lambda} (N_{i\alpha} - N_{i\alpha\lambda} + N_{i\alpha-\lambda})$$

$$-2 a^{+}_{p\lambda} a_{p'-\lambda} a^{+}_{i\alpha-\lambda} a_{i\alpha\lambda} \Big) \Big) \tag{3.38}$$

Carrying out the sum over λ on the first term and using (3.5) gives,

$$\tfrac{1}{2} . \sum_{\lambda} \left(a^{+}_{p\lambda} a_{p'\lambda} N_{i\alpha} - \sigma^{\lambda}_{pp'} S^{-\lambda}_{i\alpha} \right) - \tfrac{1}{2} . \left(a^{+}_{p+} a_{p'+} - a^{+}_{p-} a_{p'-} \right) (N_{i\alpha+} - N_{i\alpha-}) \tag{3.39}$$

Using Eq. (3.7) for $S^{z}_{i\alpha}$ the final result is

$$\sum_{\lambda} \tfrac{1}{2}.N_{i\alpha}\, a^{+}_{p\lambda}\, a_{p'\lambda} \;-\; \underline{\sigma}_{pp'}.\,\underline{S}_{i\alpha} \tag{3.40}$$

If this is now used in Eq.(3.36) the first term of (3.40) is incorporated with the second of (3.36) to give a contribution H_{dir} so,

$$H_{rest} = H_{ex} + H_{dir} \tag{3.41}$$

With

$$H_{ex} = -\tfrac{1}{2}.\sum_{\substack{ipp'\\ \alpha}} J^{ip'\alpha}_{ip\alpha}\, \underline{\sigma}_{pp'}.\,\underline{S}_{i\alpha} \tag{3.42}$$

and

$$H_{dir} = \sum_{\alpha\lambda ipp'} \left(W^{ip'\alpha}_{ip\alpha} + \tfrac{1}{2}.J^{ip\alpha}_{ip\alpha}\, N_{i\alpha} \right) a^{+}_{p\lambda}\, a_{p'\lambda} \tag{3.43}$$

These terms in the Hamiltonian can be further simplified if the orbital labels do not appear explicitly in the co-efficients J and W. Eq. (3.34) implies that the mixing co-efficients $V_{ip\alpha}$ should be independent of the orbital suffix α , while Eq.(3.27) implies that the levels are degenerate i.e. ξ_α and U_α do not depend on α , so that J (and W) can be rewritten as,

$$J^{jp'\beta}_{ip\ \alpha} = J_{pp'}(\underline{R}_i - \underline{R}_j)$$

assuming that only spatial differences are important. Then carrying out the summation over the 2S values of α on each atom, and using Eq. (3.7) for the spin operators, the final result for the 4 terms in H_2 is,

$$H'_o = -\tfrac{1}{2}.\sum_{\substack{ijp\\ \alpha\beta\lambda}} \left(W_p(\underline{R}_i - \underline{R}_j) + \tfrac{1}{2}.\, J_p(\underline{R}_i - \underline{R}_j)[N_{i\alpha-\lambda} + N_{j\beta-\lambda}] \right) a^{+}_{j\beta\lambda} a_{i\alpha\lambda} \tag{3.44}$$

This can be incorporated into H_0 by altering the definitions of ε_α and represents an exchange term between the d-electrons themselves.

$$H_{dir} = \sum_{\substack{ipp' \\ \alpha\lambda}} \left(W_{pp'}(\underline{R}_i) + \tfrac{1}{2} J_{pp'}(\underline{R}_i) N_{i\alpha} \right) a^{+}_{p\lambda} a_{p'\lambda}$$

In the sub-space where there are N_i d-electrons on each atom, H_{dir} is just a one-electron scattering term for the conduction band which can be incorporated again in H_0 . In fact, for $r_\gamma \ll 1$ the resultant shifts of their wave-functions and energies are negligible.

$$H_{ch} = \tfrac{1}{4} \sum_{\substack{ipp' \\ \alpha\lambda}} J_{pp'}(\underline{R}_i)\, a^{+}_{i\alpha\lambda} a^{+}_{i\alpha-\lambda} a_{p\lambda} a_{p'-\lambda} + \text{h.c.} \tag{3.46}$$

This is the only term which does not conserve the number of d-electrons and represents a double-mixing term between the d-orbitals and the conduction band. However this only occurs for doubly occupied orbitals with opposite spins ar , since in this model the orbitals are taken to be independent, this term can be neglected. This leaves only,

$$H_{ex} = -\tfrac{1}{2} \sum_{ipp'} J_{pp'}(\underline{R}_i)\, \underline{\sigma}_{pp'} \cdot \underline{S}_i \tag{3.47}$$

This is the localized - moment s-d exchange Hamiltonian which will be analysed further in Chapter 5. Near the Fermi surface of the conduction band, Eq. (3.34) becomes,

$$J_{p_f p_f}(\underline{R}_i) \equiv J(\underline{R}_i) = \frac{2 |V_{ip_f}|^2 U}{\xi_d (\xi_d + U)} \tag{3.48}$$

Now a localized moment is most likely to exist if

$\varepsilon_d < \mu$ and $\varepsilon_d + U > \mu$ i.e. $\gamma \xi_d^\gamma > 0$

then $J(\underline{R}_i)$ is negative so that the coupling is anti-ferromagnetic. As will be shown in section (5.3) this is necessary to produce an observable resistance minimum.

(3.4) Holstein-Primakoff and Decoupling Approximations.[16)]

Holstein and Primakoff (H.P.) presented the first and most well-known representation of the quantum-mechanical spin operators by introducing a boson operator A, (the lowering operator for a simple harmonic oscillator), and its Hermitian conjugate A^+ with the commutation rule,

$$[A, A^+] = 1 \qquad (3.49)$$

The H.P. transformation (which is a particular example of a wider class of transformations), retains the hermiticity of the general spin operators, magnitude S, and has the form,

$$S^z = N - S \quad \text{and} \quad S^+ = A^+ (2S - N)^{1/2} \qquad (3.50)$$

with $N = A^+ A$, the number operator of the bosons. Since N measures the deviation from the maximum spin down state, which if small $(N \sim 1)$ and $S \gg 1$ enables the roots to be approximated by their leading terms, that is,

$$S^+ = (2S)^{1/2} A^+ \quad , \quad S^- = (2S)^{1/2} A \qquad (3.51)$$

The diagonal part of the s-d Hamiltonian Ho is still diagonal in the boson representation, so,

$$H_0 = \sum_{p\lambda} \xi_{p\lambda} N_{p\lambda} + \omega_0 (N - S) \qquad (3.52)$$

with the one-electron energies measured relative to the Fermi energy μ , that is,

$$\xi_{p\lambda} = \varepsilon_p - \mu + \tfrac{1}{2}\lambda\omega_0 \quad \text{and} \quad \omega_0 = g\,\mu_B h^z \qquad (3.53)$$

In the thermal interaction picture (with $\tau = it$,where t is the time) the operators are defined by equations of the form,

$$X(\tau) = e^{H_0\tau} X e^{-H_0\tau} \qquad (3.54)$$

So for the bose-fields and the conduction electron operators,

$$A^+(\tau) = e^{\omega_0\tau} A^+ \quad \text{and} \quad a^+_{p\lambda}(\tau) = e^{\xi_{p\lambda}\tau} a^+_{p\lambda} \qquad (3.55)$$

For the representation in which the σ^z component of the Pauli matrices is diagonal, one has,

$$\underline{S}\cdot\underline{\sigma}_{\lambda\lambda'} = \lambda S^z \delta_{\lambda\lambda'} + (S^+\delta_{\lambda,-} + S^-\delta_{\lambda,+})\delta_{\lambda',-\lambda} \qquad (3.56)$$

The interaction part of the s-d Hamiltonian H_1 for a single impurity at the origin with a δ -function range of interaction (or $J_q = J$) can be re-written in terms of the appropriate Wannier operators α[87], where,

$$a_\lambda = N^{-\frac{1}{2}} \sum_p a_{p,\lambda} \qquad (3.57)$$

If this is used in Eq. (5.5) then H_1 becomes,

$$H_1 = -J\, \underline{S} \cdot \sum_{\lambda\lambda'} a^+_\lambda \underline{\sigma}_{\lambda\lambda'} a_{\lambda'} \qquad (3.58)$$

or,

$$H_1 = -J \left(S^+ a^+_- a_+ + S^- a^+_+ a_- + \sum_\lambda \lambda S^z a^+_\lambda a_\lambda \right) \qquad (3.59)$$

In terms of the H.P. representation, Eq.s (3.50) and (3.51), this becomes,

$$H_1 = -J \sum_\lambda \left(A^\lambda a^+_{-\lambda} a_\lambda + \lambda a^+_\lambda a_\lambda (A^+ A - S) \right) \qquad (3.60)$$

where the following abbreviated notation for the bosons has been adopted,

$$A^\lambda = \Theta(\lambda) A^+ + \Theta(-\lambda) A \qquad (3.61)$$

The single particle Green's functions can be defined in a similar way to those in Appendix A. The Wannier Green's function at the origin is given by,

$$G^0_{\nu\lambda} (\tau - \tau') = < Tw\, (a_\nu(\tau) , a^+_\lambda(\tau')) >_0 \qquad (3.62)$$

In terms of the temperature difference $\bar{\tau} = \tau - \tau'$, and the one electron fermi factors,

$$f^-_{p\lambda} = (e^{\beta\xi_{p\lambda}} + 1)^{-1} = 1 - f^+_{p\lambda} \qquad (3.63)$$

and since G^0 is diagonal in the momentum representation, one has,

$$G^0_{\nu\lambda} (\bar{\tau}) = \frac{\delta_{\nu\lambda}}{N} \sum_p e^{-\beta\xi_{p\lambda}\bar{\tau}} \left(\Theta(\bar{\tau}) f^+_{p\lambda} - \Theta(-\bar{\tau}) f^-_{p\lambda} \right) \qquad (3.64)$$

Similarly the bose propagator $B^{o}(\tau)$ is given by,

$$B^{o}(\tau-\tau') = <Tw(A(\tau), A^{+}(\tau'))>_{o} \quad (3.65)$$

which is evaluated in terms of the bose factors,

$$b^{-}(\omega_{o}) = (e^{\beta\omega_{o}}-1)^{-1} = b^{+}(\omega_{o}) - 1 \quad (3.66)$$

so

$$B^{o}(\tau) = e^{-\omega_{o}\tau}(\Theta(\tau)\, b^{+}(\omega_{o}) + \Theta(-\tau)\, b^{-}(\omega_{o})) \quad (3.67)$$

Since $G(\tau)$ is add periodic with respect to τ, its (odd) Fourier transform (see Appendix A. 40) is,

$$G^{o}_{\lambda}(\bar{\nu}) = \frac{1}{N}\sum_{p}(\xi_{p\lambda} - i\bar{\nu})^{-1} \quad (3.68)$$

The corresponding (even) Fourier transform of $B^{o}(\tau)$ is,

$$B^{o}(\bar{\alpha}) = (\omega_{o} - i\bar{\alpha})^{-1} \quad (3.69)$$

The restriction to large S can be seen by evaluating the thermal average of S^{z} in the two representations with respect to the eigenstates of H_{o}.

In the spin-space with the restriction to the first 2S eigenstates of N, one has,

$$< S^{z} >^{s}_{o} = < N - S >^{s}_{o} = -B_{s}(\tfrac{1}{2}.\beta\,\omega_{o}) \quad (3.70)$$

where $B_{s}(x)$ is the Brillouin function of paramagnetism for spin S

$$B_{s}(x) = (S+\tfrac{1}{2})\coth(2S+1)x - \tfrac{1}{2}\coth x . \quad (3.71)$$

However

$$\langle N \rangle_{0}^{A} = b^{-}(\omega_0) \neq \langle N \rangle_{0}^{s} \qquad (3.72)$$

but in the limit $S \gg 1$ then $B_S(x) = S - b^{-}(2x)$, so in this limit,

$$\langle S^{z} \rangle_{0}^{A} = \langle S^{z} \rangle_{0}^{s} \qquad (3.73)$$

This could have been anticipated, for in this limit both representations satisfy $[S^{-}, S^{+}] = -2S^{z} = 2S$.

So a diagrammatic perturbation theory can now be constructed from Eq. (3.60) using Gaudin's[88] proof of Wick's theorem for the bose-fields A and A^{+} (Appendix B.) The electronic Green's function is represented by a directed solid line and the bose propagator by a directed curly line, Fig. (1.), (see later).

The lowest order diagrams in each case are just the simple "bubble" graphs, Fig. (3.). The corresponding lowest order irreducible self-energy $\Pi(\tau)$ for the bose propagator is given by,

$$\Pi(\tau) = J \sum_{\lambda} \lambda\, G_{\lambda}^{0}(0^{-})\, \delta(\tau) \qquad (3.74)$$

which has the simple Fourier transform,

$$\Pi(\bar{a}) = 2J\zeta^{0} \qquad (3.75)$$

where the electronic magnetization ζ is defined by,

$$\zeta^{0} = \frac{\tfrac{1}{2}(N_{+}^{0} - N_{-}^{0})}{N} = \tfrac{1}{2}\sum_{\lambda} \lambda\, G_{\lambda}^{0}(0^{-}) \qquad (3.76)$$

Similarly the effective potential (see Chapter 5.) $V_\lambda(\tau)$ for the Wannier propagator is given to first-order by,

$$V_\lambda(\tau) = \lambda J (B^0 (0^-) - S) \delta(\tau) \qquad (3.77)$$

which has the transform $V_\lambda(\bar{\nu}) = \lambda J (b^- - S)$ (3.88)

In the large S limit (Eq.(3.73)) one has,

$$V_\lambda(\bar{\nu}) = \lambda J < S^z >_0 \qquad (3.89)$$

These two first order results can also be obtained by decoupling the Green's functions equations of motion. Writing $F(\omega) = << S^- , S^+ (\omega) >>$ with $\eta = 1$ for the spin operators, the corresponding equation of motion (C. 18.) with the Kondo Hamiltonian Eq.s (3.52) and (3.58) is,

$$(\omega_0 - \omega) << S^- ; S^+ (\omega) >> + < \{ S^-, H_1] ; S^+(\omega) >> = < [S^-, S^+] > \qquad (3.90)$$

Evaluation of the commutator gives,

$$(\omega_0 - \omega) F(\omega) + 2J << \alpha_-^+ \alpha_+ S^z ; S^+(\omega) >> - J \sum_\lambda \lambda << \alpha_\lambda^+ \alpha_\lambda S^- ; S^+(\omega) >> = -2 < S^z > \qquad (3.91)$$

This is approximated by neglecting the higher order Green's function $<< \alpha_{-1}^+ \alpha_{+1} S^z ; S^+ >>$ and decoupling the other term in the non-vanishing form,

$$<< \alpha_\lambda^+ \alpha_\lambda S^- ; S^+ >> \cong < \alpha_\lambda^+ \alpha_\lambda > << S^- ; S^+ >> \qquad (3.92)$$

With these approximations Eq. (3.91) has the solution,

$$F(\omega) = \frac{-2 < S^z >}{\omega_0 - \omega - 2J\zeta} \qquad (3.93)$$

If this is compared with the result for the bose propagator using Eq. (3.75),

$$B(\omega) = \frac{B^{\circ}(\omega)}{1 - \Pi(\omega)\, B^{\circ}(\omega).} = (\omega_0 - \omega - 2J\zeta\ )^{-1} \qquad (3.94)$$

Now $F(\omega) = 2S\ B(\omega)$ in the large S limit, and also in this approximation $< S^z > = -2S$, so the two results, Eq.s (3.93) and (3.94) are equivalent. In fact, if this result is compared with the exact result, to first order in J for S = ½ or S = 1, Eq. (5. 18), it will be seen to be correct. This demonstrates the relative insensitivity of first order results, which can always be found by almost all methods to this accuracy. A similar result is obtained by using the same decoupling approximation for the Wannier equation of motion.

(3.5) Yolin's Wick Theorem and Abrikosov's Method.

The proof of a spin-Wick's theorem for S = ½, given by Yolin,9) depends on the fact that the two anomalous states $| 0,0 >$ and $|+,->$ (using the same notation as in section (3.2)) , are null eigenvectors of all the spin operators i.e. Eq. (3.4). Consequently a trace over this set of states, (denoted generically by "a"), of any product of spin operators X(S), which does not involve any additive constants, will only involve non-zero contributions from the two spin-states $|+,0>$ and $|0,->$. This property is maintained even when the states are weighted by the Boltzmann factor $\exp(-\beta H_o)$, with H_o diagonal in S^z , say $\omega_c S^z$, then,

$$\mathrm{Tr}_a \left(e^{-\beta\omega_o S^z} X(S) \right) = \mathrm{Tr}_s \left(e^{-\beta\omega_o S^z} X(S) \right) \quad (3.95)$$

where the operators on the L.H.S. are written in the coupled fermion representation, Eq. (3.1).

However, the partition function Z^o involves a trace over the Boltzmann factor which picks up contributions from the two anomalous states, so,

$$Z_a^o = \mathrm{Tr}_a\left(e^{-\beta\omega_o S^z}\right) = 2 + e^{\frac{1}{2}\beta\omega_o} + e^{-\frac{1}{2}\cdot\beta\omega_o} \quad (3.96)$$

This is <u>not</u> equal to the partition function evaluated in the true spin space for $S = \frac{1}{2}$, for,

$$Z_s^0 = \mathrm{Tr}_s\left(e^{-\beta\omega_o S^z} \right) = e^{\frac{1}{2}\beta\omega_o} + e^{-\frac{1}{2}\beta\omega_o} \quad (3.97)$$

Now using the usual definition of a thermal average, evaluated in the interaction picture, one has,

$$< X(S) >_o^s = \frac{\mathrm{Tr}_s\left(e^{-\beta\omega_o S^z} X(S) \right)}{Z_s^o} = \frac{Z_a^o}{Z_s^o} \cdot \frac{\mathrm{Tr}_a\left(e^{-\beta\omega_o S^z} X(S)\right)}{Z_a^o}$$

or in an obvious notation,

(3.98)

$$< X(S) >_o^s = \bar{Y} < X(S) >_o^a \quad (3.99)$$

where

$$\bar{Y} = \frac{Z^{\overset{o}{a}}_{\sigma}}{Z_s} = \frac{\cosh\left(\frac{1}{2}\beta\,\underline{\omega}_o\right) + 1}{\cosh\left(\frac{1}{2}\beta\,\omega_\sigma\right)} \qquad (3.100)$$

The bar over the Y has been used to differentiate this compensation factor from later ones.

The difficulty of all such compensation schemes is that when there are N different sites contributing spin operators in the product X(S) the factor must become $\bar{Y}^N$, (see section (6.3)). Once an equivalence relation between the spin space, and its representational space, has been established, for example Eq. (3.99), for complete traces; then Gaudin's method of deriving Wick's theorem (Appendix B) can be used in the new space to obtain single particle contractions between the representational operators.

As can be seen from the generalization of this representation for spins greater than ½, one can always find a sub-set of eigenstates corresponding to a given S value, but some of the remaining anomalous states give non-aero contributions to any average, (for example S = 1, Eq. (3.9.)), so the previous technique cannot be used. This is not the case for the general drone representation where all states are spin states, Unfortunately, in this case, linear combinations must be used, which introduces problems of normalization within the trace.

Abrikosov[10)] generalized this procedure in a novel way by introducing a 2S + 1 bilinear form of fermi operators c_m and c_m^+ (note: 2S + 1 = 2 × 2S only for S = ½, so either extension has the same spin half form.) The spin operators $\underline{S_i}$ for spin S are written in terms of their 2S + 1 matrix representation $\underline{S}_{mm'}$, so that,

$$\underline{S} = \sum_{m,m'=-s}^{s} c_m^{+} \underline{S}_{mm'} c_{m'} \qquad (3.101)$$

where

$$\underline{S}_{mm'} = < S,m \mid \underline{S} \mid S, m' > \qquad (3.102)$$

and

$$[c_m , c_{m'}^{+}]_{+} = \delta_{mm'} \qquad (3.103)$$

This representation was discovered independently by the present author, for it is obviously true for any operator which can be represented by a finite matrix: (Usual second quantization involves infinitely dimensional matrices in Many-body Physics).

The representation given by Eq. (3.101) is readily seen to obey the correct commutation rules for spin operators, as pairs of fermions occur for each operator. Moreover in the usual matrix representation in which S^z is diagonal with its eigenvalues, occuring in an ordered manner down the leading diagonal of the matrix, one has,

$$S^z = \sum_{m=-s}^{s} m \, c_m^{+} c_m \quad \text{and} \quad S^{+} = \sum_{m} ((S+m) (S+1-m))^{1/2} c_m^{+} c_{m-1} \qquad (3.104)$$

However, as has been shown already, it is not sufficient that the representation just has the correct commutation rules; there must be a 1 to 1 correspondence between the states in the two representations. Otherwise supplementary techniques must be introduced to discount the effect of the anomalous states.

In this representation the eigenstates can be obtained from the usual vacuum state $|0>$ by addition of extra fermions, the resulting states are all orthonormal. A state with n fermions can occur in ${}^{2S+1}C_n$ ways, so that altogether for spin S there are 2^{2S+1} possible states. As can be seen from Eq. (3.104), only the single fermion states, denoted $|m>$, correspond to spin states, and there are 2S + 1 of these. Thus, there will be $2^{2S+1} - (2S+1)$ anomalous states in general (check, for $S = \frac{1}{2}$ this is 2).

Since the states are orthonormal the sub-space of the one-fermion states is orthogonal to all the other anomalous states, denoted $|m^* >$, so,

$$< m | m^* > = 0 \qquad (3.105)$$

A technique based on Eq. (3.105) using projection operators was derived by the present author before the discovery of the drone -fermion technique (see Chapter 4.). Due to the complexity of this method its use was discontinued - to low orders it was found equivalent to the Abrikosov weighting method, which is described next.

In general, only the vacuum state of the set of anomalous states is a null eigenvector of the spin operators, since the representation always involves a destruction operator on the R.H.S., so an equation like the first part of Eq. (3.4) is also valid here. However for the rest of the anomalous states,

$$\underline{S} \, | \, m^* > \; \neq 0 \qquad \text{(in general).} \qquad (3.106)$$

The restriction to the spin states $| m >$ and the vacuum state $|0 >$ is obtained by altering the Hamiltonian in the Boltzmann factor to include an additional term,

$$H_Q = Q \sum_{m=-s}^{s} c_m^+ c_m \qquad (3.107)$$

This does not effect the diagonalization for originally $H_0 = \omega_o S^z$. Now an n particle state will have an extra weighting factor $e^{-\beta nQ}$. Abrikosov assigns the energy Q a value much greater than kT, so in performing thermal averages, the greatest contribution will come from the spin states (remembering that the vacuum state does does not contribute), so,

$$< X(S) >_o^s = (Z_s^o)^{-1} e^{\beta Q} \sum_m <m| e^{-\beta(H_o+H_Q)} X(S)| m > \qquad (3.108)$$

Hence, to order 1 this can be extended to a trace over all fermion states,

$$< X(S) >_o^s = (Z_s^o)^{-1} e^{\beta Q} Tr_c (e^{-\beta(H_o+H_Q)} X(S)) \qquad (3.109)$$

Similarly

$$Z_{cQ}^o = Tr_c (e^{-\beta(H_o+H_Q)}) = 1 + O(e^{-\beta Q}) \qquad (3.110)$$

so in the limit of large Q or Q >> kT then, in the notation of Eq. (3.110)

$$< X(S) >_o^s = \left(\frac{e^{\beta Q}}{Z_s^o}\right) < X(S) >_o^{cQ} \qquad (3.111)$$

For $\omega_o = 0$ then $Z_s^o = 2S + 1$,which is just Abrikosov's factor.

If Eq. (3.104) is used for the spin operators in X(S) of the R.H.S. of Eq. (3.111), the usual Wick's theorem can be used for the fermion fields. Their zero order Green's function is denoted by,

$$\overset{o}{C}_{mm'}(\bar{\tau}) = \langle T_W (c_m(\tau), c^{+}_{m'}(\tau')) \rangle_{o}^{CQ} \tag{3.112}$$

This has the odd-Fourier transform,

$$\overset{o}{C}_{mm'}(\bar{\nu}) = \delta_{mm'} (Q + m\omega_o - i\bar{\nu})^{-1} \tag{3.113}$$

So the evaluation of Eq. (3.112) leads to,

$$\overset{o}{C}_{mm'}(\tau) = e^{-(m\omega_o + Q)\tau} (\Theta(\tau) f^{+}_{mQ} - \Theta(-\tau) f^{-}_{mQ}) \tag{3.114}$$

with

$$f^{+}_{mQ} + 1 = f^{-}_{mQ} = (e^{\beta(m\omega_o + Q)} + 1)^{-1} \cong e^{-\beta(m\omega_o + Q)} \tag{3.115}$$

All measurable averages must be multiplied by the factor $e^{\beta Q}(\overset{o}{Z}_{s})^{-1}$ so only diagrams with one factor $e^{-\beta Q}$ will produce a finite contribution in the infinite Q limit. Moreover as the spin matrices $S_{mm'}$ are cyclic inside the trace, the self-energy contributions to any electron propagator can only involve <u>one</u> $f^{-}_{m\,Q}$ factor, so all other time orderings of that graph are exponentially small.

The other main difficulty with this method is that it is restricted to only one spin impurity (for $S > \frac{1}{2}$) or equivalently the low concentration limit. For example, if 2 spins are present, the factor $e^{-2\beta Q}$ could arise from either one of the sites having 2 fermions excited (a non-spin case), or one fermion on each site,(a true spin state, for two sites).

To avoid such difficulties, the next chapter introduces the drone - fermion representation, which for $S = \frac{1}{2}$ suffers from none of these troubles and for $S = 1$ they can be compensated for in a manner similar to Yolin's treatment for $S = \frac{1}{2}$.

Chapter 4.

WICK'S THEOREM FOR THE DRONE-FERMION REPRESENTATION.

(4.1) Introduction.

The drone-fermion representation previously given by Mattis for $S = \frac{1}{2}$ is generalized to all S values and once more the small S eigenstate properties are analysed. This representation has the fundamental advantage that all the fermion states can be formed into linear combinations which are always eigenstates of $\underline{S}^2$ and S^z leaving no anomalous states. Unfortunately, these linear combinations have differing normalization co-efficients so that a general Wick's theorem cannot be readily derived. However for $S = \frac{1}{2}$, a direct correspondence can be established which results in a very simple form of the Wick theorem for these operators. This result is established in section (4.3) and the method is then used in the following chapters. The analogous result is then proved for $S = 1$ in a somewhat less elegant manner in section (4.4) and apart from an additional multiplicative factor (Y) is very similar to the result for $S = \frac{1}{2}$. These results, it should be emphasized, can be incorporated immediately into standard many-body theory and do not necessitate any specialized manipulation or special diagrams, in contrast to most other spin-Wick treatments mentioned in Chapter 1.

(4.2) The general Drone Representation for Spin S.

The drone-fermion representation for spin-half operators localized at the spatial sites R_i is,$^{5)}$

$$S_i^z = c_i^+ c_i - \tfrac{1}{2} , \qquad S_i^+ = c_i^+ \varphi_i \qquad (4.1)$$

where the real fermion operator φ_i is defined by,

$$\varphi_i = d_i + d_i^+ \qquad (4.2)$$

The anti-commutation rules for these fermion fields are,

$$[c_i , c_j^+]_+ = [d_i , d_j^+]_+ = \delta_{ij} \qquad (4.3)$$

while all other pairs anti-commute amongst themselves. The use of Eq. (4.3) shows that $\varphi_i^2 = 1$, which is why the D-ons are known as drones, as they only produce the commutation rules between different sites, (Eq. (2.19)),

$$[S_i^z , S_j^{\pm}] = \pm S_i^{\pm} \delta_{ij} \; ; \; [S_i^+ , S_j^-] = 2S_i^z \delta_{ij} \qquad (4.4)$$

It is readily seen that the representation given by Eq. (4.1) satisfies these commutation rules and is also Hermitian. It will be shown later that this representation corresponds to S = ½; for the moment it will be generalized in a similar manner to the coupled-fermion representation of Chapter 3. Thus an additional subscript α (α = 1, ... , 2S) is added to each spin-half operator in the C-D fermion space giving,

$$S_i^z(\alpha) = c^+_{i\alpha}\, c_{i\alpha} - \tfrac{1}{2}, \quad S_i^+(\alpha) = c^+_{i\alpha}\, \varphi_{i\alpha} ,$$

$$\varphi_{i\alpha} = d_{i\alpha} + d^+_{i\alpha} \qquad (4.5)$$

with the complete non- vanishing anti-commutation rules,

$$[c_{i\alpha} , c^+_{j\beta}]_+ = [d_{i\alpha}, d^+_{j\beta}]_+ = \delta_{ij}\, \delta_{\alpha\beta} \qquad (4.6)$$

Moreover in terms of the vacuum state $|0>$ defined by,

$$c_{i\alpha} |0> = d_{i\alpha} |0> = 0 \qquad (4.7)$$

each site and representation is associated with a vector space $|\tfrac{1}{2}, i, (\alpha)>$ spanned by the vectors

$$|0> , \quad d^+_{i\alpha}|0> , \quad c^+_{i\alpha} |0> , \quad d^+_{i\alpha}\, c^+_{i\alpha} |0> \qquad (4.8)$$

Tensor products of these different vector space representations (all with the same vacuum state), can now be constructed to give a space for spin S ,

$$|S, i> = |\tfrac{1}{2}, i, (1) > |\tfrac{1}{2}, i, (2)> \ldots\ldots |\tfrac{1}{2}, i, (2S)> \qquad (4.9)$$

The operators in this larger space are merely the sum of the individual spin ½ operators at each site,

$$S_i^z = \sum_{\alpha=1}^{2S} (c^+_{i\alpha}\, c_{i\alpha} - \tfrac{1}{2}) , \quad S_i^+ = \sum_{\alpha=1}^{2S} c^+_{i\alpha}\, \varphi_{i\alpha} \qquad (4.10)$$

Now all the individual components are vector spin operators, then ipso facto, the spin commutation rules Eq. (4.4) are preserved. (This may be checked directly). In this representation all fermion states can be grouped to form eigenstates of the same $\underline{S}^2$ and different values of m i.e. $| S,M >$.

In general, one can evaluate all the eigenstates for a given S value by finding all the different fermion states corresponding to $| S, -S >$ and then construct the remainder by repeatedly using the raising operator S^+ on each, using the equation,

$$S^+ |S,m> = \sqrt{(S - m)(S+ m+1)}\, |S,m+1> \qquad (4.11)$$

This will exhaust the complete set of c - d operator states in the form of 2^{2S} independent spin equivalent series. It is then found that the root co-efficient in Eq. (4.11) (which is a direct consequence of the general spin commutation rules) is merely the required normalization of the states in the new representation.

(4.3) A Wick's Theorem for S = ½.

For S = ½, there is only one representation for each site, so that there are only 3 operators in this space, namely, 1, c_i^+ and d_i^+ which can act on the vacuum state. This generates a complete double representation of the spin - half eigenstates (dropping the site label i for the present) $|\frac{1}{2}, \pm\frac{1}{2}>$ as can easily be verified.

So,

$$|\tfrac{1}{2}, -\tfrac{1}{2}> \; = \; |0> \qquad \text{or } d^{+}|0>$$

and

$$|\tfrac{1}{2}, +\tfrac{1}{2}> \; = \; c^{+} d^{+}|0> \quad \text{or } c^{+}\,|0> \qquad (4.12)$$

Using the notation of section (3.5) for $S = \frac{1}{2}$, a simple Wick theorem for the spin operators in this representation will now be demonstrated.

In evaluating a trace in the spin-space and C- space (including the D-ons) of any product of spin operators $X(S)$, a mere double- overcounting will occur, for all the states in the C- space correspond to spin states, and are orthonormal one to another, so,

$$Z_s^o \; = \; \tfrac{1}{2} \; . \; Z_c^o \qquad (4.13)$$

Similarly for <u>any</u> product of spin operators,

$$\mathrm{Tr}_s \; (e^{-\beta\,\omega_o S^z} \; X(S) \;) \; = \tfrac{1}{2}\,\mathrm{Tr}_c \; (e^{-\beta\omega_o S^z} \; X(S) \;) \qquad (4.14)$$

where the operators in the R.H.S. take their fermion forms, Eq. (4.1). So upon dividing Eq. (4.13) and using the notation of Eq. (3.98) for the definition of a thermal average in the interaction representation, one has,

$$< X\,(S) >_o^s \; = \; < X\,(S) >_o^c$$

If this is compared with Eq. (3.99) one can see an advantage of this representation immediately, namely, there is no need for any normalization factor like Y . This is very useful in many-spin problems. Moreover, the D-ons have very simple properties which are also useful in any Quantum Field Theory approach. Once more, the resulting Wick's theorem is straight-forward, after an equivalence relation like Eq. (4.15) has been established. (See discussion after Eq. (3.100)).

In the interaction representation with the simple Zeeman- like Hamiltonian, Eq. (2.35) the "temperature" dependence of the fermions fields is simply (c.f. Eq. 3.54),

$$c^+(\tau) = e^{H_0\tau} c^+ e^{-H_0\tau} = e^{\omega_0\tau} c^+ ; \quad \varphi(\tau) = \varphi \tag{4.16}$$

The τ - dependence of the D- ons is merely to order them under the Wick operator Tw.

Thus,

$$< c_i \, c_j^+ >_0 = \delta_{ij} f^- \; ; \quad < d_i \, d_j^+ >_0 = \tfrac{1}{2} \delta_{ij} \tag{4.17}$$

where the simple fermi functions have been defined,

$$f^{\pm} = \left(e^{\mp \beta\omega_0} + 1 \right)^{-1} \tag{4.18}$$

In analogy to (A.15 and A.16) this enables the free (denoted by zero superscript) temperature ordered C-on and D- on (symmetrized) propagators $C^0(\tau)$ and $D^0(\tau)$ to be defined ($\eta = -1$),

$$\begin{aligned} C^0_{ij}(\tau) &= < \mathrm{Tw}\,(c_i(\tau) \, , \, c_j^+(0) \,) >_0 \\ &= \delta_{ij} e^{-\omega_0\tau} (\theta(\tau) f^+ - \theta(-\tau) f^-) \end{aligned} \tag{4.19}$$

and $D^0_{ij}(\tau) = < \mathrm{Tw}\,(\varphi_i(\tau), \varphi_j(0) >_0 = \delta_{ij} (\theta(\tau) - \theta(-\tau))$

The C- on propagator can be represented diagrammatically by a directed wavy-line from the point τ' to the point τ and the D- on propagator, by an undirected checked - line between τ and τ' (Fig. 1 (a) and (b)). The propagator of most interest in spin problems is the spin- flip propagator Eq.(2.31), which in the free case, is represented by a parallel pair of C- on and D- on lines (Fig. 1 (c)) ,

$$F^{o}_{ij}(\tau) = \langle T(S^{-}_{i}(\tau), S^{+}_{j}(o))\rangle^{s}_{o} = \delta_{ij}C^{o}(\tau)D^{o}(\tau) \qquad (4.20)$$

This well illustrates the nature of the drone propagator, for it converts the fermion properties ($\eta = -1$) of the C- on to "boson - like" properties ($\eta = 1$), as one requires for spin - waves, for example. The term "boson - like" is used to indicate that the spins obey commutation rules rather than anti-commutation rules (C.1). These functions also have simple Fourier series transforms (A.35 - 40) defined by,

$$C^{o}(\tau) = \beta^{-1}\sum_{\nu} e^{-i\bar{\nu}\tau} C^{o}(\bar{\nu}) \; ; \quad C^{o}(\bar{\nu}) = (\omega_{o} - i\bar{\nu})^{-1} \qquad (4.21)$$

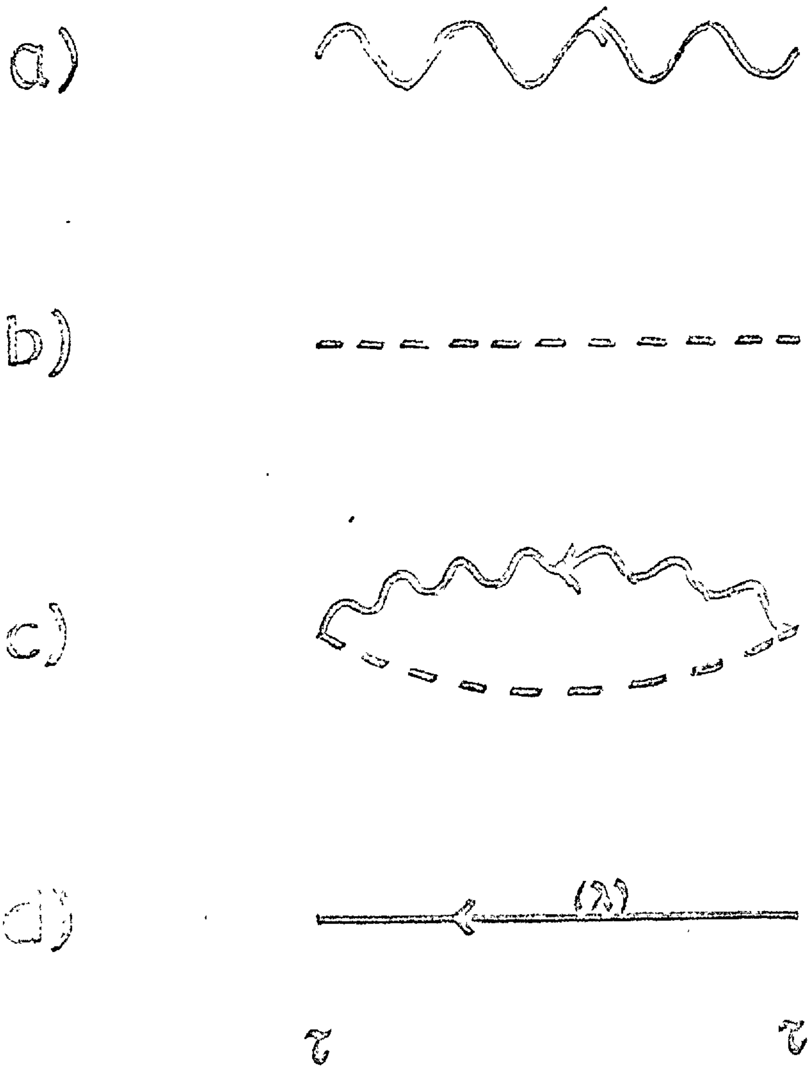
and

$$D^{o}(\tau) = \beta^{-1}\sum_{\nu} e^{-i\bar{\nu}\tau} D^{o}(\bar{\nu}) \; ; \quad D^{o}(\bar{\nu}) = -2\,(i\bar{\nu})^{-1} \qquad (4.22)$$

Similarly for the bose-like ($\varepsilon = \alpha$) propagator, with

$$F^{o}(\bar{\alpha}) = \frac{\tanh(\frac{1}{2}\beta\omega_{o})}{\omega_{o} - i\bar{\alpha}} = \frac{-2\,\langle S^{z}\rangle_{o}}{\omega_{o} - i\bar{\alpha}} \qquad (4.23)$$

FIG. 1.



This could have been anticipated from Eq. (2.38) N. B. $F^{o}(\bar{\alpha})$ is not defined for $\omega_o = 0$, unless it can be non-vanishingly renormalized, although $F^{o}(\tau)$. is well defined (in fact, $\frac{1}{2}$).

(4.4) A Wick's Theorem for S = 1.

In order to demonstrate the Wick theorem for S = 1 the complete set of states for S = 1 are needed. In this case there are four independent operators "c_1^+, c_2^+, d_1^+, d_2^+".(The site label will be dropped for the present) so one can construct from them all possible non-zero combinations operating on the vacuum state (remembering all destruction operators on this state vanish). The four independent sets which are both normalized and satisfy Eq. (4.11) are listed in Table 1, (P.72). In order to preserve the sign of these vectors (as the operators are fermions) the following convention for their normal order is adopted: The smallest D-on operator acts first on the vacuum state (furthest to the R.H.S.) followed by its corresponding C-on (if present), then the next lowest D-on and its C-on etc. up to the highest numbered C-on on the L.H.S. It is at this stage one can see the difficulty of deriving a general Wick theorem for finite temperature averages, as some of these states are only present in linear combinations and so have different normalization factors. This means there cannot be a general correspondence between a trace over spin states and a trace over C-on(and D-on) states. This difficulty can be avoided for the case of S = 1 by noting that the "under-weight" states only occur for $m = 0$. Now both the individual states and their linear combinations (i.e. true spin states) possess the crucial property $< c \mid S^z \mid c > = 0$. Thus a trace over the spin states of functions of S^z (which involves no constants before transforming to C, D-ons, and denoted $X(S^z)$) only picks up the contributions from $m = \pm 1$, which are over-counted 4 times (the independent series - 4 in this case) in the sum over the equivalent C-on and D-on states. Thus (c.f. Eqs. (3.95) and (4.14)

$$\mathrm{Tr}_s\, X(S^z) = \tfrac{1}{4}.\ \mathrm{Tr}_c X(S^z) \tag{4.24}$$

in an obvious notation, and the operators on the R.H.S. take their c- d forms. This zero contribution from linear functions of S^z however, cannot be invoked for constants which are diagonal in these extra states; the equivalent statement to Eq. (4.24) is,

$$\mathrm{Tr}_s\, 1. = \tfrac{1}{4}.\ \mathrm{Tr}_c\, 1. - 1 \ . \tag{4.25}$$

The correspondence exhibited in Eq. (4.25) is also true for exponential functions of S^z. This is particularly so for the case of the partition function Z^o, evaluated in the interaction representation of the two spaces. In the same notation as section (3.5), the appropriate equation is then,

$$Z_S^o = \tfrac{1}{4} Z_C^o - 1 \ , \tag{4.26}$$

with (4.27)

$$Z_c^o = 4.\,(e^{\beta\omega_o} + e^{-\beta\omega_o} + 2) = 4.(e^{\beta\omega_o} + 1)(e^{-\beta\omega_o} + 1)$$

This latter factorization is crucial to the whole argument for it helps to cancel out the fermi factors Eq. (4.18). Moreover the factor of ½ in the C-on form of S^z is just sufficient to introduce an inverse bosefactor (Eq(3.66)) in the $< S^z >^c_o$ type averages. This eventually will relate the fermion-like anti-commutation rules of the C-ons with the "boson-like" commutation rules of the actual spin operators for S =1.

Now, as can be checked by either explicit calculation, or cycling one of the C-ons around the trace (see later), one has,

$$\mathrm{Tr}_c (e^{-\beta\omega_o S^z} c^+_\alpha c_\alpha) = 4 (1 + e^{-\beta\omega_o}) \qquad (4.28)$$

So, upon defining averages with respect to the C-D space, by;

$$< c^+_\alpha c_\alpha >^c_o = (Z^c_o)^{-1} \mathrm{Tr}_c (e^{-\beta\omega_o S^z} c^+_\alpha c_\alpha) = f^- (\tfrac{1}{2} \omega_o) \qquad (4.29)$$

using Eq. (4.29) and after using Eq. (4.10) for S= 1, with the spin operators represented by their C-D form, one obtains,

$$< S^z >^c_o = 2 (e^{\beta\omega_o} + 1)^{-1} - 1 = \frac{1 - e^{\beta\omega_o}}{1 + e^{\beta\omega_o}} = \mu \frac{1 - e^{\mu\beta\omega_o}}{1 + e^{\mu\beta\omega_o}} \qquad (4.30)$$

In the last form, the compact notation $\mu = \pm 1$ has been introduced for later use. The magnetization in the two spaces can now be related,

$$\begin{aligned} < S^z >_o^s &= (Z_s^o)^{-1} \cdot \mathrm{Tr}_s(e^{-\beta\omega_o S^z} S^z) \\ &= (4Z_s^o)^{-1} \cdot \mathrm{Tr}_o(e^{-\beta\omega_o S^z} S^z) \end{aligned} \qquad (4.31)$$

Then multiplying and dividing by Z_o^o and using Eq. (4.29), this introduces the normalization factor $Y(\omega_o)$,

$$< S^z >_o^s = Y \cdot < S^z >_o^o \qquad (4.32)$$

where

$$Y(\omega_o) = Z_o^o \ (4Z_s^o)^{-1} = (f^+f^- Z_s^o)^{-1} \qquad (4.33.)$$

Moreover for S = 1, one can always use the following closure relations for products of S^z, ("n" is any integer)

$$(S^z)^{2n+1} = S^z \quad \text{or} \quad (S^z)^{2n} = (S^z)^2$$

So any polynomial in S^z, $X(S^z)$ also satisfies

$$< X(S^z) >_o^s = Y \cdot < X(S^z) >_o^o \qquad (4.34)$$

This is the equation which restricts the proof to S = 1 and S = ½, in the latter case $Y = 1$, (see Eq. (4.15)).

The next stage of the proof is to generalize this to products of the raising and lowering operators S (remembering $\mu = \pm 1$). So, on re-writiong Eq. (4.4), for one site, in the useful form

$$[S^{\mu}, S^{-\mu}] = 2\mu S^z \quad \text{and} \quad [S^z; S^{\mu}] = \mu S^{\mu} \qquad (4.35)$$

Since spin averages are diagonal in S^z, there must be an equal number of S^μ and $S^{-\mu}$ operators. The general proof is inductive so one starts out with the simplest products $< S^+ S^- >_o^s$ or $< S^- S^+ >_o^s$ and uses the property of cyclically transferring the operators around the trace, as in (A.10) and using,

$$e^{\lambda S^z} S^\mu e^{-\lambda S^z} = e^{\lambda\mu} S^\mu \qquad (4.36)$$

then finally commuting them back to their usual position in the product. The final result is,

$$< S^\mu S^{-\mu} >_o^s = \frac{2\mu < S^z >_o^s}{1 - e^{\mu\beta\omega_o}} \qquad (4.37)$$

This approach can be equally well applied to the spin operators in their C-D form since the trace now covers the complete representation of the C-D states and so maintains the crucial cyclic property, so immediately,

$$< S^\mu S^{-\mu} >_o^c = \frac{2\mu < S^z >_o^c}{1 - e^{\mu\beta\omega_o}} \qquad (4.38)$$

Upon multiplying by the factor Y and using Eq. (4.32), then,

$$< S^\mu S^{-\mu} >_o^s = Y < S^\mu S^{-\mu} >_o^c \qquad (4.39)$$

The same argument is used for the next product, so,

$$< S^{\mu} S^{-\mu} S^{z} >_{o}^{s} = \frac{2\mu \quad <(S^{z})^{2} >_{o}^{s}}{1 - e^{\mu\beta\omega_o}} + \frac{< S^{\mu} S^{-\mu} >_{o}^{s}}{1 - e^{-\mu\beta\omega_o}} \qquad (4.40)$$

There is an identical result for $< S^{\mu} S^{-\mu} S^{z} >_{o}^{c}$ but now all the averages on the R.H.S. are just replaced by C-on averages $< \; >_{o}^{c}$, but from Eq.s (4.34) and (4.39), each of these is related to a spin - space average like $<>_{o}^{s} = Y < \; >_{o}^{c}$, so,

$$< S^{\mu} S^{-\mu} S^{z} >_{o}^{s} = Y < S^{\mu} S^{-\mu} S^{z} >_{o}^{c} \qquad (4.41)$$

Similarly it can be shown that a product of n spin operators can be reduced to ones involving (n - 1) spin operators. Then the rest of the proof is simply inductive, so need not be stated here; this immediately leads to the crucial result for a general product of spin-one operators,

$$< X (S^{\mu} , S^{-\mu} , S^{z}) >_{o}^{s} = Y < X(S^{\mu}, S^{-\mu}, S^{z}) >_{o}^{c} \qquad (4.42)$$

where the operators on the R.H.S. take their C-D form for $S = 1$, Eq. (4.10). The corresponding result for a product of spin operators referring to N different sites is to convert Y to Y^{N} on the R.H.S. of Eq. (4.42)

TABLE 1 .

The Spin States	The Equivalent C-on , D-on States .			
	1	2	3	4
1,-1	1	d_1	d_2	$d_2\ d_1$
1, 0	$2^{-1/2}(c_2d_2+c_1d_1)$	$2^{-1/2}(c_1+c_2d_2d_1)$	$2^{-1/2}(c_2+d_2c_1d_1)$	$2^{-1/2}(c_2d_1+d_2c_1$
1, 1	$c_2d_2c_1d_1$	$c_2d_2c_1$	$c_2c_1d_1$	$c_2\ c_1$

The four independent sets of C-on , D-on states for one site corresponding to the three spin states $| S , m >$ for $S = 1$ and $m = \pm 1 , 0$. Each is to be interpreted as a creation operator (in the same order) acting on the vacuum state $| 0 >$.

Chapter 5.

THE CONDUCTION-ELECTRON LOCALIZED MOMENT INTERACTION.

(5.1) The Interaction Hamiltonian.

The model considered in this chapter will be one where the conduction electrons in a metal of N well - localized atoms (in a periodic lattice) interact with n magnetic atoms. Three cases will be considered. In the next 3 sections dilute alloys with non - interacting impurities ($n \ll N$) will be considered, then the case of interacting impurities ($n < N$) and finally the periodic lattice ($n = N$) or rare - earth metals.

A phenomenological approach is taken here, rather than an attempt to show the equivalence between the present s - d (or s - f) Hamiltonian and some other model, as was done in section (3.3) with the Anderson Hamiltonian. However, such an exchange Hamiltonian is expected to be a good approximation in the case of the rare - earths (Doniach,84) de Gennes),30) for in these isolated atoms the 4-f shells are known to be very tightly bound and well - localized. Moveover, in their metallic state these bands are far below the conduction bands, so their behaviour can be expected to be well described by only their angular momentum degrees of freedom. In S - state ions such as Gd, this will reduce to using only their spin vectors $\underline{S}$. In a non S- state ion the J states will be sufficient to describe the dynamics of the magnetic ion.

Consequently, a general exchange Hamiltonian H_1 is introduced which is assumed to well describe the dynamics of the many - body system. This will be taken to be of the form of an interaction of strength J $(\underline{x})$ between the spin-density of the conduction electrons $S_e(\underline{x})$ (section (2.4)) and the spin - density of the magnetized ions $S(\underline{x})$, so that

$$H_1 \quad = \quad -2 \iint d^3 x \, d^3x' J \, (x - x') \, \underline{S}_e \, (x) \, \underline{S} \, (x') \qquad (5.1)$$

For well - localized f - shell electrons on the magnetic ions the spin - density for n spins is taken to be

$$\underline{S}(x) \quad = \quad N^{-1} \sum_{j=1}^{n} \underline{S}_j \; \delta(\underline{x} - \underline{R}_j) \qquad (5.2)$$

If both the electron - spin density and the range function are Fourier transformed with respect to the inverse lattice vectors (Eq. (2.49)), so that

$$J \, (\underline{x}) \quad = \quad \sum_{q} J_q \, e^{i\underline{q}\cdot\underline{x}} \quad \text{with} \ \sum_{q} e^{i\underline{q}\cdot\underline{x}} = \text{Vol} \quad \delta \, (\underline{x}) \qquad (5.3)$$

If Eq.'s (5.2) and (5.3) are used in Eq. (5.1) with the identity

$$\text{Vol.}^{-1} \int d^3x \; e^{i(\underline{q}-\underline{q}')\cdot\underline{x}} \; = \; \delta_{qq'} \qquad (5.4)$$

the general form of the interaction is then obtained

$$H_1 \quad = \quad -N^{-1} \sum_{qj} J_q \; \underline{\sigma}_q \cdot \underline{S}_j \quad e^{-i\underline{q}\cdot\underline{R}_j} \qquad (5.5)$$

The term $e^{-i\underline{q}.\underline{R}_j}$ appears in the function $\rho(q)$ which is the Fourier transform of the spatial distribution of the magnetic ions $\rho(\underline{x})$, where

$$\rho(\underline{x}) = \sum_{j=1}^{n} \delta^3(\underline{x} - \underline{R}_j) \qquad (5.6)$$

so

$$\rho(q) = \sum_{j=1}^{n} e^{-i\underline{q}.\underline{R}_j} \qquad (5.7)$$

In ge neral , it is difficult to evaluate any results with the general form J_q, so this is always approximated by a constant co - efficient $J_q = J$. Thisis equivalent to restricting $J(\underline{x})$ to a point contact model $J(\underline{x}) = \text{Vol.}\, J\, \delta^3(\underline{x})$ or that all overlaps of the f - shell electrons with neighbouring magnetic ions are small. Finally, the constant J is taken to be a fundamental parameter of the model and is found from experimental checks on the resulting theories. Finally, if there is also an extra spin independent potential (e.g. direct Coulomb interaction) $V(\underline{x})$ this will give an extra term in the Hamiltonian H_V, where

$$H_V = \int d\,\underline{x}\; \Psi^+(\underline{x})\, V(\underline{x})\Psi(\underline{x}) = \sum_{pq\lambda} V_q\, a^+_{p\lambda} a_{p-q\,\lambda} \qquad (5.8)$$

This will merely affect the lowest order Green's function for the electrons Eq. (3.64) to give a correction (dropping the spin index, λ)

$$G^{(v)}_{pp'}(\bar{\tau}) = \int_0^\beta d\tau_1\; V_{p-p'}\, G^o_p(\tau-\tau_1)\, G^o_{p'}(\tau_1-\tau') \qquad (5.9)$$

This can be completely re - summed (at least, formally) in terms of the mass - operator $M^{V}(\tau)$ or its transform

$$M^{V}_{pp'}(\nu) = V_{p-p'} \tag{5.10}$$

The corresponding Dyson equation is then

$$G^{V}_{pp'}(\bar{\nu}) = G^{0}_{pp'}(\bar{\nu}) + \sum_{qq'} G^{0}_{pq}(\bar{\nu})\, M^{V}_{qq'}(\bar{\nu})\, G^{V}_{q'p'}(\bar{\nu}) \tag{5.11}$$

The formal solution of this equation in terms of the inverse matrix in the momentum representation is

$$G^{V}_{pp'}(\bar{\nu}) = \left(\delta_{pp'} - G^{0}_{p}(\bar{\nu})\, V_{p-p'}\right)^{-1} G^{0}_{p'}(\bar{\nu}) \tag{5.12}$$

This is exactly solvable in the simple case of a constant range interaction, or $V_q = V\,\delta_{qo}$ then

$$G^{V}_{pp'}(\nu) = \frac{\delta_{pp'}}{G^{0}_{p}(\bar{\nu})^{-1} - V} = \delta_{pp'}\,(\xi_p - V - i\bar{\nu})^{-1} \tag{5.13}$$

Thus, such a spin - independent potential can be accurately accounted for by just a change in the Fermi level $\mu \to \mu + V$. However, in more realistic cases of an $\underline{x}$ - dependent potential this cannot be done so readily. No striking effects of such potentials are expected, in contrast to the spin - dependent case (as will be seen) where the dynamical degree of internal freedom of $\underline{\underline{S}}$ can lead to quite unexpected results.

(5.2) Low - order Corrections in Dilute Alloys.

The case of dilute alloys well illustrates the effect of coupling two relatively simple systems. In the present model calculation interference effects between different magnetic atoms are neglected, (so the concentration of impurities $c = \frac{n}{N}$ is very small). Even so, high temperature susceptibility measurements verify that the magnetic moment on rare - earth atoms still persists when in dilute solutions, in other non - magnetic rare - earths (e.g. La, Lu, Y), or in noble metal solvents. The case of the transition metals (Mn, Fe, Co) in noble metal solvents is less clear - cut, for, although a magnetic moment still persists , there are no integral (or half integral) S or J values, so the localized moment model cannot be expected to be so good for these metals as for the rare - earth alloys.

Since interference effects will be assumed negligible (however, see section (5.5)) only one impurity will be considered, and its location will define the co - ordinate origin. Edwards' averaging process[89)] will then be used to introduce the concentration dependence of the resulting effects.

The Hamiltonian for this model has been introduced earlier in section (3.4), where it is written in terms of the Wannier operators at the origin . The spinor form is Eq. (3.59), in terms of the drone - fermion representation for spin - ½ , Eq. (4.1) ; this becomes

$$H_1 = -J\left[\left(c^+ \varphi\, a_-^+ a_+ + \varphi\, c\, a_+^+ a_- + \sum_\lambda \lambda (c^+ c - \tfrac{1}{2})\, a_\lambda^+ a_\lambda \right)\right] \tag{5.14}$$

The diagonal part of the Hamiltonian is still given by Eq.(3.52) or

$$H_0 = \sum_{p\lambda} \xi_{p\lambda} \, a^+_{p\lambda} a_{p\lambda} + \omega_0 \left(c^+ c - \tfrac{1}{2} \right) \quad (5.15)$$

The Wannier Green's function (at the origin) is defined by Eq.s (3.62) and (3.64) and its transform by Eq. (3.68). The C -on and D -on propagators are defined as in Chapter 4, viz. Eq.s (4.19), as is the spin - flip propagator F by Eq.s (4.20).

For convenience the g factors of the conduction electrons and of the localized moment will be taken to be equal; moreover, the constant density of states model for the conduction electrons will always be used,

$$\rho(\omega) = \pi^{-1} \text{Im. } G^0_\lambda (\omega + is) = \rho \text{ only if } -D < \omega - \tfrac{1}{2}\omega_0 < D \quad (5.16)$$

Although only one magnetic impurity is present , the d operators must be retained throughout the calculation. In the evaluation of the Green's functions, by equations like (A.28), the transformed interaction Hamiltonian must be bose-like, for the substitution of the Wick - ordering operator in the development operator ((A.23) and (A.27)) for the Dyson - ordering operator, is only valid for even - order products of fermion operators. The usual fermion form of temperature perturbation theory (Appendix A) can now be applied to the Hamiltonian given by Eq.s (5.14 - 15), using the usual diagrammatic rules (Abrikosov et al).[18] The interaction vertices corresponding to Eq. (5.14), are illustrated in Fig.(2). The one - electron properties (for nth - order scattering off the impurity) are evaluated in terms of the effective potential $V_\lambda^{(n)}(\tau)$ defined by the criterion that this part of the graph is irreducible (between the n vertices) with respect to any one electron line. This differs from Doniach's effective potential, where the contributions diagonal in the combined spin of the impurity, and of one electron, are chosen. This is convenient in the case when no external field is present, as it leaves the Hamiltonian rotationally invariant. Thus the perturbation terms represented by Figs. (3a and 3b) give the total first order contribution

$$V_\lambda^{(1)}(\tau_1 - \tau_2) = \lambda J \left(\langle c^+ c\rangle_0 - \tfrac{1}{2}\right) \delta(\tau_1 - \tau_2) = \lambda J \langle S^z\rangle_0 \delta(\tau_1 - \tau_2) \tag{5.17}$$

Its (odd - periodic) Fourier series transform is therefore

$$V_\lambda^{(1)}(\bar{\nu}) = \lambda J \langle S^z\rangle_0 \tag{5.18}$$

This is the expected first - order field - splitting of the two spin bands which vanishes as the field decreases to zero, c.f. Eq. (3.89).

When one considers the second - order effects Fig. (3c and 3d), one can immediately appreciate the dynamics of the situation, as the graphs show explicitly which terms in the Hamiltonian are contributing in each case. For example in Fig. (3c) the electron is scattering longitudinally and

FIG. 2.

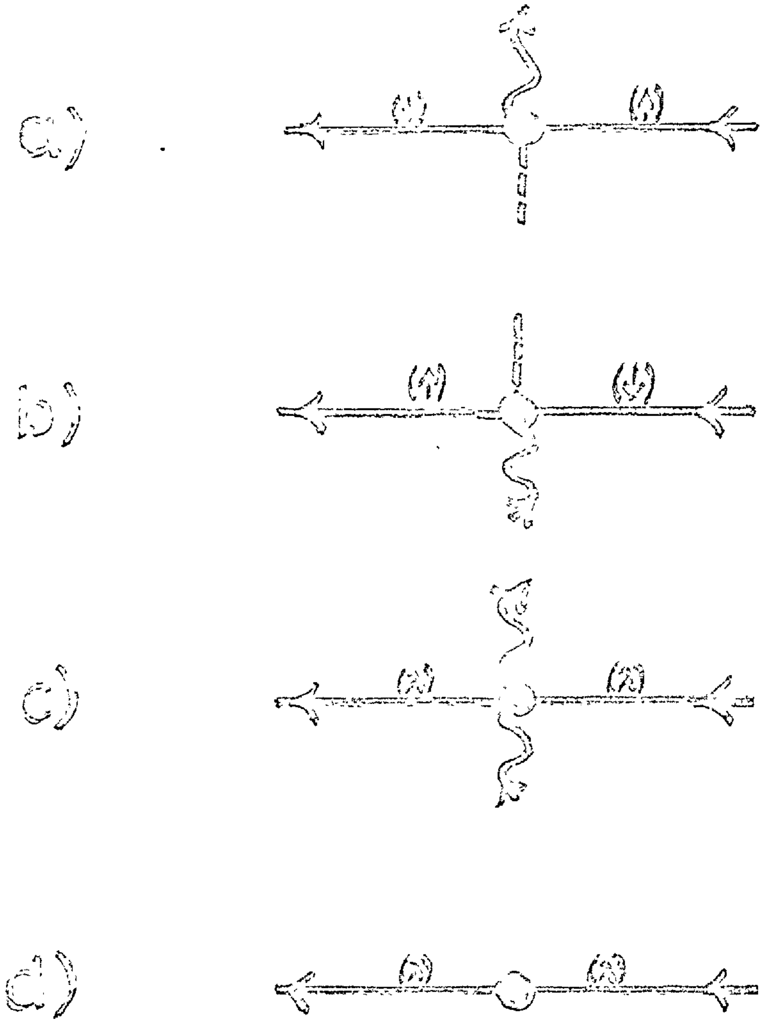
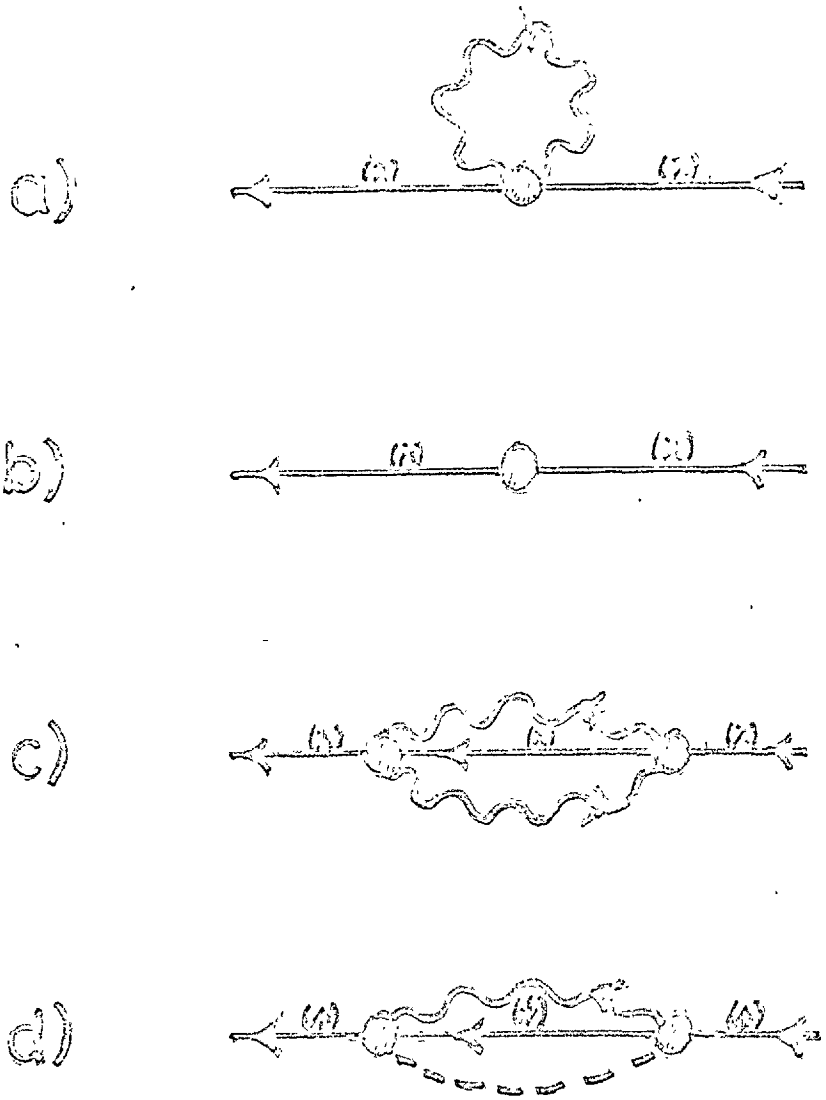


FIG. 3.



coherently off the impurity ; in contrast to the second order reducible graph, when the scattering is incoherent (i.e. the two spin averages are quite independent; see later). The contribution of this coherent graph is:

$$V_{\lambda}^{(2L)}(\tau) = -J^{2} G_{\lambda}^{o}(\tau)\, C^{o}(\tau)\, C^{o}(-\tau) = -J^{2} f^{+} f^{-} G_{\lambda}^{o}(\tau) \qquad (5.19)$$

Similarly Fig. (3d) corresponds to transverse coherent scattering, with the excitation of a spin - flip (or spin - wave, in a lattice) in the intermediate state. Its contribution is

$$V_{\lambda}^{(2T)}(\tau) = J^{2}\, G_{-\lambda}^{o}(\tau)\, F^{o}(\lambda\tau). \qquad (5.20)$$

The transform becomes

$$V^{(2)}(\bar{\nu}) = \frac{J^{2}}{N} \sum_{p} \frac{\left(f^{+} f^{-} + f^{\lambda} f^{+}_{p,-\lambda} + f^{-\lambda} f^{-}_{p,-\lambda} \right)}{\xi_{p,\lambda} - i\bar{\nu}} \qquad (5.21)$$

This form exhibits the symmetry due to the choice $g_e = g_s$. Using the constant density - of - states for the electrons one can write down the analytic continuation of this quantity (i.e. $\omega = i\bar{\nu}$) just above and below the real ω-axis.

$$V^{(2)}(\omega \pm is) = \rho J^{2} \int_{\mu - D}^{\mu + D} dE\, \frac{\left(f^{+} f^{-} + f^{\lambda} f^{+}_{-\lambda}(E) + f^{-\lambda} f^{-}_{-\lambda}(E) \right)}{E + \frac{\lambda\omega_{o}}{2} - \mu - \omega \mp is}$$

(5.22)

Thus, the absorbtive part is given by

$$\text{Im.}\ V_{\lambda}^{(2)}(\omega \pm is) = \pm\, \pi \rho J^{2}(f^{+}f^{-} + f^{\lambda}\, f^{-\lambda}(\omega_o - \lambda\omega) + f^{-\lambda}\, f^{\lambda}(\omega_o - \lambda\,\omega)). \tag{5.23}$$

where the following identity has been used

$$\frac{1}{x \mp is} = \frac{\text{Pr.}}{x} \pm i\,\pi\,\delta(\,x\,).$$

This can be considered in several limits, for example, in zero magnetic field one has (Subscript zero for $h^z = 0$).

$$\text{Im.}\ V_{o}^{(2)}(\omega \pm is) = \pm\, \tfrac{3}{4}\, \pi\, \rho\, J^{2} \tag{5.24}$$

This is essentially Abrikosov's[10)] lowest order result, for spin - disorder scattering, since for $S = \tfrac{1}{2}$, $S(S+1) = \tfrac{3}{4}$, so exhibiting the rotational invariance. Similarly, for the real part,

$$\text{Re.}\ V_{o}^{(2)}(\omega) = \tfrac{3}{4}\, \rho J^{2}\ \text{ln.} \left| \frac{D - \omega}{D + \omega} \right| \tag{5.25}$$

In fact, one could have anticipated this result from Eq. (5.21)

$$V_{o}^{(2)}(\omega) = \tfrac{3}{4}\ J^{2}\ G_{o}^{o}(\,\omega\,) \tag{5.26}$$

In the same manner one can calculate the first and second - order corrections to C (τ) and D (τ), whose self - energy parts are denoted by $\Sigma\ (\tau)$ and $\Lambda\,(\tau)$ respectively. The evaluation of Σ itself will give the magnetization; the first order result Fig. 4 (a) merely involves the electronic magnetisation ζ ., Eq. (3.76) and (3.75).

i.e.
$$\Sigma(\bar{\nu}) = 2J\zeta^{o} = -\rho J \omega_{o} \qquad (5.27)$$

No self - consistent soln's (i.e. molecular field) for $\Sigma^{(1)}$ and $V^{(1)}$ when $h^{z} = 0$ can be found, as expected,(contrary to the case when there are interacting impurities, when the Curie temperature is finite).

When $\Sigma^{(2)}$ is evaluated the first order corrections on the first - order internal electron lines must not be forgotten, (Fig. 4 (b i,ii)), as these give a large contribution, which can-cel exactly with parts of the other second-order graphs, involving the excitation of an electron-hole pair (Fig. 4 b iii, iv).

$$\Sigma^{(2I)}(\tau) = -J^{2}\, C^{o}(\tau) \sum_{\lambda} G^{o}_{\lambda}(\tau)\, G^{o}_{\lambda}(-\tau) ; \Sigma^{(2T)}(\tau) = -J^{2} D^{o}(\tau)\, G^{o}_{+}(\tau) G^{o}_{-}(-\tau) \qquad (5.28)$$

The sum total of self - energy corrections to C (τ) up to 2nd order in the usual limit of $k_B T >> \omega$ or ω_o is

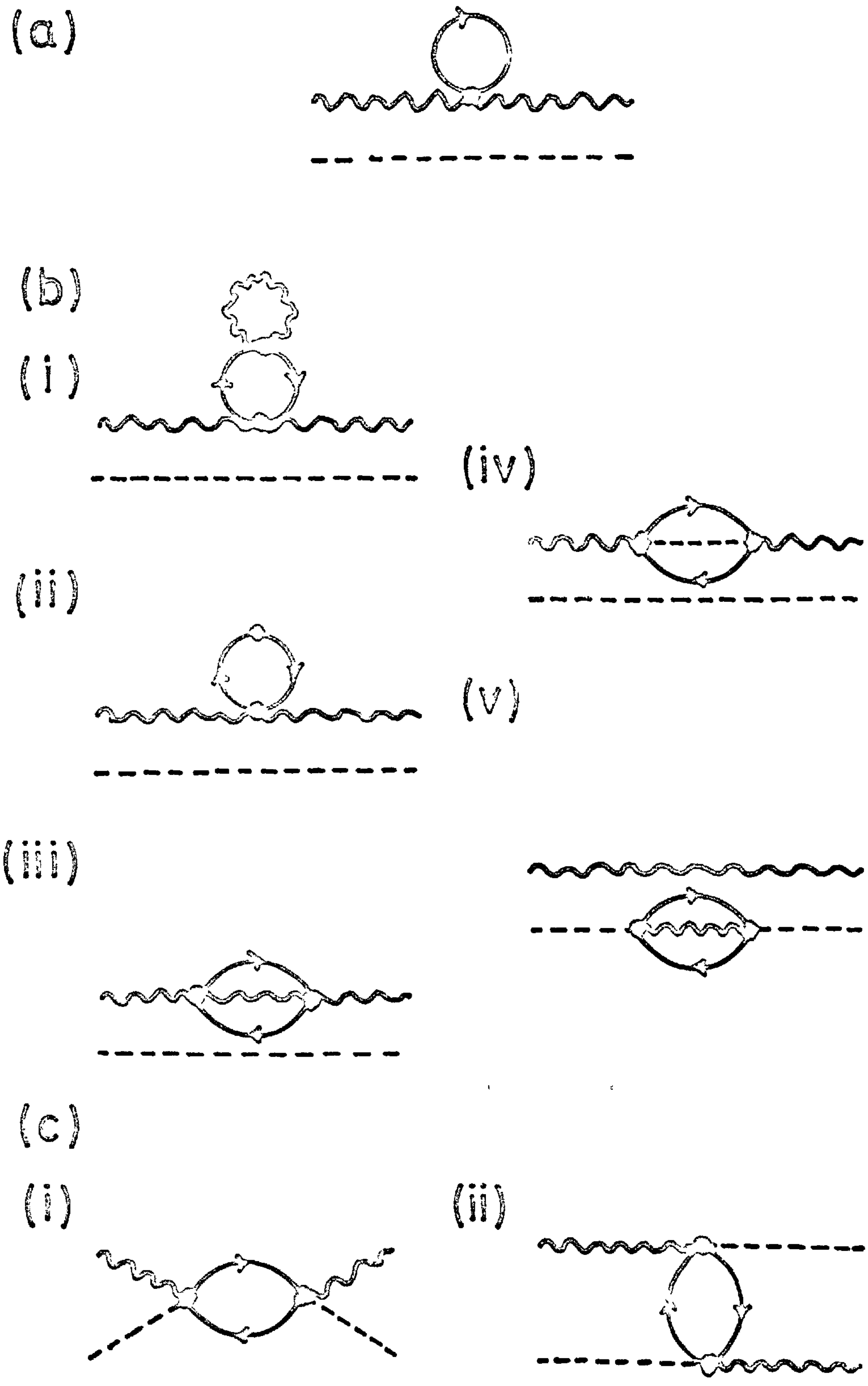
$$\Sigma^{(1+2)}(\omega \pm is) = -\rho J \omega + 4(\rho J)^{2} \left[\left(\omega - \frac{\omega_o}{2}\right)\left(1 + \ln . \frac{2\gamma\beta D}{\pi}\right) + (\omega_o - \omega) \ln . 2 \pm i\pi k_B T \right] \qquad (5.29)$$

where log γ = 0.58 is Euler's constant. So from Dyson's equation

$$C(\omega \pm is) = (\omega - \omega - \Sigma(\omega \pm is))^{-1} = (\omega_R \mp i\Gamma - \omega)^{-1} \qquad (5.30)$$

where, on the energy - shell, $\omega = \omega_o$,

FIG. 4.



$$\omega_R - i\Gamma = \omega_0\left(1 + \rho J - 2(\rho J)^2\left(1+\ln \frac{2\gamma\beta D}{\pi}\right)\right) - i4\pi(\rho J)^2 k_B T. \qquad (5.31)$$

The magnetization is obtained by replacing the sum over ν by an integral over ω on the Fermi - Dirac contour, C_f encircling the imaginary ω -axis; this is then evaluated by deforming the contour around the pole off the real axis (Appendix A.42)

$$\langle c^+ c \rangle = \frac{1}{2\pi i} \oint_{cf} \frac{d\omega}{e^{\beta\omega} + 1} C(\omega) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{d\,\omega}{e^{\beta\omega} + 1} \, \mathrm{Disc.}C(\omega) \qquad (5.32)$$

or
$$R^{(2)} + \tfrac{1}{2} = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{d\,\omega}{e^{\beta\omega} + 1} \, \frac{\Gamma}{[(\omega_R - \omega)^2 + \Gamma^2]} = \frac{1}{e^{\beta\omega_R} + 1} \qquad (5.33)$$

Thus
$$R^{(2)}(\omega_0) = -\tfrac{1}{2} \tanh\left(\frac{\beta\,\omega_R}{2}\right) \cong R^0(\omega_0)\left(1 + \rho J - 2(\rho J)^2\left(1+\ln . \frac{2\gamma\beta D}{\pi}\right)\right) \qquad (5.34)$$

Apart from the factor of one, this agrees with Yosida and Okiji's[52)] result, in second order but not in first order where they find no contribution. This latter point contradicts Nagaoka's[41)] result, unfortunately his differs from ours in a factor of 2 (after conversion to same form of J - theirs differs by a factor of two initially i.e. J Nagaoka = 2J).

The result (5.34) agrees exactly with Yosida & Miwa[50)] and with Scalapino's[25)] result for the Anderson model evaluated to second order. The D -on self-energy $\Lambda(\omega)$, (Fig. 4,(b v)) is only needed for the evaluation of the spin - flip propagator and hence the dynamic g-shift, of the localized transverse susceptibility $F(\omega)$. Eq.(2.31).

The contributions of Fig. (4 c) do not give a logarithmic temperature shift and cancel exactly (in the static limit, minus factor, due to interchange of the fermion - like D-on line) and so in the limit $\beta\,\omega \ll 1$ are neglected.

This just leaves the self - energy effects on the individual C -ons and D -ons, which then become a convolution to give $F(\tau)$:

$$F(\bar{\alpha}) = \beta^{-1} \sum_{\nu} D(\bar{\nu})\, C(\bar{\alpha} - \bar{\nu}) \qquad (5.35)$$

$$F(\omega) = \frac{1}{\pi i} \oint_{c} \frac{dz}{e^{\beta z}+1} \left((z + 2\Lambda(z))(\omega - \omega + z - \Sigma(\omega - z)) \right)^{-1}$$

(5.36)

This is deformed around the discontinuities of D and C at Im. z = 0 and Im. z = Im. ω respectively;

writing $z = z_1 + i\, z_2$, $\Lambda(z_1 + is) = \Lambda_1(z_1) + i\Lambda_2(z_1)$ etc.

$$F(\omega) = -2\pi^{-1}\int dz_1\, f^{-}(z_1)$$

$$\times [[(\omega_o - \omega + z_1 - \Sigma)^{-1} 2\Lambda_2(z_1)[(z_1 + 2\Lambda_1)^2 + (2\Lambda_2)^2]^{-1}$$

$$- (z_1 + \omega_2 + 2\Lambda)^{-1} \Sigma_2(\omega_1 - z_1)[(\omega_o - \omega_1 + z_1 - \Sigma_1)^2 + \Sigma_2^2]^{-1}]] \tag{5.37}$$

Eq. 5.37 has been written out in full to show the nature of the approximation to follow, which can only be done if the widths are small compared to $k_B T$; however this may no longer be true in higher orders, as both the real and imaginary parts of the self - energies appear to diverge in the anomalous temperature region (see later). But in simple second - order calculations there is no problem; thus taking into account the form of $\Sigma_1(\omega)$ and noting that

$$\Lambda^{(2)}(\omega \pm is) = 2(\rho J)^2 \left(\omega \left(1 + \ln. \frac{\gamma \beta D}{\pi}\right) \pm i\pi k_B T \right) \tag{5.38}$$

one can see that the first square bracket in Eq. (5.37) is strongly peaked around $z_1 = 0$ while the second peaks at $z_1 = \omega_R$

After ensuring a unique analytic continuation,

$$F(\omega) = 2f^{+}(\omega_R)[\omega_R - \omega - 2\Lambda(\omega - \omega_R)]^{-1} - [\omega_0 - \omega - \Sigma(\omega)]^{-1}$$

(5.39)

but to $O(J^2)$, near ω_R, $\Lambda(\omega - \omega_R + is) = \frac{1}{2} i\Gamma$,
so fially

$$F(\omega \pm is) = \frac{\tanh\left(\frac{\beta\omega_R}{2}\right)}{\omega_R - \omega \mp i\Gamma} \qquad (5.40)$$

There is an internal check on the correctness of Eq. (5.40) through using the sum rule for $s = \frac{1}{2}$.

$$< S^z > = \frac{1}{2} - < S^- S^+ > = R \qquad (5.41)$$

Thus

$$R = \frac{1}{2} - \frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{d\omega}{1 - e^{-\beta\omega}} \quad \text{Disc. } F(\omega).$$

(5.42)

$$\cong \frac{1}{2} - f^{-}(\omega_R) = -\frac{1}{2} \tanh\left(\frac{\beta\omega_R}{2}\right) \qquad \text{c.f.Eq.(5.34)}$$

The above results can be neatly summarized by stating that the impurity transverse susceptibility has the Lorentzian form

$$\chi^{T}_{ret.}(\omega) = \tanh(\tfrac{1}{2}\beta\,\omega_R)\,(\omega_R - \omega + i\Gamma)\,[(\omega_R - \omega)^2 + \Gamma^2]^{-1} \tag{5.43}$$

which is illustrated in Fig. 5.

(5.3) Higher order Effects.*

In this section complete sub - series of higher order graphs are summed which result in expressions evaluated to $O(J^2)$ in the (divergent) denominators. This is accomplished by calculating the self - energy parts to $O(J^2)$ of more complex propagators. This extends the work of previous authors whose results were evaluated to $O(J)$ in the denominator and also avoids the difficulties (especially $T < Tk$) which have previously arisen. Although various explicit formulae for the self - energies are obtained for finite magnetic fields, they are, in fact, evaluated in the zero field limit where rotational symmetry introduces several simplifying features. This leads to equations which are stable (see later) through the critical temperature (Tk, for the case of anti-ferromagnetic coupling, $(J < 0)$ and to a new ferromagnetic resonance $(J > 0)$ which occurs at a much lower temperature.

The first "log T" term in the electronic effective potential appears in third order $O(J^3)$ and is the first internal correction to the second - order skeleton graphs (which themselves were seen to exhibit no abnormalities, Eq. (5.26).

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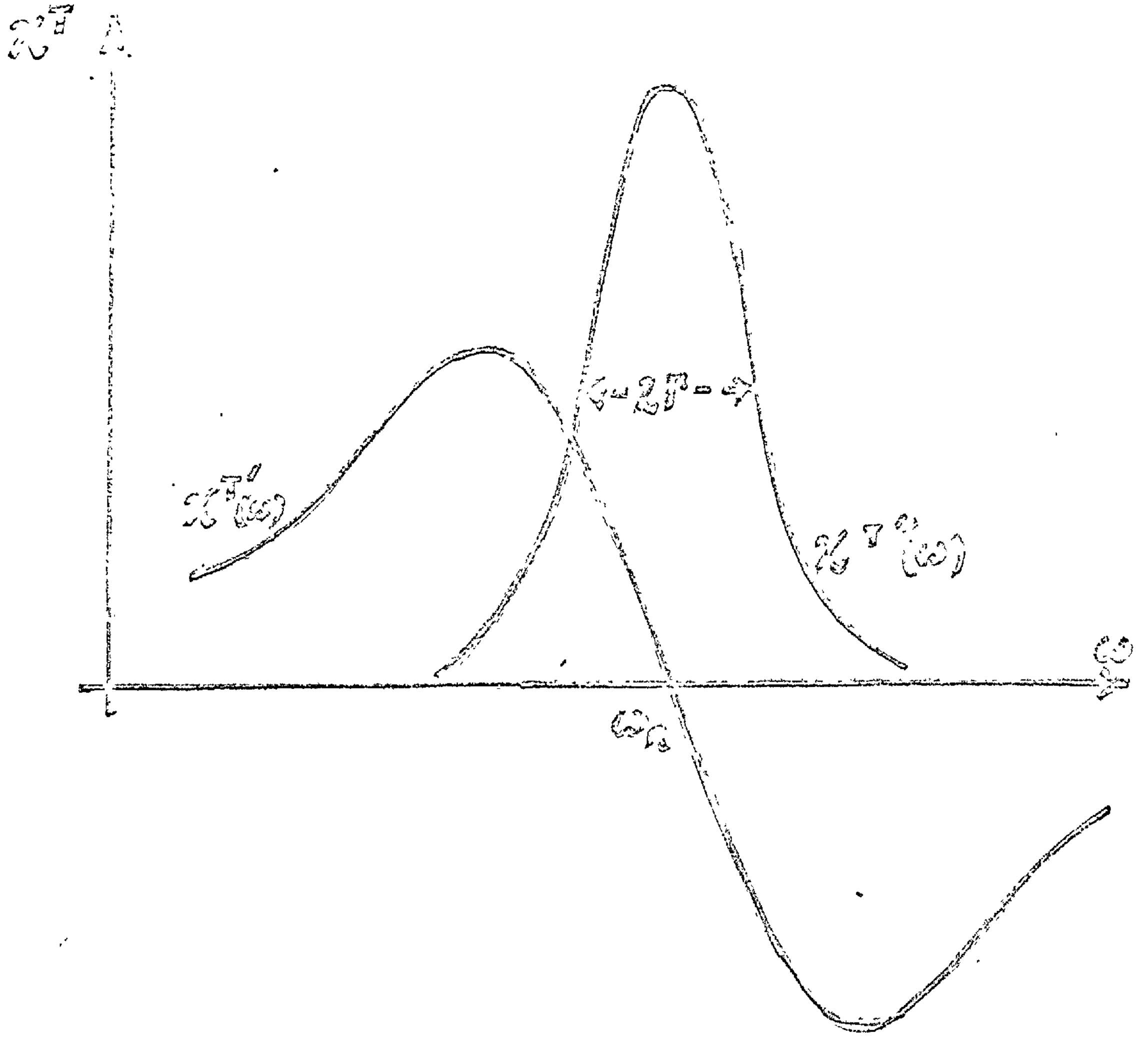
* See Addenda.

FIG. 5.


χ^H
$\chi^{H'}(\omega)$
$\leftarrow 2\Gamma \rightarrow$
$\chi^{H''}(\omega)$
ω
ω_0

This suggests that all higher order internal corrections to the simple skeleton graphs, will be divergent. So propagators are constructed from these skeletons and their own self - energy parts are constructed to $O(J^2)$. In fact, a further series of graphs is also included, arising from third - order skeleton graphs, which have the same structure as before; this maintains the correct co - efficient to $O(J^3)$ in the numerator. By considering those irreducible graphs which occur within an initial and final interaction there will always be a factor of J^2 contributed to the numerator. In practice, this means that one looks for repeated scatterings of any two internal lines, within the second - order skeleton graphs, while the third line remains unaffected from the initial to final vertex.

Physically, this 'bare' line effectively maintains the local spin (in the case of the electron self - energy) ina definite orientation with respect to the external electronic spin i. e. the spin is "polarized" between the initial and final interaction and effectively behaves as if in a magnetic field (even in the case when there is no external magnetic field, the quantization of the electronic spin direction determines that of the local spin). This agrees with Abrikosov's 10) intuitive choice of cutting only one electron line and two spin lines at any internal point, and with Silverstein & Duke. 92)

In all cases we will need the following propagators (similar to the $\Gamma(\omega)$ of Nagaoka 41) etc.) defined by

$$S^{z_o}_{\lambda\lambda'}(\tau) = G^o_\lambda(\tau)\, C^o(\lambda'\tau).$$

see Fig.6. (5.44)

$$S^{T_o}_{\lambda}(\tau) = G^o_{-\lambda}(\tau)\, D^o(\lambda\tau).$$

The Fourier series transforms (bose - like, as pair of fermions) are

$$S^{z_o}_{\lambda\lambda'}(\bar{a}) = \lambda' N^{-1} \sum_p (f^{\lambda'} f^{+}_{p\lambda} - f^{-\lambda'} f^{-}_{p\lambda})[\xi_{p\lambda} + \lambda'\omega_o - j\bar{a}]^{-1}$$

$$S^{T_o}_{\lambda}(\bar{a}) = \lambda N^{-1} \sum_p (f^{+}_{p-\lambda} - f^{-}_{p-\lambda})[\xi_{p-\lambda} - i\bar{a}]^{-1}$$

(5.45)

A longitudinal scattering matrix T is defined by

$$S^{z}_{\lambda\lambda'}(\bar{\tau}) = S^{z_o}_{\lambda\lambda'}(\bar{\tau}) + \int\int_0^{\beta} d\tau_1 d\tau_2\, S^{z_o}_{\lambda\lambda'}(\tau - \tau_1)\, T^{z}_{\lambda\lambda'}(\tau_1 - \tau_2) S^{z}_{\lambda\lambda'}(\tau_2 - \tau')$$

or

$$S^{z}_{\lambda\lambda'}(\bar{a}) = \frac{S^{z_o}_{\lambda\lambda'}(\bar{a})}{1 - S^{z_o}_{\lambda\lambda'}(\bar{a})\, T^{z}_{\lambda\lambda'}(\bar{a})} \qquad (5.46)$$

On evaluation of the graph in Fig. 7 and using Eq.s (5.45 - 6)

$$T^{z}_{\lambda\lambda}(\tau) = \lambda J\, \delta(\tau), \quad \text{so} \quad S^{z}_{\lambda\lambda}(\bar{a}) = \frac{S^{z_o}_{\lambda\lambda}(\bar{a})}{1 - \lambda J\, S^{z_o}_{\lambda\lambda}(\bar{a})} \qquad (5.47)$$

FIG. 6.

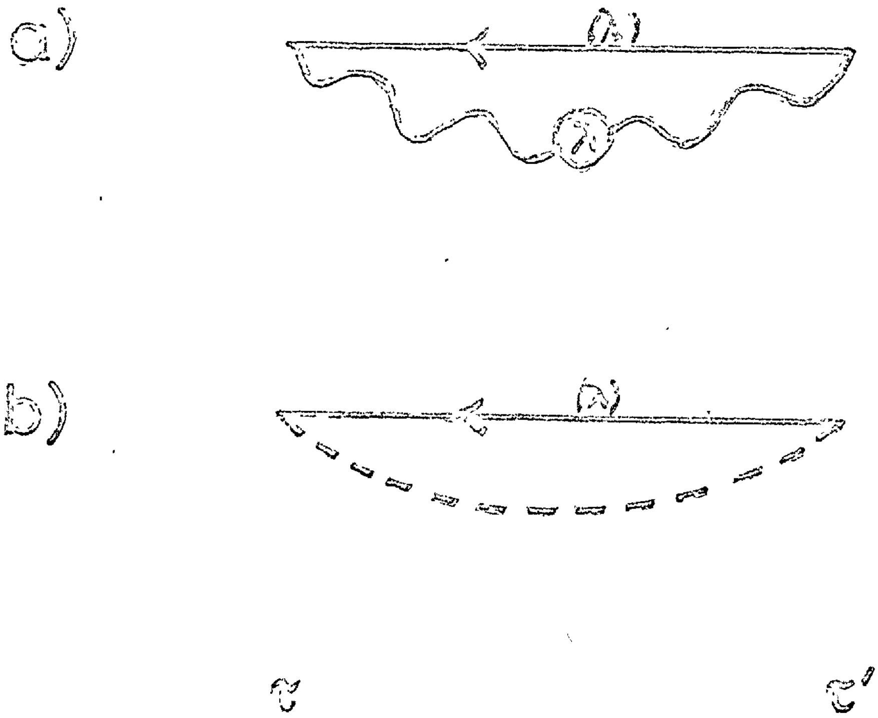
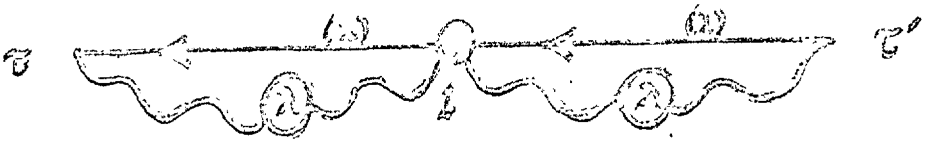


FIG. 7.



For the off - diagonal longitudinal matrix elements, both graphs illustrated in Fig. 8 are necessary to be accurate to $O(J^2)$.

$$T^z_{\lambda,-\lambda}(\tau) = \lambda J\delta(\tau) - J^2 S^{To}_{\lambda}(\tau), \qquad (5.48)$$

$$\text{so} \quad S^z_{\lambda,-\lambda}(\bar{\alpha}) = \frac{S^{zo}_{\lambda,-\lambda}(\bar{\alpha})}{1 - \lambda J\, S^{zo}_{\lambda,-\lambda}(\bar{\alpha})\,(1 - \lambda J\, S^{To}_{\lambda}(\bar{\alpha}))}$$

The result for $S^T_\lambda(\tau)$ can be simply obtained by examining Fig. 9 and realizing that the complete series can be obtained by replacing $S^{zo}_{\lambda,-\lambda}(\bar{\alpha})$ in the second term by the complete $S^z_{\lambda-\lambda}(\bar{\alpha})$, remarkably, this results in a form very similar to Eq.(5.48). The equation corresponding to Fig. 9 is;

$$S^T_\lambda(\bar{\alpha}) = S^{To}_\lambda(\bar{\alpha}) - J^2 S^{To}_\lambda(\bar{\alpha})\, S^{zo}_{\lambda-\lambda}(\bar{\alpha})\, S^{To}_\lambda(\bar{\alpha})$$

Thus

$$S^T_\lambda(\bar{\alpha}) = \frac{S^{To}_\lambda(\bar{\alpha})\,(1 - \lambda J\, S^{zo}_{\lambda,-\lambda}(\bar{\alpha}))}{1 - \lambda J\, S^{zo}_{\lambda,-\lambda}(\bar{\alpha})(1 - \lambda J\, S^{To}_\lambda(\bar{\alpha}))} \qquad (5.49)$$

These propagators and their transforms will first be used in evaluating the effective potential for the electrons in a systematic way to $O(J^2)$.

The longitudinal scattering potential (Fig. 3c) is

FIG. 8.

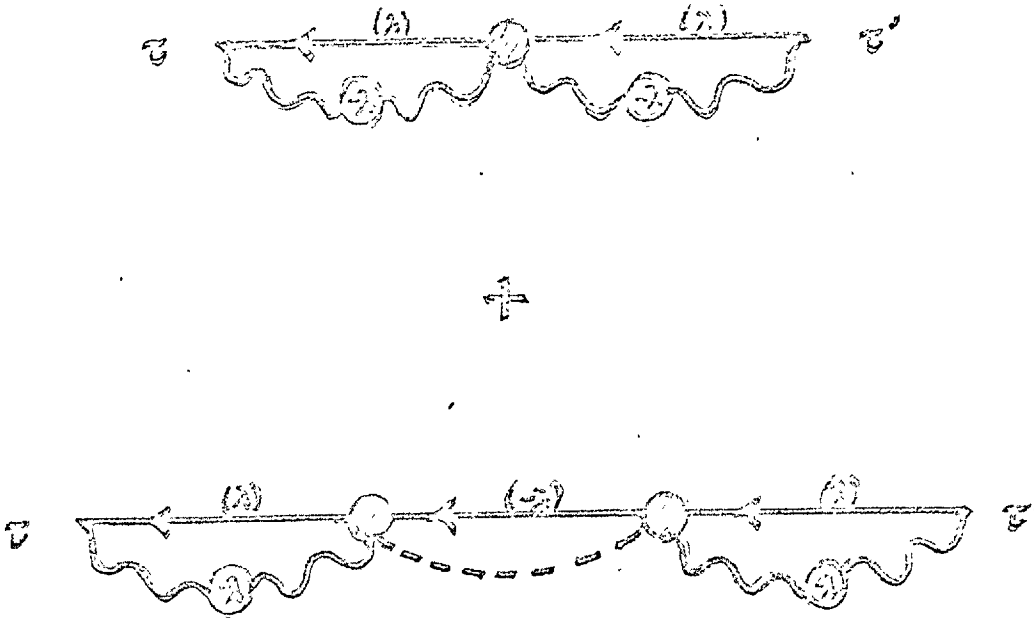
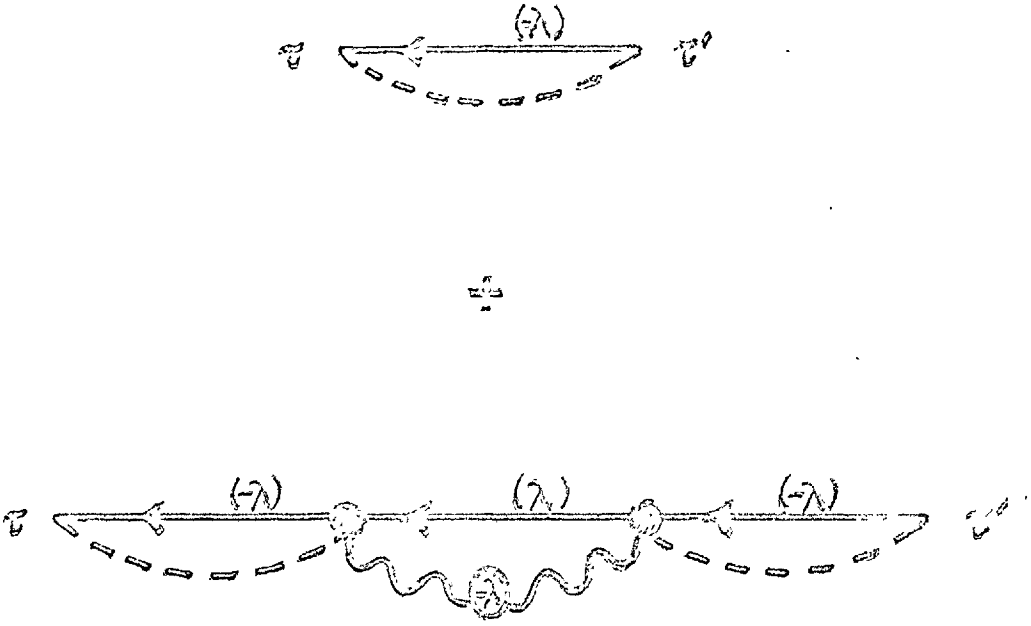


FIG. 9.



renormalized by splitting Eq. (5.19) into two equal contributions, then renormalizing the appropriate pair of free propagators, thus,

$$V_\lambda^{(2L)}(\tau) = -\frac{J^2}{2} \left(C^o(\tau)\, S^{z_o}_{\lambda-}(\tau) + C^o(-\tau)\, S^{z_o}_{\lambda+}(\tau) \right))$$

$$= \tfrac{1}{2} \left(V_\lambda^{(2La)}(\tau) + V_\lambda^{(2Lb)}(\tau) \right)$$

Then upon affecting a Fourier series transform

$$V_\lambda^{(2L)}(\bar{\nu}) = \frac{-J^2}{2\beta} \sum_\alpha \left(C^o(\bar{\nu} - \bar{\alpha})\, S^{z_o}_{\lambda-}(\bar{\alpha}) + C^o(\bar{\alpha} - \bar{\nu})\, S^{z_o}_{\lambda+}(\bar{\alpha}) \right) \tag{5.50}$$

Now each of these parts can scatter independently and repeatedly (i.e. $S^{z_o} \rightarrow S^z$) but this would involve overcounting the first term twice (see Fig. 10). The renormalized terms corresponding to the correct summation (note absence of brackets around superscript) are defined as follows

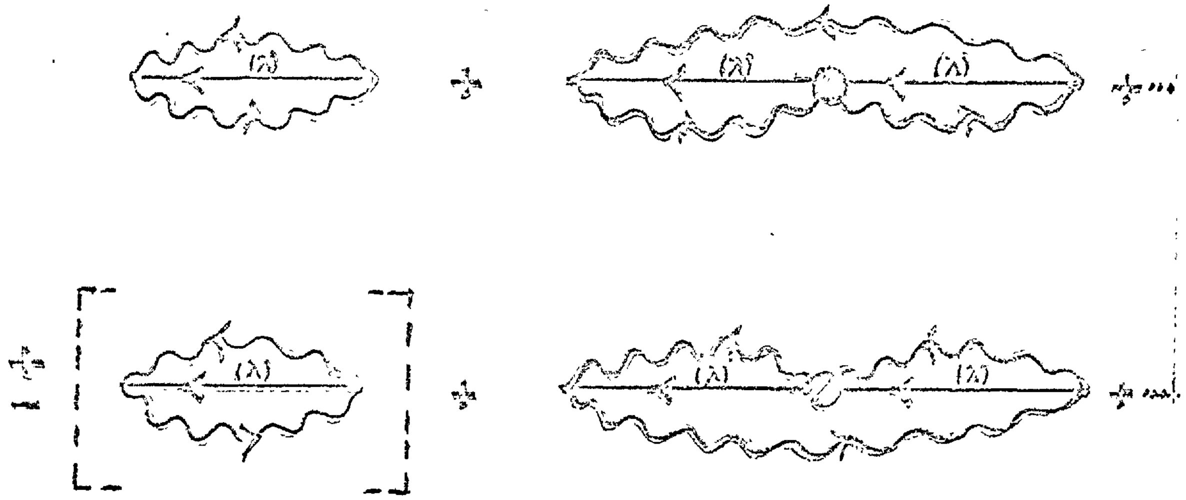
$$V_\lambda^{2L}(\bar{\nu}) = V_\lambda^{2La}(\bar{\nu}) + V_\lambda^{2Lb}(\bar{\nu}) - V_\lambda^{(2L)}(\bar{\nu}) \tag{5.51}$$

So

$$V^{2L}(\nu) = \frac{-J^2}{\beta} \sum_{\alpha\lambda'} C^o(\lambda'(\bar{\alpha} - \bar{\nu})\left(S^z_{\lambda\lambda'}(\bar{\alpha}) - \tfrac{1}{2} S^{z_o}_{\lambda\lambda'}(\bar{\alpha}) \right) \tag{5.52}$$

Similarly for the transverse part (Fig. 3d), Eq. (5.20) becomes

FIG. 10.



$$V_{\lambda}^{(2T)}(\tau) = \tfrac{1}{2} J_{-}^{2} \left(D^{o}(\lambda\tau)\, S^{z_o}_{-\lambda,\lambda}(\tau) + C^{o}(\lambda\tau)\, S^{T_o}_{\lambda}(\tau) \right) \tag{5.53}$$

which, on transforming and renormalizing, like Eq. (5.51) becomes,

$$V_{\lambda}^{2T}(\bar{\nu}) = \frac{J^{2}}{\beta} \sum_{\alpha} D^{o}(\lambda(\bar{\nu} - \bar{\alpha}))[S^{z}_{-\lambda,\lambda}(\bar{\alpha}) - \tfrac{1}{2} S^{z_o}_{-\lambda,\lambda}(\bar{\alpha})] + C^{o}(\lambda(\bar{\nu}-\bar{\alpha}))[S^{T}_{\lambda}(\bar{\alpha}) - \tfrac{1}{2} S^{T_o}_{\lambda}(\bar{\alpha})] \tag{5.54}$$

Before proceeding it must be noted that this procedure is not quite complete, as a whole sub - series of graphs is being neglected which have the same structure as those already considered. These are the two third order skeleton graphs (Fig. 11) which are needed when $h^{z} = 0$ to preserve rotational symmetry. They give contribution

$$V_{\lambda}^{(3T)}(\tau) = \lambda J^{3} C^{o}(\lambda\tau) \left(R^{o}_{\lambda}(\tau) + \bar{R}^{o}_{\lambda}(\tau) \right) \tag{5.55}$$

where

$$R^{o}_{\lambda}(\bar{\tau}) \equiv \int_{0}^{\beta} d\tau_{1}\, S^{T_o}_{\lambda}(\tau-\tau_{1})\, S^{z_o}_{\lambda-\lambda}(\tau_{1}-\tau'); \quad \bar{R}^{o}_{\lambda}(\tau) \equiv \int_{0}^{\beta} d\tau\, S^{z_o}_{\lambda-\lambda}(\tau-\tau_{1})\, S^{T_o}(\tau_{1}-\tau') \tag{5.56}$$

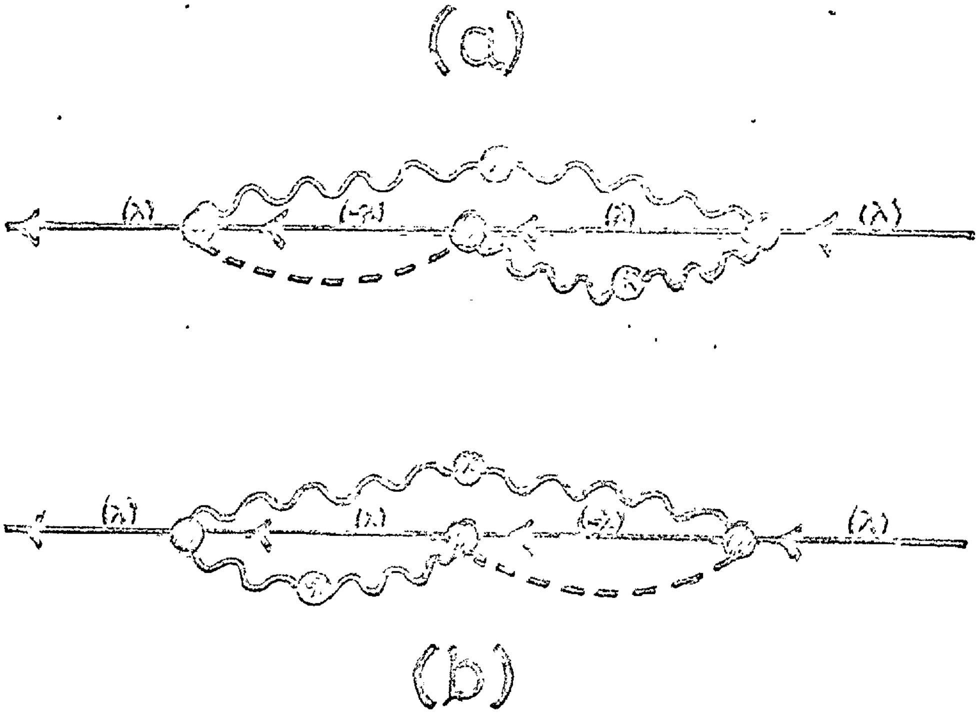
$$R^{o}_{\lambda}(\bar{\alpha}) = R^{o}_{\lambda}(\bar{\alpha}) = S^{T_o}_{\lambda}(\bar{\alpha})\, S^{z_o}_{\lambda,-\lambda}(\bar{\alpha}) \tag{5.57}$$

So,

$$V_{\lambda}^{(3T)}(\bar{\nu}) = \frac{2\lambda J^{3}}{\beta} \sum_{\alpha} C^{o}(\lambda(\bar{\nu}-\bar{\alpha})\, R^{o}_{\lambda}(\bar{\alpha}). \tag{5.58}$$

This is simply renormalized by <u>only</u> converting $S^{z_o} \rightarrow S^{z}$

FIG. 11.



in $R^{o}_{\lambda}(\bar{\alpha})$ (renormalizing $S^{To}_{\lambda}(\bar{\alpha})$ also would lead to some over-counting.)

$$V^{3T}_{\lambda}(\bar{\nu}) = 2\lambda\, \beta^{-1}\, J^{3} \sum_{\alpha} \frac{C^{o}(\lambda(\bar{\nu}-\bar{\alpha}))\, S^{To}_{\lambda}(\bar{\alpha})\, S^{zo}_{\lambda-\lambda}(\bar{\alpha})}{1 - \lambda J\, S^{zo}_{\lambda-\lambda}(\bar{\alpha})[1-\lambda J S^{To}_{\lambda}(\bar{\alpha})]}$$

The complete second order effective potential, or "polarization potential", V^{p}_{λ} can now be defined as the sum of these 3 terms,

$$V^{p}_{\lambda} \equiv V^{2L}_{\lambda} + V^{2T}_{\lambda} + V^{3T}_{\lambda} \qquad (5.60)$$

The above expressions are somewhat inelegent, so they will be evaluated in the zero external field limit, (where many other graphs, due only to field splitting, also vanish.) Thus from Eq. (4. 19) $\mathrm{Lt.}_{\omega_0 \to 0}\, C^{o}(\lambda\tau) \to \frac{1}{2} D^{o}(\lambda\tau)$; $D^{o}(\lambda\bar{\nu}) = \lambda D^{o}(\bar{\nu})$. so the zero - field correlation propagator $S^{o}(\bar{\alpha})$ is defined by

$$\lim_{\omega_0 \to 0} S^{zo}(\bar{\alpha}) = \frac{1}{2} S^{To}(\bar{\alpha}) = \frac{\lambda'}{2N} \sum \frac{(f^{+}_{p} - f^{-}_{p})}{\xi_{p} - i\bar{\alpha}} \equiv \frac{\lambda}{2} S^{o}(\bar{\alpha}) \qquad (5.61)$$

In this limit Eq.s (5.47 - 9) become

$$S^{z}_{\lambda,\lambda}(\bar{\alpha}) = \tfrac{1}{2}.\lambda S^{o}(\bar{\alpha})[1-\tfrac{1}{2}.\, JS^{o}(\bar{\alpha})]^{-1};$$

$$(5.62)$$

$$S^{z}_{\lambda,-\lambda}(\bar{\alpha}) = -\frac{\lambda}{2}\, S^{o}(\bar{\alpha})\ [\ 1 - \tfrac{1}{2}.\, JS^{o}(\bar{\alpha})\ ]^{-1}.[1 + J\ S^{o}(\bar{\alpha})\ ]^{-1}$$

$$S^{T}_{\lambda}(\bar{\alpha}) = \lambda\ S^{o}(\bar{\alpha})(1+\tfrac{1}{2}JS^{o}(\bar{\alpha}))[1 - \tfrac{1}{2}.\, JS^{o}(\bar{\alpha})]^{-1}.[\ 1 + JS^{o}(\bar{\alpha})\ ]^{-1}$$

This exhibits the unexpected property of factorizable denominators, as will be seen, this leads to ferromagnetic - resonance behaviour, as well as the usual anti - ferromagnetic. In fact, if this calculation had only been carried out to $O(J)$ in the denominator, only the anti - ferromagnetic result would have been obtained but witha factor "$\frac{1}{2}$" instead of unity; this factor is important, as the Kondo temperature, "Tk" depends exponentially upon it, (see next section).

Before evaluating $V^{p}(\bar{\nu})$ the propagator $S^{o}(\bar{\alpha})$ will be examined in alittle more detail. One can see that the effect of the spin operators in the interaction Hamiltonian (represented here by fermion - like C -ons and D -ons) has converted a bare fermion - like electron line to a bose - like propagator. This introduces a temperature dependent factor which changes sign as the momentum "p" passes through the Fermi surface. So from Eq. (5.61), with the constant density of states, the analytically continued form is;

$$S^{o}(\omega \pm is) = \rho\ (\ A\ (\omega) \pm i\pi\, B\ (\omega)\ )$$

where

$$A(\omega) = \text{Pr.}\int_{\mu - D}^{\mu + D} dE.\ \frac{\tanh \frac{\beta}{2}(E - \mu)}{E - \mu - \omega} \tag{5.63}$$

and $$B(\omega) = \tanh \frac{\beta\,\omega}{2} \quad \text{if} \quad |\omega| < D, \text{zero otherwise.}$$

It will also be useful to introduce the fuction $Q(\bar{\alpha})$ defined by

$$Q(\bar{\alpha}) = \frac{1 - \frac{J}{2} S^{o}(\bar{\alpha}) + \frac{1}{2}\left(J\, S^{o}(\bar{\alpha})\right)^{2}}{\left[1 - \frac{J}{2} S^{o}(\bar{\alpha})\right]\left[1 + J\, S^{o}(\bar{\alpha})\right]}$$

Or in its analytically continued form (to O(J) in the numerator) ;

$$Q(\omega \pm is) = \frac{1 \mp i\pi\rho\, J\, B(\omega)}{\left|\left[1 - \frac{J}{2} S^{o}(\omega)\right].\left[1 + J\, S^{o}(\omega)\right]\right|^{2}} \tag{5.64}$$

The effective potential $V^{p}(\omega)$ can now be evaluated as follows,

$$V^{p}_{o}(\bar{\nu}) = \frac{3}{4}\, \frac{J^{2}}{\beta} \sum_{\alpha} D^{o}(\bar{\nu} - \bar{\alpha})\, S^{o}(\bar{\alpha})\, Q(\bar{\alpha}) \tag{5.65}$$

so

$$V^{p}(\omega) = -\frac{3J^{2}}{2N} \sum_{p} \tanh \frac{\beta \xi_{p}}{2} \times \frac{1}{2\pi i} \oint_{\delta'} \frac{dz \qquad Q(z)}{(1 - e^{-\beta z})(\omega - z)(\xi_{p} - z)}$$

The latter form defines the complex integral $I_p(\omega)$, in terms of the bose - contour C_b (Appendix A.) and the usual analytic continuations, $\omega = i\bar{\nu}$, $i\bar{\alpha} = z = z_1 + iz_2$, have been used. To evaluate $I_p(\omega)$ one can see that for $|\omega| < D$ discontinuities occur in the complex z plane at $z_2 = 0$ and $z_2 = \xi_p$. However the discontinuity along the real axis takes in the pole at $z = \xi_p$ as well as the discontinuity from Q (z), that is

$$\text{Disc.}\left(\frac{Q(z_1)}{\xi_p - z_1}\right) = \text{Disc.}\,Q(z_1)\,\frac{\text{Pr.}}{(\xi_p - z_1)} + 2\pi i\,\delta(\xi_p - z_1)\,\text{Pr}\,Q(z_1)$$

This procedure is necessary to pick up the simple 2nd order result when $Q(z_1) = 1$.

Thus deforming C_b around the two above - mentioned discontinuities, one obtains, just above the real ω - axis

$$I_p(\omega + is) = \begin{aligned}[t] & -\frac{1}{4}\,\text{Disc}Q(\omega)\cdot\left[(\xi_p - \omega)\tanh\tfrac{1}{2}\beta\omega\right]^{-1} \\ & -\tfrac{1}{2}\cdot i\pi\,\delta(\xi_p - \omega)\,Q(\omega)\left[\tanh\tfrac{1}{2}\beta\omega\right]^{-1} \\ & +\tfrac{1}{2}\cdot\left(Q(\omega) - \tfrac{1}{2}Q(\xi_p)b^{+}(\xi_p)\right)\left[\xi_p - \omega\right]^{-1} \\ & +\frac{1}{2\pi i}\int dz_1 b^{+}(z_1)\,\text{Disc.}Q(z_1)\left[(\xi_p - z_1)(\omega - z_1)\right]^{-1} \end{aligned} \tag{5.66}$$

The convention has been used that, when the phase is not specified, the principal part is to be taken. After noting the approximations made above, and the explicit dependence of J in Eq. (5.65) then Eq. (5.66) will only be evaluated to O(1) in the numerator of the real part, and to O(J) in the numerator of the imaginary part.

$$I_p\,(\omega+is) = -\tfrac{1}{2}.\Big\{[(\xi_p-\omega)^{-1}.\,(\tanh\tfrac{1}{2}\beta\xi_p)^{-1}] + i\pi[\,\delta(\xi_p-\omega).(\tanh\tfrac{1}{2}\beta\omega)^{-1} - \rho J(\xi_p-\omega)^{-1}\,]\Big\} \times \big|\,[1-\tfrac{1}{2}.J\,S^{o}(\omega)].[1+J\,S^{o}(\omega)]\,\big|^{-2} \tag{5.67}$$

Thus, by Eq. (5.65), one obtains in the limit $\omega \ll k_B T$,

$$V^{\,p}_{o}(\omega+is) = \frac{\tfrac{3}{4}.\,\rho J^2[\,\ln.\big|\frac{D-\omega}{D+\omega}\big| + i\,\pi(\,1-\rho J\,A(\omega)\,)\,]}{\big|\,[\,1-\tfrac{1}{2}.\rho JA(\omega)].\,[\,1+\rho J\,A(\omega)]\,\big|^{2}} \tag{5.68}$$

For excitations near the Fermi surface ($\omega = 0$), one can use,

$$A(0) = \int_{-D}^{D} dx.x^{-1}.\tanh\tfrac{1}{2}\beta x = 2.\ln.(\zeta\beta D),\ \zeta = \frac{2\gamma}{\pi} = 1.13 \quad \text{c.f. Eq.(5.29)}$$

$$V^{\,p}_{o}(0+is) = \frac{i\,\tfrac{3}{4}.\,\rho J^2[\,1-2\rho J\ \ln.(\zeta\,\beta D)\,]}{\big|\,[1-\rho J\ \ln.(\zeta\beta D)][\,1+2\rho J\ \ln.(\zeta\beta D)]\,\big|^{2}} \tag{5.69}$$

One can see that this diverges under TWO conditions,

$$\text{a)}\quad 1 + 2\rho J\ \ln.\Big(\frac{\zeta\,\beta D}{k_B\,T_{c-}}\Big) = 0$$

$$\text{b)}\quad 1 - \rho J\ \ln.\Big(\frac{\zeta\beta\,D}{k_B\,T_{c+}}\Big) = 0 \tag{5.70}$$

Using Nagaoka's values for the parameters.41)

$$D = 5 \times 10^4 \ {}^\circ K \quad , \quad \rho |J| = 0.05$$

Eq. (5.70) becomes

$$\begin{aligned} &a) \quad k_B T_{c-} = \zeta D e^{\frac{1}{2\rho J}} = \zeta D e^{10\,\varepsilon(J)} \\ &b) \quad k_B T_{c+} = \zeta D e^{\frac{-1}{\rho J}} = \zeta D e^{-20\varepsilon(J)} \end{aligned} \qquad (5.71)$$

These only have low - temperature solutions ($k_B T_c < D$), if in Eq. (5.71a) J is negative giving $T_{c-} = 3^\circ K$, and if J is positive in Eq. (5.71 b), giving $T_{c+} = 2 \times 10^{-4}$ °K. Thus T_{c-} is the usual anti - ferromagnetic "transition - point found by Nagaoka, which will in future be denoted by "T_k" while T_{c+} is a new ferro - magnetic characteristic temperature. However, this latter is only of academic interest, for

$$\frac{T_{c+}}{T_k} = \frac{k_B T_k}{\zeta \ D} \qquad (5.72)$$

Before proceeding further a comment regarding the stability of this solution should be made i.e. the sign of the imaginary part of $V^p(\omega + is)$ which, in the present notation should take the sign of s. This is true for the anti-ferromagnetic case in the temperature range from zero to the unphysically high value of $\zeta D \exp.(\frac{1}{2\rho |J|})$. However an instability occurs below T_k for the ferromagnetic case, before its own T_c is reached, but no significance is attached to this result as it seems quite possible that higher order terms would counteract this change in sign.

Although the effective potential V appears to diverge at T_k, this is not the quantity of direct physical significance. The single particle-like times "τ_p" are determined by the imaginary part of the electron self-energy $M_{p;\lambda}(\omega)$. This is given by Edward s'method of taking an ensemble average over all impurity sites in the low concentration limit, $c \to 0$.

$$G_{\underline{p},\lambda}(\omega) = (\xi_{\underline{p}\lambda} - \omega - cM_{\underline{p}\lambda}(\omega))^{-1} \qquad (5.73)$$

where

$$M_{\underline{p}\lambda}(\omega) = \frac{V_\lambda(\omega)}{1 - V_\lambda(\omega)\, G^{o}_{\lambda}(\omega)} \qquad (5.74)$$

The one - electron quasi - particle life - time is given by

$$\tau^{-1}_{\underline{p},\lambda} = c\, M_{\underline{p},\lambda}(\xi_{\underline{p},\lambda} + is) \qquad (5.75)$$

However Eq.s (5.25 - 6) show that the real part of $G^{o}(\omega)$ vanishes at the Fermi surface (as does the real part of $V^{p}(\omega)$, in the above approximation. So, on using the form of $V^{p}_{0}(0 + is)$ valid in the temperature range $e^{-10} < \frac{T}{T_k} < e^{10}$ for $J < 0$, and using Eq.s (5.69, -74, -75) the life - time is given by

$$\tau^{-1}_{F} = \frac{c\pi}{\rho} \frac{1}{(\pi^{2} + 6\,|\ln.(\frac{T}{T_k})|^{2})} \qquad (5.76)$$

Equation (5.74) must be used in the temperature range $\frac{1}{4} < \frac{T}{T_k} < 4$ but outside this range $V^p_o(\omega)$ may be used to sufficient accuracy.

Then, using the following form for the resistivity (at temperature T) $\rho_{Res.}(T)$, the calculated result for the resistivity is given by

$$\rho_{Res.}(T)^{-1} = \frac{2e^2}{3m^2}\int d\,\xi_{\underline{p}}\,\tau_{\underline{p}}\,p^2\,\frac{\partial}{\partial\xi_{\underline{p}}}f^-_p = \frac{ze^2}{2m\rho}\,\tau_F \qquad (5.77)$$

$$\rho_{Res}(T) = c\,\frac{2m\pi}{ze^2}\,\frac{1}{\pi^2 + 6\left|\ln.\left(\frac{T}{T_k}\right)\right|^2} \qquad (5.78)$$

where z is the number of conduction electrons (mass m) per atom.

(5.4) Nagaoka's "Perturbational" Result. 41)

Nagaoka's results for his high temperature (perturbation) solution of his truncation scheme, for the equations of motion of the Green's functions, will be analysed first to cast them into a form comparable with the present results. Equation (2.17), for the diagonal element of the one electron's Green's function (using the same notation as in his first paper, denoted NI), can be written,

$$2\pi G_{pp}(\omega) = \frac{1}{(\omega-\xi_p)}\left(1 - \frac{J^2}{(\omega-\xi_p)}\,\frac{\Gamma(\omega)}{(1+2J\,g(\omega)+J^2F(\omega)\,\Gamma(\omega))}\right) \qquad (5.79)$$

This is then inverted and expanded to $O(J^2)$ in the numerator, to give

$$G^{-1}_{pp}(\omega) = 2\pi\left(\omega - \xi_p + \frac{J^2\,\Gamma(\omega)}{1 + 2J\,g(\omega) + J^2\,F(\omega)\,\Gamma(\omega)} \ldots\ldots\right)$$

(5.80)

This is Nagaoka's result (NI 3 - 2) apart from the term of $O(J^2)$ in the denominator; however, this must be retained to remove the divergence at T_k. In the limit $\omega +$ is the damping co - efficient is obtained

$$\tau_p^{-1} = \text{Im.}\ \frac{J^2\Gamma(\omega)}{1 + 2Jg(\omega) + J^2 F(\omega)\Gamma(\omega)} .$$

(5.81)

Now in NI, the zeroth approximation of $n_p = f_{-p}$ and $m_p = 0$ were used; in the present notation this becomes,

$$2g^{o}(\omega + is) = \overset{o}{S}(\omega + is) = \rho\left(A(\omega) + i\pi\tanh\frac{\beta\omega}{2}\right)$$

and

$$4/3\ \Gamma^{o}(\omega + is) = -F^{o}(\omega + is) = G^{o}_{o}(\omega + is) = \ln.\left|\frac{D - \omega}{D + \omega}\right| + i\pi\rho$$

This results, near the Fermi surface, in

$$\tau_F^{-1} = \frac{c\,\tfrac{3}{4}\,\pi J^2\rho}{\tfrac{3}{4}(\pi\rho J)^2 + 1 + 2\rho J.\ln.(\zeta\beta D)} = \frac{c\,\pi\,\rho^{-1}}{\pi^2 + \frac{8}{3\rho|J|}\ln.\left(\frac{T}{T_k}\right)}$$

(5.82)

The initial expansion to $0(J^2)$ was necessary for a meaningful result, otherwise Eq.(5.80) would be

$$G^{-1}_{pp}(\omega + is) = \frac{2\pi(\omega - \xi_p)^2}{(\omega - \xi_p + \Delta + \frac{i}{\tau_p})} \qquad \text{where } \Delta \text{ is the shift.}$$

As one can see, this vanishes at the Fermi surface ($\xi_F = 0$, $\omega = 0$).

In his second paper N II, Nagaoka starts with the perturbational approximation $n_p = f_p^-$ and $G^0_{pp'}(\omega)$ and upon neglecting higher order effects (NII 4.2), finds for m_p (see NII 4.7)

$$m_{pF} = \frac{3/2\, \rho J \ln.(\zeta\beta D)}{1 + 2\rho J \ln.(\zeta\beta D)} \qquad (5.83)$$

This can now be used to find

$$\mathrm{Im.}\,\Gamma(0 + is) = \mathrm{Im.}\,\frac{1}{N}\sum_p \frac{m_F - 3/4}{is - \xi_p} = -\pi\rho(m_F - 3/4).$$

Finally, on neglecting the real part of $\alpha(\sigma)$, the self-consistent result is

$$\tau_F^{-1} = \frac{c\, 3/4\, \pi\rho J^2}{[3/4(\pi\rho J)^2 + (1 + 2\rho J \ln.\zeta\beta D)^2]} = \frac{c\,\pi\,\rho^{-1}}{[\pi^2 + \frac{16}{3}|\ln.(\frac{T}{T_k})|^2].}$$

(5.84)

On comparing this result with Eq. (5.69), using (5.74), one can see that this is in agreement for $J < 0$ if terms of $O(J)$ which appear to be unimportant near T_k, had been neglected. In fact they do give a numerical contribution of order unity, as can be seen by comparing the above result with Eq. (5.76). The difference has been lost somewhere in the decoupling scheme along with the ferromagnetic result. These high temperature results contrast markedly with the self - consistent solution found at low temperatures (below T_k) which indicates a possible type of phase - transition. This latter result is found by the use of equations analogous to those in Superconductivity and the self - consistent assumption that m_F diverges at absolute zero. However, Fischer, who follows Nagaoka in his truncation formulation, adopts a different self - consistent low temperature assumption, and finds that $m_F = \frac{3}{4}$(see Eq. (5.83)) with the result that the resistivity vanishes like $\log^{-2}(T)$ at absolute zero, in agreement with Eq. (5.78).

Abrikosov's result (in the present notation) is

$$\tau_F^{-1} = \frac{c\pi}{\rho} \frac{\frac{3}{16}}{\left| \ln. \frac{T}{T_k} \right|^2} \qquad (5.85)$$

This could agree with Nagaoka's second result if the resonant part "II^2" had been included.

(5.5) Interacting Impurities.

The low concentration limit for dilute magnetic alloys exhibits the unexpected effect of a "bottle - neck" in the relaxation process of the localized moments, to the lattice, via the conduction electrons. The experimental results of Gossard et al[53)] have been given a theoretical foundation using the present techniques, in a letter published in Physical Review Letters. This work forms the basis of the present section. The Hamiltonian is that used in earlier sections of this Chapter, with $J_q = J$, but now, with several impurities, Eq. (5.5). The same notation for the C,D and F propagators, introduced in Chapter 4 for several spins, is used in the diagonalized momentum representation for the one - electron propagators, that is

$$G^{o}_{pp',\lambda}(\tau) = \delta_{pp'} G^{o}_{p,\lambda}(\tau) = \delta_{pp'} e^{-\xi_{p\lambda}\tau} (\Theta(\tau) f^{+}_{p\lambda} - \Theta(-\tau) f^{-}_{p\lambda}) \tag{5.86}$$

This will still be represented by a directed solid - line, Fig. (1d) so the interaction vertices will be the same as Fig.2.

The spin - operators have not been Fourier transformed, for only in the perfect lattice, (next section), is $< C^{+}_{q} C_{q'} >_{o}$ diagonal. For random alloys, inthe notation of Eq. (5.7),

$$< c^{+}_{q} c_{q'} >_{o} = N^{-1} \rho(q - q') < c^{+} c >_{o} \tag{5.87}$$

Moreover, in contradistinction to earlier sections, the effective need not be used here, but the mass - operator itself, evaluated in the momentum representation, $M_{pp'}$. The term corresponding to Fig. (3a,b) (to be contrasted with Eq.(5.18)) is

$$M^{(1)}_{pp',\lambda}(\bar{\nu}) = \lambda N^{-1} J R^{o} \rho(p - p') \tag{5.88}$$

where

$$R = < S^z_j > \qquad (5.89)$$

This is then averaged over all possible impurity configurations, so

$$\bar{\rho}\ (q) = (\mathrm{Vol.})^{-n} \int \int d^3 R_1 \ldots d^3 R_n\, \rho\,(q) \qquad (5.90)$$

If the impurity atoms are constrained to vacant lattice sites in the metal, then the integrals are converted to sums over all lattice points. The dotted notation of Edwards,[89)] will be used to indicate this averaging procedure - dotted lines converging on one cross, will indicate averaging at one site only. The average of a single spatial distribution function is simply

$$\bar{\rho}\,(q) = n\ \delta_{qo} \qquad (5.91)$$

So the averaged first - order mass - operator is diagonal in the momentum representation and takes the form

$$M^{(1)}_{pp', \lambda}\ (\bar{\nu}) = \lambda\, cJR^{o}\ \ \delta_{pp'} \qquad (5.92)$$

Similarly the C -on self - energy is diagonal in the site representation (c.f. Eq. (5.27)),

$$\Sigma^{(1)}_{ij}\ (\bar{\nu}) = 2J\ \ \zeta^{o}\ \ \delta_{ij} \qquad (5.93)$$

As in section (5.2), these can be self - consistently renormalized to give

$$G^{1}_{p}(\bar{\nu}) = (\xi_{p\lambda} - \lambda c J R_{1} - i\bar{\nu})^{-1} \; ; \; \sigma^{1}_{j}(\bar{\nu}) = (\omega_{0} - 2J\zeta - i\bar{\nu})^{-1} \tag{5.94}$$

The self - consistent solution for the two relative magnetizations are then (by A. 42)

$$R_{1} = -\tfrac{1}{2} \tanh \tfrac{1}{2}\beta(\omega_{0} - J2\zeta_{1}) \; ; \; \zeta_{1} = -\rho(\tfrac{1}{2}\omega_{0} - c\, JR_{1}) \tag{5.95}$$

The $\underline{k}$ - momentum component of the electronic transverse susceptibility[59)] propagator $K(\underline{k}, \tau)$ is defined in analogy to Eq. (2.31), by using Eq. (2.49)

$$K(\underline{k}; \tau) = \langle T(\sigma^{-}_{-\underline{k}}(\tau), \sigma^{+}_{\underline{k}}(0)) \rangle = N^{-2} \sum_{pp'} K_{pp'}(\underline{k}; \tau) \tag{5.96}$$

In terms of the one - electron operators, this has the form

$$K_{pp'}(\underline{k}; \tau) = 4\langle T_{W}(a^{+}_{p-k,-1}(\tau^{+}) a_{p,+1}(\tau)\, a^{+}_{p'+k,+1}(0^{+}) a_{p',-1}(0)) \rangle \tag{5.97}$$

In the interaction representation, this corresponds to a particle - hole propagating with opposite spin directions, so

$$K^{0}_{pp'}(\underline{k}, \tau) = -4G^{0}_{p,+1}(\tau)\, G^{0}_{p',-1}(-\tau)\, \delta_{p',p-k} \tag{5.98}$$

The transform of this propagator leads to

$$K^{0}(\underline{k}, \bar{\alpha}) = 4N^{-2} \sum_{p} (f^{+}_{p,+1} - f^{+}_{p-k,-1})(\xi_{p,+1} - \xi_{p-k,-1} - i\bar{\alpha})^{-1} \tag{5.99}$$

The analytically continued form of this function in the static limit (i.e. k = 0) will often occur, including first order renormalization; it is found to be

$$K^{o}\ (\underline{0}, \omega) = -\frac{8}{N}\ \zeta_1\ (\omega_o - 2cJR_1 - \omega)^{-1} \qquad (5.100)$$

The self - energy Ξ_{ij} correction to the localized spin - flip propagator for the case of interacting impurities, is given by a diagram of the type illustrated in Fig. (4.ci). The first vertex occurs on one site, while the second occurs ona different site with the electron - hole pair K connecting these two s-cattering events. In the non - interacting case, these two events would occur on the same atom.

The corresponding Dyson equation, inthe site representation, is

$$F_{ij}\ (\bar{a}) = F^{o}_{ij}\ (\bar{a}) + \sum_{nm} F^{o}_{in}\ (\bar{a})\ \Xi_{nm}\ (\bar{a})\ F_{mj}(\bar{a}) \qquad (5.101)$$

with

$$\Xi_{nm}\ (\bar{a}) = \frac{J^2}{4} \sum_{k} e^{-i\underline{k}(\underline{Rn}-\underline{Rm})}\ K^{o}\ (\underline{k};\ \bar{a})\ . \qquad (5.102)$$

Summation over the indices i and j defines the spin - flip propagator F for the whole set of localized spins, so

$$F\ (\bar{a}) = \sum_{i} F^{o}_{i}\ (\bar{a}) + J^2 \sum_{ik}\ e^{-i\underline{k}.\underline{Ri}} F^{o}_{i}(\bar{a})\ K^{o}(\underline{k};\bar{a}) \sum_{mj}\ e^{i\underline{k}\cdot\underline{R}_m} F_{mj}(\bar{a}) \qquad (5.103)$$

This equation is then averaged in a similar manner to Eq. (5.90) and the interference condition ($R_i \neq R_m$) is imposed. This eliminates all but the static limit for the electron - hole pair propagator (Eq. (5.100)) and results in a separable equation of the form

$$\bar{F}(\bar{a}) = \sum_i \overset{o}{F}(\bar{a}) + \sum_i \overset{o}{F}(\bar{a}) \frac{J^2}{4} \overset{o}{K}(\underline{0},\bar{a})\, \bar{F}(\bar{a}) \qquad (5.104)$$

This has the solution

$$\bar{F}(\bar{a}) = nF^o(\bar{a})\left(1 - n\frac{J^2}{4}F^o(\bar{a})\, K^o(\underline{0};\bar{a})\right)^{-1} \qquad (5.105)$$

The analytically continued result is then

$$\bar{F}(\omega) = \frac{2n R_1 (\omega - \omega_0 + 2cJR_1)}{(\omega_0 - \omega)(\omega_0 - 2J\zeta_1 - 2cJR_1 - \omega)} \qquad (5.106)$$

In order to describe the effect of damping of the system, the spin - lattice relaxation time $T_{sL} = \Delta^{-1}$ of the electrons is introduced as a phenomenological constant of the theory. In a similar manner to Giovannini et al,12) this is inserted in the denominator of the transverse electron susceptibility transform Eq. (5.100), ($i\bar{a} = \omega + i\varepsilon$ limit)

$$K^o(\underline{0},\omega) = -8N^{-1}\zeta_1\left[\omega_0 - 2cJR_1 - \omega - i\Delta\right]^{-1} \qquad (5.107)$$

If this new form is used in Eq. (5.105) the final result is

$$\bar{F}(\omega) = \frac{2nR_1(\omega + i\Delta - \omega_0 + 2cJR_1)}{\left[(\omega_0 - \omega)(\omega_0 - 2cJR_1 - 2J\zeta_1 - \omega - i\Delta) + i2\Delta J\zeta_1\right]} \qquad (5.108)$$

Again , in the limit $\Delta = 0$ this reverts to Eq. (5.106), which has two poles. The acoustic mode occurs at $\omega = \omega_0$, when the electrons precess with the local moments and an optical mode $\omega = \omega_0 - 2cJR_1 - 2J\zeta_1$, when the two spin systems precess in anti - phase. In the high temperature (paramagnetic region) $k_BT >> \omega_0$ then

$$R_1 = -\omega_0(4k_BT)^{-1} \quad ; \zeta_1 = -\tfrac{1}{2} \rho \omega_0 \qquad (5.109)$$

In this regime, the residues of the spin - flip function (which are proportional to their susceptibility contributions) are respectively

$$\frac{n\omega_0}{2k_BT} \quad \frac{c}{(c+c_0)} \quad \text{and} \quad \frac{n\omega_0}{2k_B T} \quad \frac{c_0}{(c+c_0)} \qquad (5.110)$$

where the characteristic concentration c_0 has been introduced; it is defined in this model by

$$C_0 = 2\rho k_B T = \zeta_1 R_1^{-1} \qquad (5.111)$$

The fact that there is no large first - order Yosida shift $\rho J \omega_0$, can be understood54) as the adiabatic following of the instantaneous local moment magnetization by the conduction electron magnetization. As was shown in Chapter 2 (see Eq. (2.63), when $\Delta = 0$ the Kondo - type Hamiltonian does not affect the dynamics of the total spin. If the electrons are heavily damped ($\Delta >> 2cJR_1$), that is, in the isothermal limit, then K^0 is very small, so only the first term is significant, Eq. (3.93) $\overline{F}(\omega) = nF^0(\omega) = 2nR(\omega + 2J\zeta_1 - \omega_0)^{-1}$

(5.112)

Thus full first - order Yosida shift $\omega = \omega_0 - 2J\zeta_1$ now appears, as the electrons always collide with the lattice before hitting the next magnetic impurity. Effectively the phase - coherence between the two spin systems is destroyed. If the calcutation is carried out to $O(J^2)$, then the pole occurs at

$$\omega_r = \omega_o - 2J\zeta_1 \left[1 - \frac{c}{c_o} \left(\frac{2J\zeta_1}{\Delta} \right)^2 \right] \tag{5.113}$$

However, if the damping is small ($\Delta << 2cJR_{\zeta}$) then dynamics of the localized systems are described by damped frequency response at $\omega = \omega_o - i\delta$, where δ^{-1} is the effective local - moment relaxation time $T_{ds}^{eff.}$ rather than the expected large Korringa width $\Gamma = T_{ds}^{-1}$ given by Eq. (5.31). In the present case, from Eq. (5.108)

$$\delta = \frac{c_o}{(c + c_o)} \cdot \Delta \tag{5.114}$$

Thus, as c tends to zero, δ tends to Δ , so the electrons successfully transfer all their spin - flip energy gained from the local spins to the lattice. However, as the concentration increases and exceeds c_o, then the line - width δ becomes narrower and narrower. This indicates that the electrons cannot remove the local - moment spin - flip energy fast enough to the lattice, before colliding with the next impurity. As Gossard, et al 53) pointed out and verified experimentally, this leads to a so - called "bottle - neck" effect in the relaxation processes.

A very similar result can be found by following Hasegawa's 54) approach, based on the phenomelogical Bloch equations for the decay of the spin systems. Equation (5.26) gives the second - order relaxation time for the conduction electrons, viz.

$$T_{sd}^{-1} = \tfrac{3}{4}\, c\, \pi\, \rho\, J^{2} \qquad (5.115)$$

So

$$\frac{T_{ds}}{T_{sd}} = \frac{3c}{16\,\rho\, kBT} = \frac{3}{8}\,\frac{c}{c_o} \qquad (5.116)$$

and in the bottleneck region $\frac{T_{ds}}{T_{sd}} >> 1$, so $c >> c_o$, as before.

Following Hasegawa, in the limit $T_{sL} >> T_{sd}$, one has

$$\delta = \frac{T_{sd}}{(T_{sL} + T_{sd})} \cdot \frac{1}{T_{ds}} = \frac{T_{sd}}{T_{sL}} \cdot T_{ds}^{-1} = 8/3\, \frac{c_o}{c}\, \Delta \qquad (5.117)$$

This can be compared with the present dynamical result given by Eq. (5.114). Gossard et al[53)] found that for 0.3% Mn in Cu $\Delta = 2.3 \times 10^{11}\,\mathrm{sec.}^{-1}$ They also found that this bottleneck could be opened by the addition of small amounts of Ti or Ni (neither of which have moments in Cu). The additional line - width broadening for an additional Ti concentration $c_{imp.}$ is found to be equal to "$a\, \frac{c}{c}\, \mathrm{imp.}\, k_B\, T$ " where 'a' is a constant. This can be derived in the Hasegawa approach, if one assumes an extra term which increases the width of the electron relaxation time to the lattice

, by a factor " $a\,(2\rho)^{-1}\, c_{imp.}$ ". This reflects the interference effects between the two types (magnetic and non-magnetic) of impurities. Moreover, on adding small amounts of Fe or Co, which do have moments in Cu, they also found that the additional broadening was a factor 10 times larger than for the addition of Ti or Ni. This is because the localized d - spin energy can be transferred , either to the s - electrons or preferably (80%) to the Fe impurities via R.K.Y. type interactions. The Fe moments then rapidly relax to the lattice because of the orbital nature of this moment.

The results for the simple alloys can easily be summarized in the interesting regime

$$\delta < \Delta < 2J\zeta < 2cJR_1 \quad \text{or} \quad \frac{\delta}{\omega_0} < \rho J$$

by quoting the main characteristics of the line - shape of the local - moment. This is given by the imaginary part of $F(\omega)$ and is proportional to the power absorbtion of the magnetic impurities (Slichter)[83] or to their neutron-scattering cross - section (Doniach)[84]. The sharp peak of this function around ω_0 has a width δ which is contrasted with the broader secondary peak at the optical resonant frequency $\omega_0 - 2cJR_1 - 2J\zeta_1$, which has a width of about Δ .

(5.6) Ferro - magnetic Rare - earth Metals.

The case of the rare - earth metals will be considered as a final example of the "Kondo" type interaction Hamiltonian. Many of the results will be found to be similar to those of earlier sections in this Chapter in the limit $c = 1$, but the derivations are sufficiently different to warrant inclusion.

If $J > 0$ the interaction favours the alignment of the two spin systems, giving a ferromagnetic ground - state. However in the absence of the interaction, the electron gas is not ferromagnetic - it is the coupling of the two systems which produces a polarization of the conduction band. This polarized band can then sustain spin - wave excitations of its own, but these are now coupled to the spin - waves of the local - moment system. The resulting dynamics are quite complicated but can be considered explicitly inthe long- wavelength limit. This result was previously found by Doniach and Wohlfarth 59) in their treatment of dilute alloys of iron in palladium, when a decoupling procedure was employed for the equations of motion of the appropriate retarded propagators.

Again, the spin - $\frac{1}{2}$ case will be condidered , so that when $n = N$, all the localized spins occupy a Bravais lattice; then Eq. (5.7) becomes

$$\rho (q) = N \delta_{qo} \tag{5.118}$$

This now implies (Eq. (5.87)) that the drone - fermions are diagonal in the momentum representation, so

$$< c_q^+ c_{q'} >_o = < c_q^+ c_q >_o \delta_{qq'} \tag{5.119}$$

where the transforms of the fermions are defined by

$$c_j^+ = N^{-\frac{1}{2}} \sum_{\underline{k}} e^{i\underline{k}\cdot\underline{R}_j} c_{\underline{k}}^+ ; \quad \varphi_j = N^{-\frac{1}{2}} \sum_{\underline{k}} e^{i\underline{k}\cdot\underline{R}_j} \varphi_{\underline{k}} \tag{5.120}$$

and since φ_j is real, then $\varphi_k^+ = \varphi_{-k}$. The interaction Hamiltonian is transformed from Eq. (5.5) to the following form, by substituting Eq. (4.1) for the spin operators $\underline{S}_j$ and then Fourier transforming the result using Eq. (5.119):

$$H_1 = \frac{-J}{N} \sum_{pqk} \left(a^+_{p-k,-1}\, a_{p',+1}\, c^+_{q+k}\, \varphi_{-q} + a^+_{p+k,+1}\, a_{p',-1}\, \varphi_{q-k}\, c_q \right.$$

$$\left. + \sum_{\lambda} \lambda\, a^+_{p+k,\lambda}\, a_{p',\lambda}\, c^+_{q-k}\, c_q \right) \qquad (5.121)$$

The same diagrammatic vertices are used, as in the previous sections, except that now all the lines carry a momentum label corresponding to Eq. (5.121). Finally the spin - flip propagator Fij, defined in Eq. (4.20) is Fourier transformed like K $(\underline{k}, \tau)$, by using $S_j = N^{-1/2} \sum_k e^{i\underline{k} \cdot \underline{R}_j}\, \underline{S}_k$, then

$$F(\underline{k};\tau) = \langle T\left(S^-_{-k}(\tau),\ S^+_k(0) \right) \rangle = N^{-1} \sum_{qq'} F_{qq'}(\underline{k};\tau) \qquad (5.122)$$

Since translational invariance now occurs, momentum is conserved, so all self - energy corrections are diagonal in the momentum representation, and so will be labelled by only one momentum suffix. Then, immediately, the first order renormalized mass - operator for the one - electron Green's function and the self -energy for the C -on (c.f. Eq. (5.92 - 3) are

$$M^1_{p,\lambda}(\bar{\nu}) = \lambda J R_1 \ , \ \Sigma^1_q(\bar{\nu}) = 2 J \zeta_1 \qquad (5.123)$$

As in Eq.s (5.94 - 5), these corrections give the two self-consistent equations for the relative magnetizations,

$$R_1 = -\tfrac{1}{2} \cdot \tanh. \tfrac{1}{2}. \beta\,(\omega_o - 2J\,\zeta_1);\; \zeta_1 = -\tfrac{1}{2}\,\rho\,(\omega_o - 2JR_1) \qquad (5.124)$$

The latter result is valid for any smoothly varying density of states curve, if the Fermi energy is much larger than ω_0 or JR_1 and is exact for the usual rectangular band. The self - consistent equation for the localized spins is then

$$R_1 = -\tfrac{1}{2} \cdot \tanh. \tfrac{1}{2}. \beta\,[\,\omega_o + \rho J\,(\omega_0 - 2JR_1)\,] \qquad (5.125)$$

In the high temperature regime tanh. x $\rightarrow$ x, this has the usual Curie - Weiss (or molecular field) type of solution

$$R_1 = -\frac{\omega_0}{4k}\,(\,1 + \rho J\,)\,(\,T - To\,)^{-1} \text{ with } k.To = \tfrac{1}{2}\,\rho J^{\,2} \qquad (5.126)$$

When the external field vanishes, the usual magnetization curve results for T < Tc,

$$R_1 = \tfrac{1}{2}. \tanh. \left(\,2R_1 \frac{Tc}{T}\,\right) \qquad (5.127)$$

These first - order corrections (internal "splittings") on the C -ons result in the Yosida shift of the resonance frequency of the spin - flip propagator (which is independent of $\underline{k}$),

$$F^1(\underline{k}, \bar{\alpha}\,) = -2R_1\,(\,\omega_o - 2J\zeta_1 - i\,\bar{\alpha}\,)^{-1} \qquad (5.128)$$

If the self - energy corresponding to the propagator $F_{qq'}(\underline{k}, \tau)$ is denoted by $\Xi_{qq'}(\underline{k}, \tau)$, then the new equation corresponding to Eq. (5.101) is

$$\overset{(2)}{F}_{qq'}(\underline{k}\,;\bar{\alpha}) = \overset{o}{F}_{qq'}(\underline{k};\bar{\alpha}) + \sum_{pp'} \overset{o}{F}_{qp}(\underline{k};\bar{\alpha})\ \overset{(2)}{\Xi}_{pp'}(\underline{k};\bar{\alpha})\overset{(2)}{F}_{p'q'}(\underline{k};\bar{\alpha}) \tag{5.129}$$

where, now $\overset{(2)}{\Xi}_{pp'}(\underline{k};\bar{\alpha}) = J^2 K^1(\underline{k}, \bar{\alpha})$

If this is now summed over the two additional indices q and q', the final result is

$$F^{(2)}(\underline{k};\bar{\alpha}) = -2R\ (\omega_o - 2J\zeta_1 - i\bar{\alpha} + 2R_1 N J^2 K^1(\underline{k};\bar{\alpha}))^{-1} \tag{5.130}$$

This is to be contrasted with Eq. (5.106), where there is no $\underline{k}$ - dependence. Now as $K^1(\underline{k};\bar{\alpha})$ is strongly dependent on $\underline{k}$ and $\bar{\alpha}$ (see Eq. (5.99)), the spectrum of these excitations is quite complicated. However, in the long - wavelength limit (k = 0), the modified form of Eq. (5.106) is recovered;

$$F^{(2)}(\underline{0}, \omega) = \frac{2R_1(\omega - \omega_o + 2JR_1)}{(\omega_o - \omega)(\omega_o - 2JR_1 - 2J\zeta_1 - \omega)} \tag{5.131}$$

Similarly for the second - order corrections to the electron transverse susceptibility, when the self - energy is just the local - moment spin - wave propagator ; that is $J^2F^1(\underline{k}, \bar{\alpha})$, so

$$K^{(2)}(\underline{k}, \bar{\alpha}) = K^1(\underline{k},\bar{\alpha})\,[1 - NJ^2\ F^1(\underline{k}, \bar{\alpha})\ K^1(\underline{k};\bar{\alpha})\ ^{-1} \tag{5.132}$$

Again , in the same limit

$$K^{(2)}(\underline{0},\omega) = \frac{8\,\zeta_1(\omega - \omega_0 + 2J\zeta_1)}{N(\omega_0 - \omega)(\omega_0 - 2JR_1 - 2J\zeta_1 - \omega)} \tag{5.133}$$

Thus, both propagator transforms have the same poles and only differ in their residues. These equations can then be interpreted in the same manner as in the discussion following Eq. (5.108), when $\Delta = 0$.

Chapter 6.

THE HEISENBERG MODEL.

(6.1) Introduction.

As a final example of the Quantum Field Theory methods for spin operators, developed in this thesis , the well-known model of a lattice of ferromagnetic spins will be considered in some detail. However, to further illustrate the usefulness of the 2S fermion representation, as a means of converting electronic many - body problems to spin problems, the equivalence is first shown in the next section between the usual exchange part of two - body Coulomb interaction and the Heisenberg model of the ferromagnet. The remaining sections of this chapter are then devoted to an extensive analysis of this Hamiltonian, using the drone - fermion representation for the spins. Thus, these two fermion representations can be used, in general, for analysing many - electron problems, instead of treating the original Hamiltonian directly. The intermediate step of converting to a spin Hamiltonian, often leads to greater physical insight into the dynamics of the system, as in the case of the Kondo model or the Heisenberg model.

(6.2) Equivalence of the Heisenberg and Exchange Models for General Spin.

In this section the Heisenberg Hamiltonian will be rederived in a simple manner, using the general 2S fermion representation introduced in section (3.2) , by a method resembling that in section (3.3). The starting point is the exchange part of the general two - body interaction, written in Wannier form. In this case the operator $a^{+}_{i\alpha\lambda}$ will create an electron on the ith site, in the [illegible] band, corresponding to the label α and with spin orientation λ. In terms of the exchange integral V_{ij}, which is taken to be independent of spin index and band in this approximation, the Hamiltonian takes the form

$$H_{Ex.} = \sum_{\substack{ij\alpha\beta \\ \lambda\lambda'}} V_{ij} \, a^{+}_{i\alpha\lambda} \, a_{j\beta\lambda} \, a^{+}_{j\beta\lambda'} \, a_{i\alpha\lambda'} \qquad (6.1)$$

with

$$V_{ij} = \tfrac{1}{2} \iint d^3 \underline{r} \, d^3 \underline{r}' \, \Psi^{*}_{i\alpha}(\underline{r}') \, \Psi_{j\beta}(\underline{r}') \frac{e^2}{(\underline{r}-\underline{r}')} \Psi^{*}_{j\beta}(\underline{r}) \, \Psi_{i\alpha}(\underline{r}) \qquad (6.2)$$

The prime indicates that self interactions $i = j$ are forbidden; this can be dropped if the definition of V_{ij} is extended by the restriction that it vanishes, if $i = j$. Also, one band only will be considered, containing $2l + 1$ possible electrons of any one spin orientation. Upon expanding the sum over λ', the operators can be anticommuted to the form

$$H_{Ex} = \sum_{ij} V_{ij} \sum_{\alpha\beta}^{2l+1} \sum_{\lambda=-1}^{+1} \left(a^{+}_{i\alpha\lambda} a_{i\alpha\lambda} a_{j\beta\lambda} a^{+}_{j\beta\lambda} - a^{+}_{i\alpha\lambda} a_{i\alpha-\lambda} a^{+}_{j\beta-\lambda} a_{j\beta\lambda} \right) \qquad (6.3)$$

Using Eq. (3.5) for $S_i^{\pm}(\alpha)$ and defining $N_{i\alpha\lambda} = a^+_{i\alpha\lambda}\ a_{i\alpha\lambda}$, and using the anti - commutation rules Eq. (3.6) for the first term, then

$$H_{Ex} = \sum_{ij\alpha\beta\lambda} V_{ij} \left(N_{i\alpha\lambda} (1 - N_{j\beta\lambda}) - S_i^{\lambda}(\alpha)\, S_j^{-\lambda}(\beta) \right) \qquad (6.4)$$

Furthermore, defining $N_j = \sum_\lambda N_{j\lambda} = \sum_\beta^{21+1} \sum_\lambda N_{j\beta\lambda}$

then Eq. (6.4) can be arranged into the form

$$\sum_{ij\lambda} V_{ij} \left(\tfrac{1}{2} N_i \left[\sum_\beta^{21+1} (2 - N_{j\beta\lambda} + N_{j\beta-\lambda}) - N_{j\lambda} \right] - S_i^{\lambda} S_j^{-\lambda} \right) \qquad (6.5)$$

Then using Eq. (3.5) for $S_i^z(\alpha)$ and summing over λ in the first term, one finds

$$H_{Ex} = \sum_{ij} V_{ij} \left(\sum_\lambda N_{i\lambda} \left[21+1 - \tfrac{1}{2} N_{j\lambda}\right] - S_i^+ S_j^- - S_i^- S_j^+ - 2S_i^z S_j^z \right) \qquad (6.6)$$

So that finally , in a ground state configuration, where there are n_λ electrons of spin orientation λ on each atomic site, the number operators can be replaced by their eigenvalues; the exchange Hamiltonian takes the form,

$$H_{Ex} = -2 \sum_{i \neq j} V_{ij}\, \underline{S}_i \cdot \underline{S}_j - \tfrac{1}{2} \sum_{i \neq j,} V_{ij}\, n_\lambda \left(n_\lambda - 2(21+1) \right) \qquad (6.7)$$

This is identical to the form Mattis[5] obtains following an argument which is the generalization of that of Dirac for for two spin $\tfrac{1}{2}$ electrons, using the permutation operation $P_{12} = (1 + \underline{\sigma}_i \cdot \underline{\sigma}_j)$.

The further merits or disadvantages of this Hamiltonian will not be further pursued here. The spin part will be used in the rest of this chapter, with the change of notation

$$4\,V_{ij} = I(\underline{R}_i - \underline{R}_j) \qquad (6.8)$$

(6.3) Molecular Field Theory.

In this section the Heisenberg Hamiltonian will be transformed, by means of the drone - fermion representation to a form convenient for a diagramatic analysis of its structure. This will initially be done in terms of the representation for $S = \frac{1}{2}$ and the analogous result for $S = 1$ will then simply be written down. A simple high - density classification of the resulting diagrams is presented valid for temperatures above the Curie temperature T_c ; this follows the analogous arguments of Stinchcombe et al.[81)] The simplest form of renormalization of the lowest order self - energy in the evaluation of the magnetization $< S^z >$(which is also consistent with this classification) results in the Weiss molecular field model. These results will later be seen to be valid in the low - temperature region and also includes those for the Ising model, which only involves the longitudinal component of the Heisenberg model used in this result.

The model of the Heisenberg ferromagnet for N equal spins, each localized on lattice sites Ri, in the presence of an external field (giving a Zeeman splitting ω_0) , is Eq, (6.7 - 8)

$$H = \omega_0 \sum_i S_i^z - \tfrac{1}{2} \sum_{i,j} I(\underline{R}_i - \underline{R}_j)\, \underline{S}_i \cdot \underline{S}_j \qquad (6.9)$$

Since the interaction integral is only non - zero between different sites, the two sums over lattice points are complete. Moreover, due to translational symmetry, its spatial Fourier transform can be introduced,

$$J(\underline{k}) = \sum_{j} I\,(\underline{R}_i - \underline{R}_j)\, e^{i\underline{k}.(\underline{R}_i - \underline{R}_j)} \qquad (6.10)$$

So the above restriction on I becomes $\sum_{\underline{k}} J\,(\underline{k}) = 0$ (6.11)

where the sum is over all momenta $\underline{k}$ in the first Brillouin zone. Substituting in Eq. (6.9) for the spin operators ($S = \frac{1}{2}$) Eq. (4.1), one obtains

$$H = \begin{array}{l} -\frac{1}{2} N\,(\omega_o + \frac{1}{4}.\ J(\underline{0})\ ) + (\omega_o + \frac{1}{2}.\ J(\underline{0})\ )\sum_i c_i^+ c_i \\ -\frac{1}{2} \sum_{ij} I\,(\underline{R}_i - \underline{R}_j).\,(c_i^+ c_i c_j^+ c_j + c_i^+ c_j \varphi_i \varphi_j\ ) \end{array} \qquad (6.12)$$

Introducing the Fourier transforms of these new operators as in Eq. (5.120), the Hamiltonian can be written inthe usual separable form (A.17). The unperturbed Hamiltonian is diagonalised with respect to all the C -on momentum operators (the constant term is also omitted, as this gives no net effect.)

$$H_o = B \sum_{\underline{k}} c_{\underline{k}}^+ c_{\underline{k}} \quad \text{with} \quad B = \omega_o + \tfrac{1}{2}J(\underline{0}) \qquad (6.13)$$

The interaction term, which conserves momenta, can be further separated into a transverse part H_1^T and a longitudinal part (or Ising term) H_1^L.

$$H_1^T = -\tfrac{1}{2}N \sum J(k+q)\, c_{k'}^{+}\, c_k\, \varphi_q\, \varphi_{-q'}\, \delta(k-k'+q-q')$$

$$H_1^L = -\tfrac{1}{2}N \sum J(k-k')\, c_k^{+}\, c_{k'}\, c_q^{+}\, c_{q'}\, \delta(k-k+q-q') \qquad (6.14)$$

The sum in each case is over all four momenta variables.

In terms of the interaction picture for these operators one finds

$$c_k^{+}(\tau) = e^{H_o\tau}\, c_k^{+}\, e^{-H_o\tau} = e^{B\tau} c_k^{+} \; ; \; \varphi_q(\tau) = \varphi_q \qquad (6.15)$$

Thus the thermal averages for the unperturbed Hamiltonian define the simple fermi functions for this model

$$< c_k^{+} c_{k'} >_o = \delta_{kk'}(e^{\beta B}+1)^{-1} = \delta_{kk'}\, f^{-} = \delta_{kk'}(1 - f^{+})$$

$$(6.16)$$

This enables a free propagator for the C -on to be defined as in Eq. (4.19), but with $\omega_o \rightarrow B$, so,

$$C_k^o(\tau) = < T_w(c_k(\tau), c_{k'}^{+}(0)) >_o = \delta_{kk'} e^{-B\tau}(\Theta(\tau) f^{+} - \Theta(-\tau) f^{-})$$

$$(6.17)$$

similarly

$$D_q^o(\tau) = < T_w(\varphi_q(\tau), \varphi_{q'}(0)) >_o = \delta_{qq'}\, \varepsilon(\tau) \qquad (6.18)$$

The periodic nature of these functions with respect to τ enables their (odd) Fourier series transforms to be written down immediately, as in Eq.s (4.21-2), so

$$C_k^o(\bar{\nu}) = (B - i\bar{\nu})^{-1} \; ; \; D_q^o(\bar{\nu}) = -2(i\bar{\nu})^{-1} \qquad (6.19)$$

The exact propagators (in the Heisenberg picture) are related to the averages in the interaction picture, as in (A.28), that* is,

$$C_k(\tau) = \langle T_w(c_k(\tau) c_k^+(\tau'))\rangle = \langle T_w(c_k(\tau)\, U(\beta)\, c_k^+(\tau'))\rangle_0^{Ld.} \qquad (6.20)$$

The propagators are illustrated in Fig. (12) , where now, the directed solid line represents a C -on propagator $C^o(\tau)$, while the dotted line again represents a D -on propagator $D^o_q(\tau)$. (In the case of S = 1, they will involve an additional index, α). The interaction can be represented by the two types of vertex, illustrated in Fig.(13) . The first vertex represents a spin - flip transition at the temperature τ_i(or a C -on,/D -on scattering) while the second corresponds to Ising scattering (C -on/C -on scattering

* The high - density classification arises from the observation that each vertex has a factor J ($\underline{k}$) (or on transforming I_{ij}), and a label τ_i which is eventually integrated from 0 to β ,so it is approximated by $\beta\bar{I}$ where $\bar{I}$ is some average value of J ($\underline{k}$). Now any internal line will carry amomentum label $\underline{k}$ (or on transforming,a site label $\underline{R}_i$) and if it is freely summed over , will give a numerical contribution of order z , which is the number of spins interacting with any other. Thus any graph with V vertices and L internal summations, will give a contribution of approximately $(\beta\bar{I})^V . z^L$; but from molecular field theory (as will be seen) the critical temperature is given

* See Addenda.

FIG. 12.

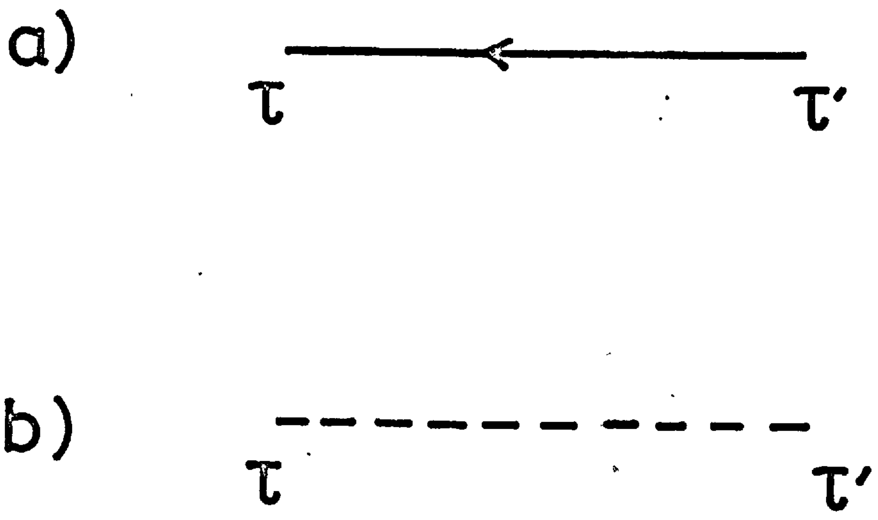
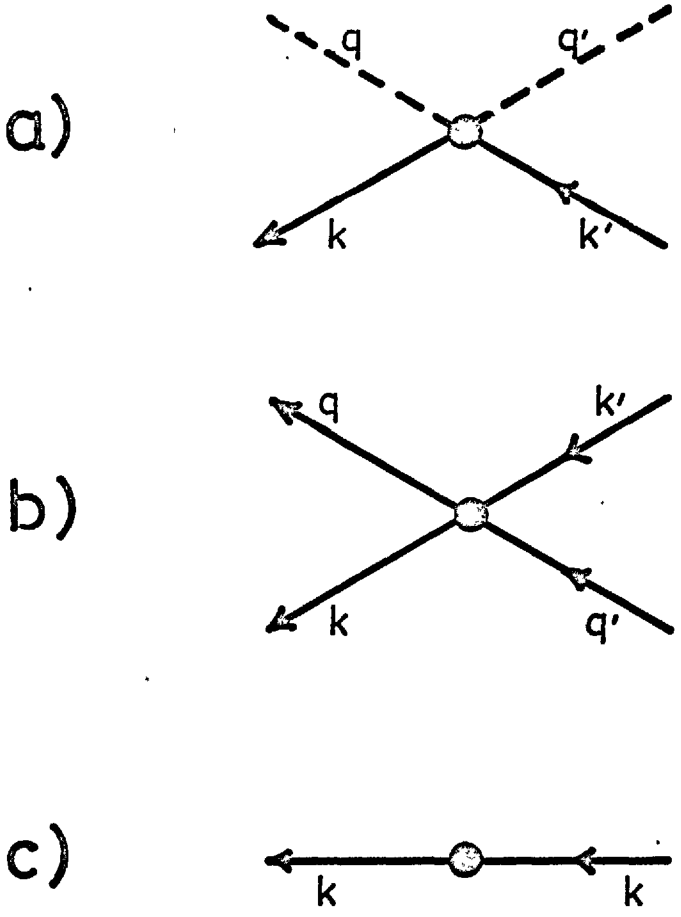


FIG. 13.



by $\frac{1}{4}\beta_c\, J(\underline{0}) = 1$ or approximately $\beta_c z \bar{I} = 1$. Such a graph will then contribute a factor $(T_c . T^{-1})^V . Z^{-L}$. Thus, for temperatures near T_c, or higher, the order of the graph in the high - density expansion is the number of vertices minus the number of free momenta summations. In general, there will always be more than one explicit summation , so we obtain an expansion in powers of $1/z$.

The lowest order self - energy correction to the magnetization is illustrated in Fig. (14a) . This gives, for the magnetic (C -on) self - energy $\Sigma^{(1)}_k(\tau)$ a total contribution,

$$\begin{aligned} &\Sigma^{(1)}_k(\tau) = J(\underline{0})\, f^- \quad \delta(\tau) \\ \text{or} \quad &\Sigma^{(1)}_k(\bar{\nu}) = J(\underline{0})\, f^- \end{aligned} \qquad (6.21)$$

Note that the exchange term in Fig. (14b) gives a zero contribution using Eq. (6.11). Using Dyson's equation for the first - order propagator

$$C^{(1)}_k(\bar{\nu}) = C^o_k(\bar{\nu}) + C^o_k(\bar{\nu})\, \Sigma^{(1)}_k(\bar{\nu})\, C^{(1)}_k(\bar{\nu}) \qquad (6.22)$$

all reducible terms of the type illustrated in Fig. (15 a) and (15b) will be included. Both of these involve no explicit k-dependence in the $\mathcal{J}(k)$ functions i.e. L = 0, so that all these graphs give a contribution O(1) in inverse powers of z . However, so do all "cacti" graphs of the type illustrated in Fig.(15c) , so these too must be included. This is quite trivial and involves , as usual, only

FIG. 14.

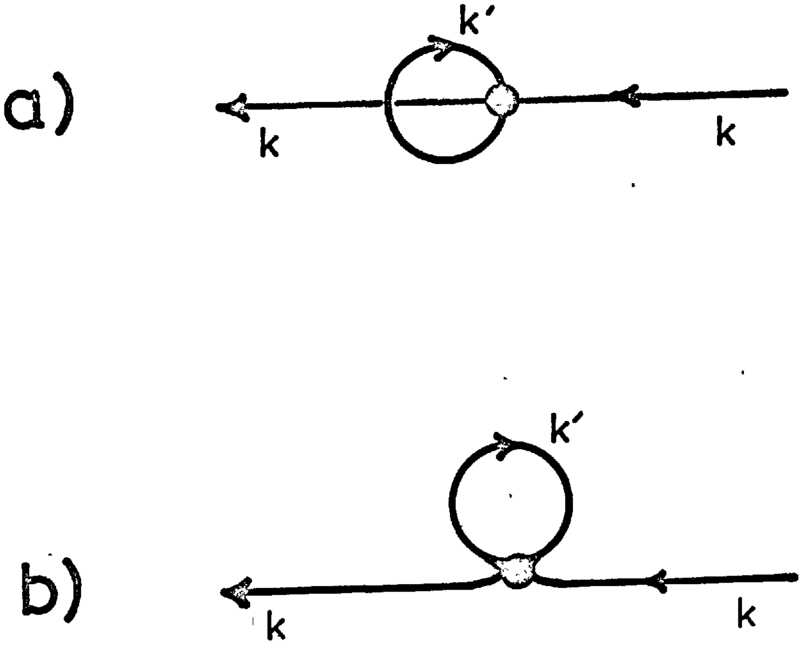
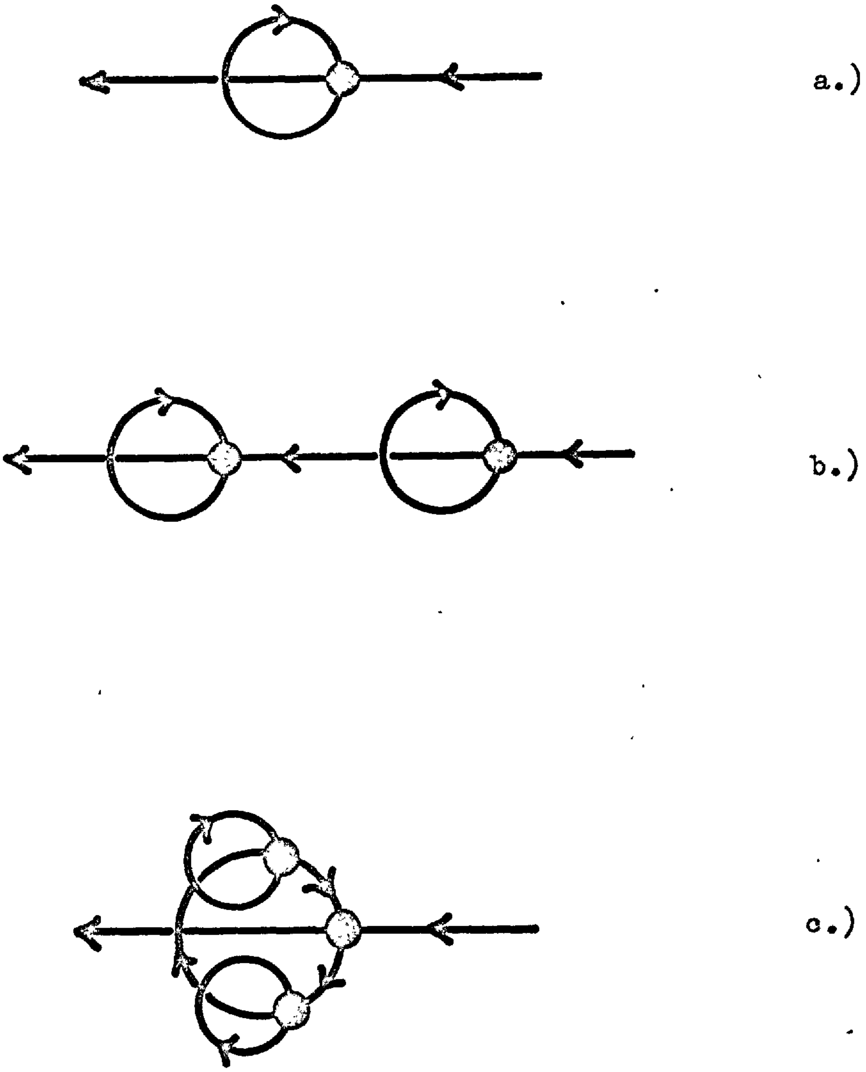


FIG. 15.



converting C -on lines in the self - energy from free averages to full self - consistent ones. This is shown in diagramatic form, in Fig. (16).

i.e.

$$\Sigma^{(1)}_k (C^o) \longrightarrow \Sigma^1_k (C^1) \qquad (6.23)$$

so

$$\Sigma^1_k (\bar{\nu}) = J(\underline{0}) \langle c^+_k c_k \rangle_1 = J(\underline{0}) (\tfrac{1}{2} + \langle S^z \rangle_1) \qquad (6.23)$$

thus,

$$C^1_k (\bar{\nu}) = (B - i\bar{\nu} - \Sigma^1_k (\bar{\nu}))^{-1} = (\omega_o - J(\underline{0}) \langle S^z \rangle_1 - i\bar{\nu})^{-1} \qquad (6.24)$$

This just introduces a real shift proportional to the net magnetization. In terms of its analytic continuation to above and below the real ω - axis (i.e. $s \rightarrow 0^+$)

$$\text{Disc } C^1_k (\omega) = C^1_k (\omega + is) - C^1_k (\omega - is) = 2\pi i \delta(\omega_o - R_1 J(\underline{0}) - \omega) \qquad (6.25)$$

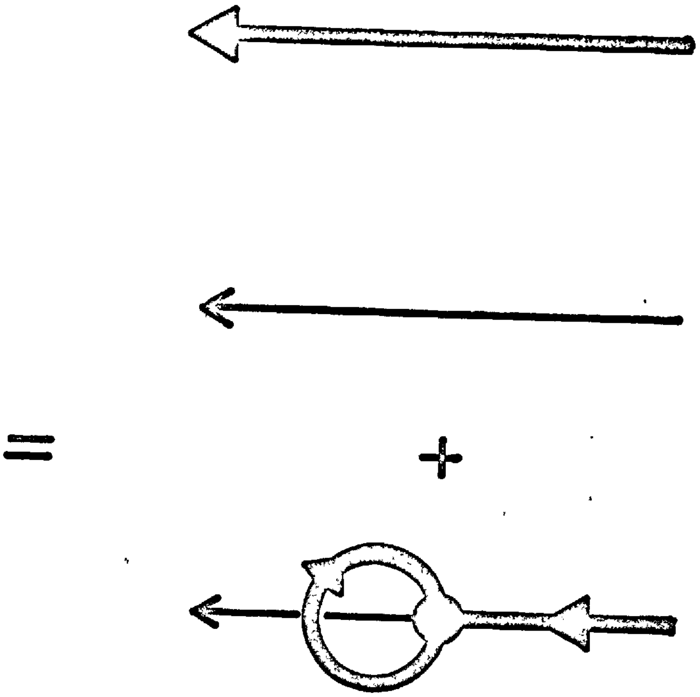
where $R_1 = \langle S^z_i \rangle_1 = \langle S^z_k \rangle_1$,

so, as in (A.42)

$$C^1_k (\tau) = \varepsilon(\tau)\, 1/2\pi i \int \frac{d\omega \quad e^{-\omega\tau}}{1 + e^{-\beta\omega}\, \varepsilon(\tau)} \,.\ \text{Disc.}\ C^1_k (\omega), \qquad (6.26)$$

where the Fermi contour has been deformed from around the imaginary ω -axis to surround the pole on the real ω-axis,

FIG. 16.



this results in

$$C^{1}_{k}(\tau) = \frac{\varepsilon(\tau)\exp-(\omega_0 - R_1 J(0))\tau}{1 + \exp-(\omega_0 - R_1 J(\underline{0}))\beta} \qquad (6.27)$$

In the limit $\tau \to 0^{+}$ and with Eq. (4.1) one obtains

$$R_1 = -\tfrac{1}{2}\tanh \tfrac{1}{2}\beta\,(\omega_0 - J(\underline{0})\,R_1) \qquad (6.28)$$

This is the usual molecular field result for $S = \tfrac{1}{2}$ (c.f. Eq.(5.124)) and only has a non - vanishing self - consistent result in zero field $\omega_0 = 0$ for temperatures below T_0 where $4T_0 = J(\underline{0})$, so, at low temperatures $R_1 \to -\tfrac{1}{2}\,\mathrm{sign}\,(\omega_0)$. As this result is correct to O(1) all future results involving C -on lines can always be renormalized by changing B to $(\omega_0 - J(\underline{0})\,R_1)$ in the Fourier transforms. This treatment can be seen to be the dual of the method of semi-invariants used by Stinchcombe et al.

The analogous result for S =1 is slightly more complicated in its calcutation, due to the presence of the counting-factor Y. If only one spin site were involved, one would simply multiply the equivalent C - space average by Y , to calculate the spin average. However, with more than one spin, counting problems enter into the calculations. These are handled as follows: the spin Hamiltonian H^{s} is first transformed to the C - space Hamiltonian H^{c} for S = 1.

$$H^{c} = \sum_{i\alpha} c^{+}_{i,\alpha}\, c_{i,\alpha} + H^{*}_{0} + H^{T}_{1} + H^{L}_{1} \qquad (6.29)$$

with

$$H_1^T = -1/(2N)\Sigma\, J(k+q)\, c^+_{k\alpha}\, c_{k'\beta}\, \varphi_{q\,\alpha}\varphi_{-q'\,\beta}\, \delta(k-k'+q-q') \tag{6.30}$$

and

$$H_1^L = -1/(2N)\Sigma\, J(k-k')c^+_{k\alpha}\, c_{k'\,\alpha}\, c^+_{q\,\beta}c_{q'\,\beta}\, \delta(k-k'+q-q')$$

The summations are over all four momenta, and the two spin indices ($\alpha, \beta = 1,2$). The term $H_o^* = \sum_{i,j,\alpha} I(\underline{R}_i-\underline{R}_j)\, c^+_{i\alpha}c_{i\alpha}$

(6.31)

cannot be immediately incorporated with the first term, as it really involves two - site summations, not just one. So this term must be included in the development operator in the C - space expansion. It is represented diagrammatically by Fig.(13c) and can be included by "zero - order" renormalization. An nth order term in the expanded development operator will contain products of 2^n different sites, but some of these will be the same as the external site labels, and also (perhaps) with several other internal labels. This will be equivalent to a series of C - space averages, all with an explicit counting factor of Y^m, for the case of m different, explicit spin operators. Application of Wick's theorem will further decompose these averages, leaving graphs involving L independent site summations, so such graphs will involve a complete counting - factor Y^{L+m}. H_o^* can only occur for reducible C -on corrections and, as it involves <u>one</u> summation over all other sites, one can always zero - order renormalize the C -on lines. This is equivalent to using the follow-ing for the unperturbed Hamiltonian, H^o_0 :

$$H^o_o = B_1(\omega_o) \sum_{i,\alpha} c^+_{i\alpha} c_{i\alpha} \tag{6.32}$$

where

$$B_1(\omega_o) = \omega_o + J(\underline{0})\, Y(\omega_o).$$

This gives, for the zero - order magnetization (in the two spaces $R^s_o = YR^o_o$ with $R^o_o = -\tanh \tfrac{1}{2}\beta(\omega_o + J(\underline{0})\,Y)$ (6.33)

The graphs generated by Fig. (15) for the calculation of the magnetization to the leading order in 1/z must also be included. The self - energy becomes,

$$\Sigma^{\alpha\beta}_{kk'}(\tau) = \delta_{\alpha\beta}\,\delta_{kk'}\,\delta(\tau)\,\frac{1}{N}\sum_{q\gamma} J(\underline{0}) \langle c^+_{q\gamma}\, c_{q\gamma} \rangle^o_o \tag{6.34}$$

The factor $J(\underline{0})$ indicates <u>one</u> sum over all other sites, so a factor Y is included to compensate for overcounting, so (in a reduced notation)

$$\Sigma^{(1)}_{k,\alpha}(\bar{\nu}) = Y\,J(\underline{0})\,2f^- = Y\,J(\underline{0})\,(R^o_o + 1) \tag{6.35}$$

Thus

$$c^{(1)}_{k,\alpha}(\bar{\nu}) = (B_1 - i\bar{\nu} - \Sigma_{k,\alpha}(\bar{\nu}))^{-1} = (\omega_o - J(\underline{0})R^s_o - i\bar{\nu})^{-1} \tag{6.36}$$

Note that this counting - factor is just sufficient to renormalize by the true (i.e. spin - averaged) magnetization

R_0^s and not the C -- space average R_0^c.

The first order magnetization is then

$$R^s_{(1)} = -Y(\omega_0) \tanh \tfrac{1}{2} \beta(\omega_0 - R^s_0 J(\underline{0})) \qquad (6.37)$$

In the same manner as $S = \frac{1}{2}$, the complete first - order renormalized line for the internal "molecular - field loop" can be used with the result

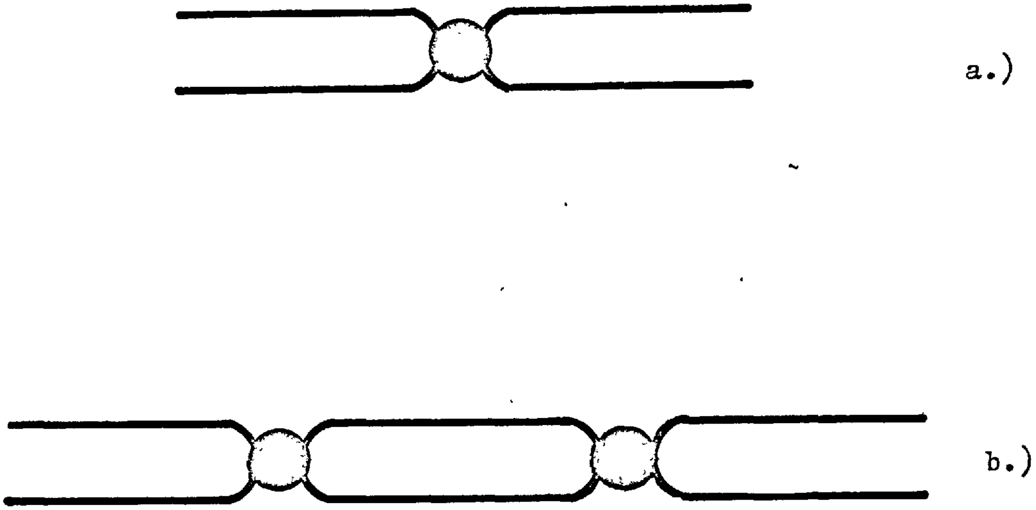
$$R^s_1 = -Y(\omega_0) \tanh \tfrac{1}{2} \beta(\omega_0 - R^s_1 J(\underline{0})) \qquad (6.38)$$

So, apart from the counting - factor Y this is identical to Eq. (6.28).

(6.4) Transverse and Longitudinal Correlations at High Temperatures.

In this section the calculation will be extended to the next order in the high - density classification,; that is, to order 1/z. This will include all graphs with one explicit k-dependence i.e. $J^n(k)$. Fig. (17) shows that these are the simple repeated scattering graphs for the two particle propagators, corresponding to the transverse and longitudinal correlations, $< S^- S^+ >$ and $< S^z S^z >$ respectively. In the next section this class of graphs chosen by the simple high - density classification, and so strictly valid only for $T > T_c$ (as shown earlier) will be shown to be the same as those corresponding to the low - order terms in the expansion in powers of the temperature. So the present results will also be valid in the whole temperature regime (apart from the

FIG. 17.



critical region) and the transverse correlations will reduce to the results of low - temperature spin - wave theory.

The case for S = ½ will again be taken, due to simplicity, and the generalization for S = 1 indicated. The spin - wave propagator F $(\underline{k}, \tau)$ is defined in terms of the Fourier transforms of the transverse correlations functions, as in Eq. (5.122).

with

$$F_{qq'}(\underline{k}, \tau) = \langle T_w(\varphi_q(\tau^+)\, c_{k+q}(\tau) c^+_{k+q'}(0^+)\, \varphi_{-q'}(0)) \rangle \tag{6.39}$$

Thus the free form of this propagator has the simple structure,

$$F^o_{qq'}(\underline{k}, \tau) = \delta_{qq'} D^o_q(\tau) C^o_{k\,q}(\tau) = \delta_{qq'} e^{-B\tau}(\Theta(\tau) f^+ + \Theta(-\tau) f^-) \tag{6.40}$$

This is illustrated in Fig. 18a and its (even) Fourier transform is given by

$$F^o_q(\underline{k}, \tau) = (\beta)^{-1} \sum_\alpha e^{-i\bar{\alpha}\tau} F^o_q(\underline{k}, \bar{\alpha}) ; F^o_q(\underline{k}, \bar{\alpha}) = \frac{\tanh \frac{1}{2}\beta B}{B - i\bar{\alpha}} \tag{6.41}$$

The 1/z series is generated from the lowest - order self - energy of this propa-gator, $\Sigma_{qq'}(\underline{k}, \;)$ is illustrated in Fig.(19)

and defined by a general correction to $F_{qq'}(\underline{k}, \tau)$, as in Eq. (5.129).

Upon evaluation this gives: (6.42)

$$\Sigma^{(1)}_{qq'}(\underline{k}, \tau) = \frac{1}{2N} J(\underline{k}) \delta(\tau) \quad ; \quad \Sigma^{(1)}_{qq'}(\underline{k}, \bar{\alpha}) = \frac{1}{2N} J(\underline{k})$$

FIG. 18.

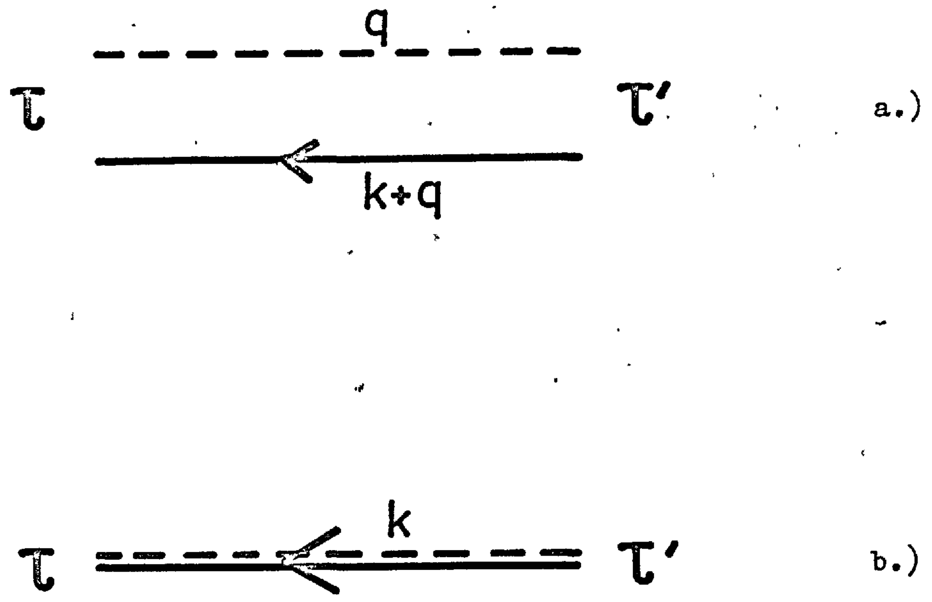
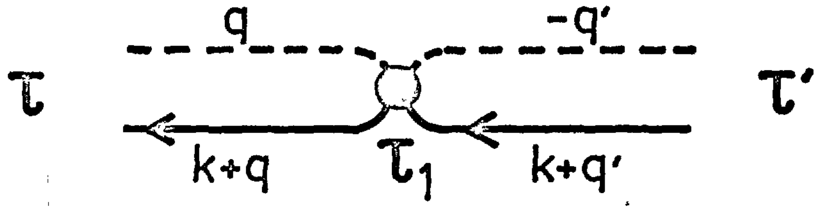


FIG. 19.



The appropriate Dyson equation for this series (including the free summations in the intermediate states) is

$$F^{(1)}_{qq'}(\underline{k},\bar{\alpha}) = F^{o}_{qq'}(\underline{k},\bar{\alpha}) + \sum_{q''} F^{o}_{q}(\underline{k},\bar{\alpha})\,\Xi^{(1)}_{qq''}(\underline{k};\bar{\alpha})\,F^{(1)}_{q'',q'}(\underline{k},\bar{\alpha}) \tag{6.43}$$

or

$$F^{(1)}(\underline{k},\bar{\alpha}) = \frac{1}{N}\sum_{qq'} F^{(1)}_{qq'}(\underline{k},\bar{\alpha}) = \{(F^{o}(\underline{k},\bar{\alpha}))^{-1} - N\,\Xi^{(1)}(\underline{k},\bar{\alpha})\}^{-1} \tag{6.44}$$

Substituting for $F^{o}(\underline{k},\bar{\alpha})$ and $\Xi^{(1)}(\underline{k},\bar{\alpha})$ by Eq.s (6.41 - 2) one finds,

$$F^{(1)}(\underline{k},\alpha) = \frac{\tanh \frac{1}{2}\beta B}{[\,\omega_o + \frac{1}{2}(J(\underline{0})-J(\underline{k})\tanh \frac{1}{2}\beta B) - i\bar{\alpha}\,]} \tag{6.45}$$

However, first - order renormalization of the constituent C -on propagators will not change the order of (1/z) of these graphs, so by Eq. (2.21) the molecular - field transverse propagator becomes:

$$F^{(1L)}_{qq'}(\underline{k},\alpha) = \frac{-\delta_{qq'}\,2R_1}{\omega_o \quad -R_1 \quad J(\underline{0}) - i\bar{\alpha}} \tag{6.46}$$

Upon including the transverse terms, one finally obtains

$$F^{1}(\underline{k},\bar{\alpha}) = -2R_1\,(\omega(\underline{k}) - i\bar{\alpha})^{-1} \tag{6.47}$$

where

$$\omega(\underline{k}) = \omega_o - R_1 \; (J(\underline{0}) - J(\underline{k})) \qquad (6.48)$$

correlations can be calculated immediately by converting the α - summation to a Bosecontour, with $z = i\overline{\alpha}$ as in (A.42) so

$$F^1(\underline{k}, \tau) = \frac{-\varepsilon(\tau) \, 2 R_1 \; \exp[-\omega(\underline{k})\tau]}{1 - \exp[-\beta\,\omega(\underline{k})\,\varepsilon(\tau)]} \qquad (6.49)$$

So the lowest - order (in powers of $1/z$) transverse interaction effects a $\underline{k}$ - dependent energy shift with no damping. Thus, at low temperatures, where $\beta J(\underline{0}) >> 1$ and $R_1 \to -\frac{1}{2}$ one recovers spin - wave theory, and for $\omega_o = 0$ the spin-waves vanish above T_c due to the factor $R_1(T)$ in the numerator, but not below T_c. In terms of the saturation magnetization M_o, the finite temperature magnetization $M(\beta)$ is given by $(T < T_c)$.

$$M(\beta) = 2M_o \left(\tfrac{1}{2} - \frac{1}{N} \sum_{\underline{k}} \langle S^+_{\underline{k}} S^-_{-\underline{k}} \rangle \right) = \tfrac{1}{2} - 0\left(\frac{T}{T_c}\right)^{3/2} \qquad (6.50)$$

Note, the energies $\omega(k)$ involve the molecular field magnetization R_1 and not the self - consistent spin - wave magnetization - so no anomalous T^3 term appears.

The result for $S = 1$ is obtained directly by remembering that the internal summation introduces a counting - factor Y, while all propagators carry two additional "spin - indices"

The corresponding Dyson equation becomes:

$$F^{\lambda\lambda'}_{qq'}(\underline{k},\bar{\alpha}) = F^{\lambda\lambda'}_{qq'}(\underline{k},\bar{\alpha})_0 + \sum_{\substack{p_1,q_1\\ \lambda_1,\lambda_1'}} F^{\lambda\lambda_1}_{qp_1}(\underline{k},\bar{\alpha})_0 \Xi^{\lambda_1\lambda_1'}_{p_1 q_1}(\underline{k},\bar{\alpha}) F^{\lambda_1'\lambda'}_{q_1 q}(\underline{k},\bar{\alpha})$$

on substituting

$$\Xi^{\lambda\lambda'}_{qq'}(\underline{k},\bar{\alpha}) = Y.\frac{1}{2N} J(\underline{k})$$

along with

$$F^{\lambda\lambda'}_{qq'}(\underline{k},\bar{\alpha})_0 = \frac{\delta_{qq'}\delta_{\lambda\lambda}\tanh\frac{1}{2}\beta(\omega_0 - J(0)R^s)}{\omega_0 - J(\underline{0})R^s - i\bar{\alpha}}$$

The result for the spin - wave (spin indices averaged) is

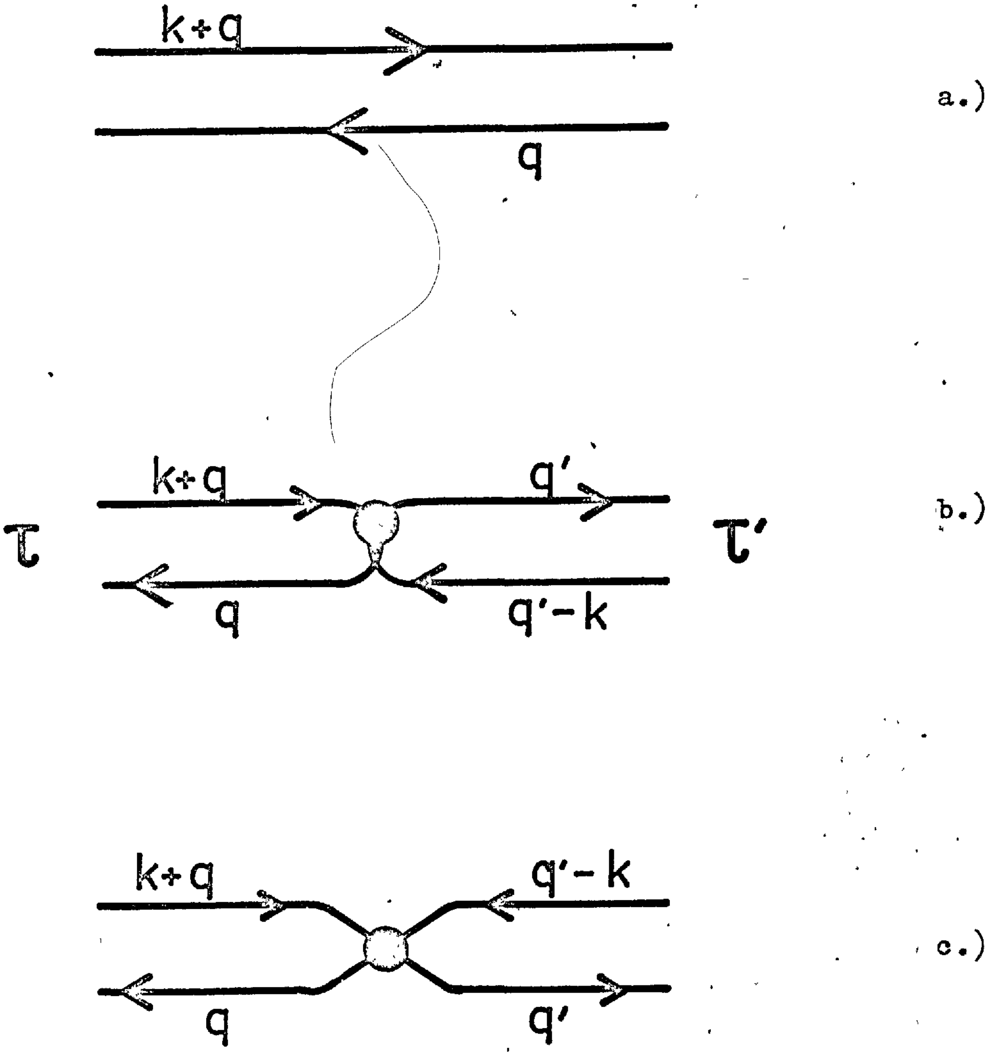
$$F^1(\underline{k},\bar{\alpha}) = \frac{-Y\ 2R^s}{\omega_0 - R^s(J(\underline{0}) - J(\underline{k})) - i\bar{\alpha}} \qquad (6.51)$$

Thus, apart from the factor Y inthe numerator (as before) the result agrees with Eq. (6.47), with the magnetizaton for $S = 1$ substituted instead of $S = \frac{1}{2}$, in Eq. (6.48). The other series of graphs, which are also of order 1/z, are the longitudinal graphs Fig. (20). However, in this case, due to the identity of the four operators, a non - propagated part must first be subtracted. Thus $\langle S_i^z\ S_j^z\rangle$ becomes

$$\langle S_i^z S_j^z\rangle = \langle c_i^+ c_i c_j^+ c_j\rangle - \frac{1}{2}\langle S_i^z\rangle - \frac{1}{2}\langle S_j^z\rangle - \frac{1}{4} \qquad (6.52)$$

So, a new two - particle propagator $K_{ij}(\tau)$ and its triple

FIG. 20.



Fourier transform (assuming an homogenous system) $K_{qq}(\underline{k}, \tau)$, is defined by

$$K_{ij}(\tau) = \langle T_w(c_i^+(\tau^+) c_i(\tau) c_j^+(0^+) c_j(0))\rangle$$

$$= \frac{1}{N} \sum_{qq'k} e^{i\underline{k}\cdot(\underline{R}_i - \underline{R}_j)} K_{qq'}(\underline{k},\tau)$$

$$(6.53)$$

Then the four - fermion propagator is defined by

$$K_{qq'}(\underline{k}, \tau) = \langle T_w(c^+_{k+q}(\tau^+) c_q(\tau) c^+_{q'-k}(0^+) c_{q'}(0))\rangle$$

$$(6.54)$$

This can always be decomposed into two parts - a self - interaction and a propagated term $\bar{K}$.

$$K_{qq'}(\underline{k},\tau) = \bar{K}_{qq'}(\underline{k},\tau) + \delta_{\underline{ko}} \langle c^+_q c_q \rangle\langle c^+_{q'} c_{q'} \rangle \qquad (6.55)$$

This separation is just sufficient to give the usual form for the longitudinal correlation

$$\langle S^z_i S^z_j \rangle - \langle S^z_i \rangle\langle S^z_j \rangle = \frac{1}{N} \sum_{qq'k} e^{i\underline{k}\cdot(\underline{R}_i - \underline{R}_j)} \bar{K}_{qq'}(\underline{k}, 0^+)$$

$$(6.56)$$

The lowest order component graph of the propagated type is the simple particle - hole pair of non - interacting C -ons;

this is illustrated in Fig.(20 a), and is given by the simplest contractions;

$$\overline{K}^{o}_{qq'}(\underline{k},\tau) = \delta_{q',k+q}\, C^{o}_{q}(\tau)\, C^{o}_{k+q}(-\tau) = \delta_{q',k+q} f^{+} f^{-}$$

(6.57)

The self - energy terms of $O(1/z)$ in the high - density expansion are illustrated in Fig. (20 b and 20 c). Explicit evaluation of the "exchange" graph Fig.(20c) demonstrates that it gives no net contribution, as it involves a self - contained interaction sum Eq. (6.11). However , the "direct" graph Fig.(20b) gives a non - vanishing self - energy contribution $A_{pp'}(\underline{k}) = \frac{1}{N} \beta J(\underline{k})$. This series is summed by using the Dyson equation

$$\overline{K}^{o}_{qq'}(\underline{k}) = \overline{K}^{o}_{qq'}(\underline{k}) + \sum_{pp'} \overline{K}^{o}_{qp}(\underline{k})\, A_{pp'}(\underline{k})\, \overline{K}_{pq}(\underline{k}) \qquad (6.58)$$

The temperature - variables τ have been dropped in this equation as each component of the equation (to this order) has no explicit τ dependence, so leading immediately to an algebraic equation. Summing over the indices q and q', and substituting Eq. (3.17) for $\overline{K}^{o}_{qq'}(\underline{k})$ leads to the final result

$$< S^{z}_{i} S^{z}_{j} > - <S^{z}_{i}> <S^{z}_{j}> = \frac{1}{N} \sum_{\underline{k}} \frac{e^{i\underline{k}.(\underline{R}i - \underline{R}j)} f^{+} f^{-}}{(1 - \beta J(\underline{k}) f^{+} f^{-})}$$

(6.59)

Thus, the complete $O(\frac{1}{z})$ result is obtained by renormalizing the individual C -on propagators - this is equivalent to the substitution $f^{\pm} \longrightarrow \frac{1}{2} \mp R_1$ giving

$$\langle S_i^z S_j^z \rangle - \langle S_i^z \rangle \langle S_j^z \rangle = \frac{1}{N} \sum_k \frac{e^{i\underline{k}\cdot(\underline{R}_i - \underline{R}_j)} \left(\frac{1}{4} - R_1^2\right)}{1 - \beta J\beta(\underline{k})\cdot\left(\frac{1}{4} - R_1^2\right)} \tag{6.60}$$

(6.5) Low - Temperature Expansion and Spin - Wave Scattering.

At this stage the calculations will be extended to low temperatures for $S = \frac{1}{2}$ and the validity of the above results to temperatures below Tc will be exhibited, as well as recovering the low temperature spin - wave results found by other methods. In this temperature regime the graphs can be classified by their contributions to the free - energy F in powers of the temperature (in fact, the reduced temperature T/Tc). In order to do this systematically, the contributions of each individual type of element in the graphs must be analyzed. Upon summation over ν of $C^0(\bar{\nu})$

there will result a factor f^+ or f^- which with simple molecular field renormalization becomes $f^{\pm} \rightarrow \frac{1}{2} \mp R_1$. Then in the two limits $T \rightarrow 0$ and $\omega_0 \rightarrow 0^+$ these become $f^+ \rightarrow 1 - e^{-\frac{1}{2}\beta J(\underline{0})}$ and $f^- \rightarrow e^{-\frac{1}{2}\beta J(\underline{0})}$ or in the

corresponding limit of $\omega_0 \rightarrow 0^-$ the roles of $f^{\pm}$ are reversed as $R_1 \rightarrow -\frac{1}{2}\,\mathrm{sgn}\,(\omega_0)$. So, at low temperatures, in zero magnetic field, with ferromagnetic interactions $J(\underline{0}) > 0$ the factor $e^{-\frac{\beta}{2} J(\underline{0})}$ is negligible compared with any finite power of T. This implies that any "particle - hole " pair of C -ons occuring between any two vertices, will introduce a factor $f^+ f^-$ upon integration over the internal temperature variables, so all such graphs will be exponentially small, and can be neglected. D -ons always give a finite contribution of O(1) as do unpaired C -ons in the correct limit. The next contributing element is the simple spin - wave (i.e. with $\underline{k}$ - dependence, introduced through one transverse vertex). Since at low temperatures Eq. (6.47) gives,

$$F(\underline{k}, \bar{\alpha}) = [\, \tfrac{1}{2}(J(\underline{0}) - J(\underline{k})) - i\,\bar{\alpha} \,]^{-1} \qquad (6.61)$$

or

$$F(\underline{k}, \tau) = e^{-\omega(\underline{k})\tau} \; (\Theta(\tau) b_k^+ + \Theta(-\tau) b_k^-) \qquad (6.62)$$

with

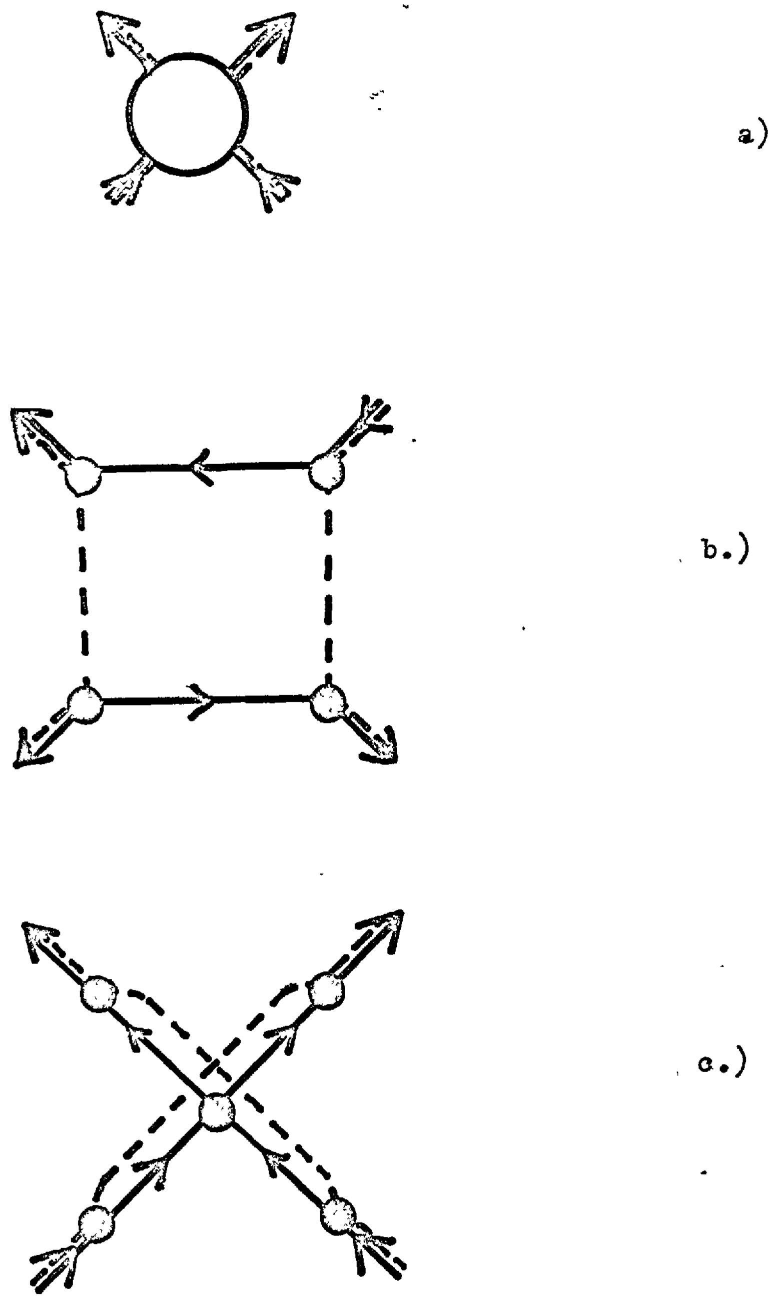
$$\omega(\underline{k}) = \tfrac{1}{2}(J(\underline{0}) - J(\underline{k})) \; ; \quad b_k^+ = 1 + b_k^-$$

$$b_k^+ = (1 - e^{-\beta\omega(\underline{k})})^{-1} \qquad (6.63)$$

This will be represented by a simple - line Fig.(18 b).

All graphs can now be simplified by isolating all spin-wave lines which then interact via equivalent vertices V represented by Fig.(21 a); these vertices will contain only C -on and D -on substructure and correspond explicitly to the kinematical corrections in ideal spin - wave theory. As this is now a standard type of Quantum Field Theory, the contributions to the change in the free - energy F , due to the interations, are given by the usual sum of distinct

FIG. 21.



connected graphs, that is (A.32).

Again the low - temperature classification method used by Stinchcombe et al[81] for their semi - invariant analysis, will be followed, and a very close correspondence for the present Green's function approach will be found. The equivalent vertices only involve functions of $J(\underline{k})$ and poles of the form $(B - i\bar{\alpha})^{-n}$ which lead to exponentially small corrections at B, but are converted to $(\tfrac{1}{2}J(\underline{k}))^{n}$ at the spin - wave poles $i\bar{\alpha} = \omega(\underline{k})$; so only result in one power of β per vertex as a result of equivalent energy conservation at this "vertex". Thus for a graph with N spin - wave lines interaction through V equivalent vertices results in S independent $\underline{k}$ and α summations. Each of the S sums over α_j is converted into a bose - contour around the whole of the imaginary ω_j axis, where $\omega_j = i\bar{\alpha}_j$. This is then distorted in the usual manner to pick up the residues of the poles from the product of the spin - wave denominators. The net result is a product of spin - wave bose occupation factors $\bar{b}_k$ multiplied by a product of (N - S) denominators, each of the form $\Sigma_j \omega(\underline{k}_j)$. The contribution of such a graph to $-\beta\Delta F$ has the form (retaining only temperature dependent factors) -

$(\beta)^{V-N+S} \, \Sigma \, (\bar{b}_k)^{S} (\bar{\omega})^{S-N}$ which is proportional to $T^{(3/2.S-V)}$.

However, in all but the simplest cases, this rule needs two modifications. The first exception occurs when there are D degenerate spin - waves in the graph, i.e. D have the same momentum and energy $(\underline{k}, \bar{\alpha})$. Then the pole from this will give a contibution obtained by differentiating (D-1) entiating (D-1) times the rest of the integrand with respect to α, so reducing the power of $\bar{\omega}$ in the denominator from (N-S) by a further (D-1). This gives a contribution to $-\beta\,\Delta F$ of the form $\beta^{(V-N+S)} \sum_{k_1 . k_s} (b_k^-)^S (\bar{\omega})^{-N+S+D-1}$ which is proportional to $T^{3/2 . S-V+D-1}$.

The second case arises when the frequency of one spin - wave appears with opposite sign in the frequency of another, due to frequency (or energy) conservation at the vertices. Effectively there exists particle and hole spin - wave states between some of the vertices. These two poles contribute to the sum over this frequency, one yielding b_k^- leading to the usual $T^{3/2}$ contribution, the other b_k^+ which involves no temperature dependent cut - off and so fails to give an $O(T^{3/2})$ contribution. However, it does still give a factor $\bar{\omega}$ in the denominator, so for S' spin - wave holes the contribution to $-\beta\Delta F$ will be $\Sigma\ \beta^{V} \left| \frac{b_{k'}^{+}}{\beta\bar{\omega}} \right|^{S'} (b_k^-)^{S-S'} (\beta\bar{\omega})^{S+S'-N}$

which is proportional to $T3/2\,(S - S') + S' - V$.

So, in general, a graph involving S - independent spin - waves, of which S' appear both with positive and negative sign in the energies, interacting through V equivalent vertices and with N_D groups of D - degenerate resulting spin - waves, will contribute to $-\beta\Delta F$ a term

$$\beta\Delta F(S, S', V, N_D) \propto T^{3/2(S-S')+S'-V+\sum_D N_D(D-1)} \tag{6.64}$$

Since $S \geq V + 1$, the lowest order graphs are those with V and N_D small, all graphs with $N_D > 0$ are at least of $O(T^{\frac{7}{2}})$ and increase rapidly with N_D ; similarly one must minimize the number of independent spin - waves. The only diagrams which give a contribution to ΔF of T^3 or less are those illustrated in Fig.(22, 23) . Thus the two lowest order diagrams in powers of T are also the same as those classified in powers of 1/z, so the results of sections (6.3) and 6.4) are also valid at low temperatures.

The low - temperature diagrams involved in spin - wave scattering will now be evaluated to exhibit the degree of correspondence with earlier theories. This will involve calculating the effects of the vertices illustrated in Fig. (21b and c) in the first diagram of the Born series Fig.(23) Since the spin - waves involve a C -on and D -on pair, then the structure of the simple interaction vertices Fig. (21) indicates that the lowest order spin - wave interactions will occur in 4th order; this vertex will be denoted by $V^{(4)}$, (the diagram obtained by interchanging the D -on pair will be included in this). If the contribution of the two spin-waves is denoted by $W(\underline{k}_1 \tau_1 , \underline{k}_2 \tau_2 ; \underline{k}_3 \tau_3 , \underline{k}_4 \tau_4)$ then the contribution of this graph to $-\beta\Delta F$ is given by,

$$\frac{1}{(2N)^4} \sum_{\underline{k}_i} \int_0^\beta d\tau_1 \dots d\tau_4 \quad W(\underline{k}_1 \tau_1 , \dots \underline{k}_4 \tau_4) \, V^{(4)}(\underline{k}_1 \tau , \dots , \underline{k}_4 \tau_4) \tag{6.65}$$

which on Fourier transforming, with repect to the τ-labels

FIG. 22.

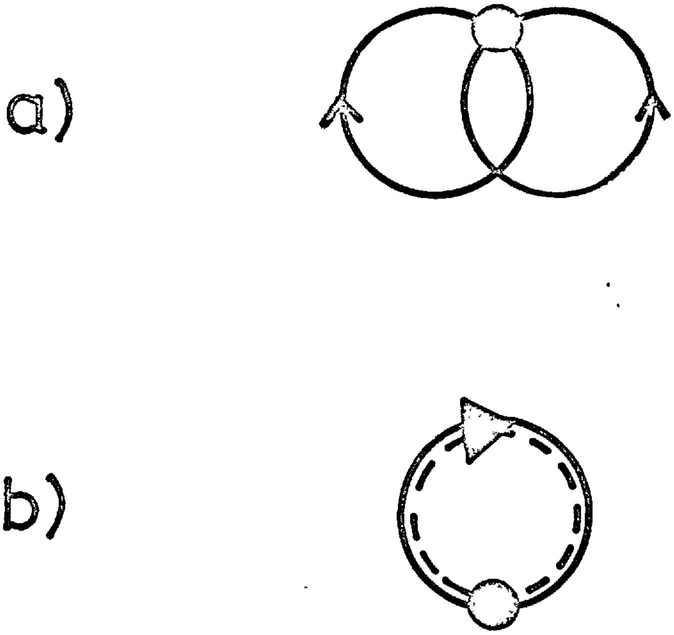
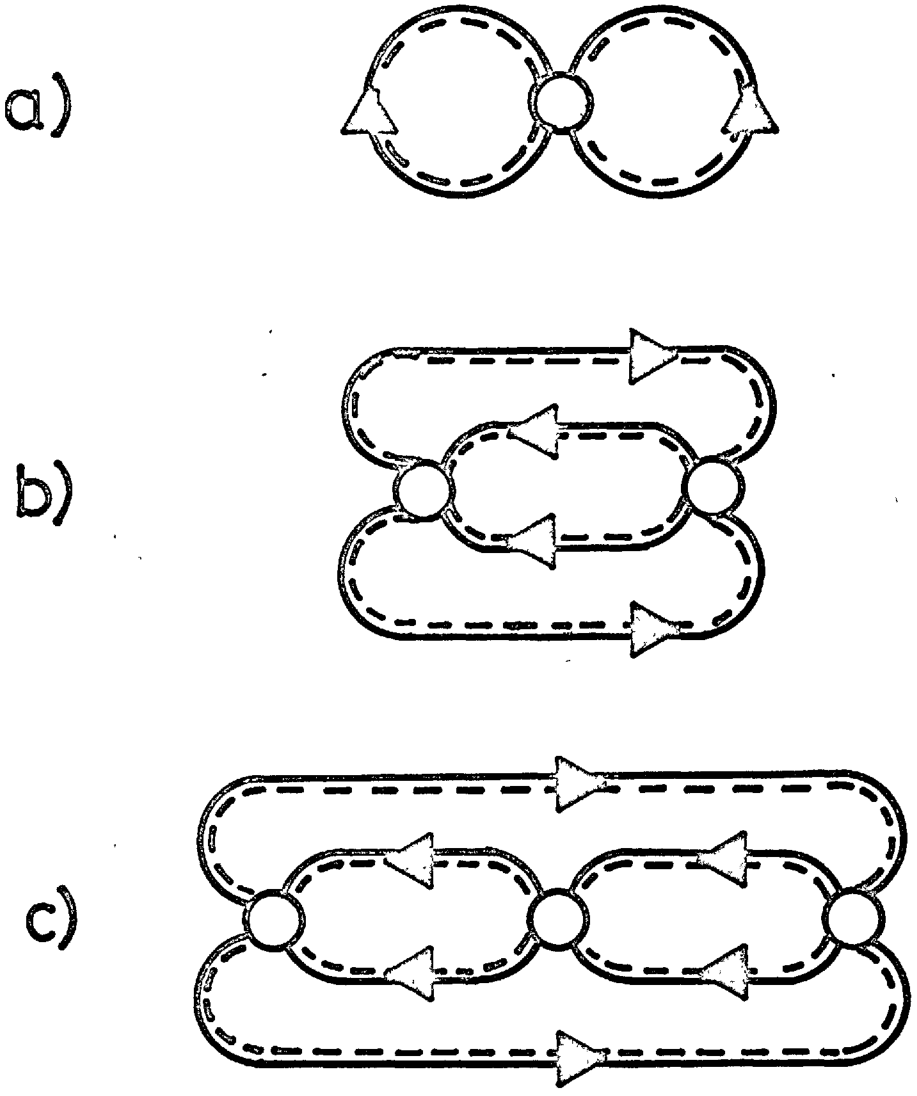


FIG. 23.



and integrating , gives (in terms of the reduced vertex $\bar{V}$)

$$\frac{N^2}{2(2N)^4} \sum_{\underline{k}\underline{k}'} J^2(\underline{k}) J^2(\underline{k}') \frac{1}{\beta^2} \sum_{\alpha\alpha'} F(\underline{k},\bar{\alpha}) F(\underline{k}'\bar{\alpha}) \bar{V}^{(4)}(\bar{\alpha}\,\bar{\alpha}';\bar{\alpha}'\,\bar{\alpha}) \tag{6.66}$$

where $\bar{V}^{(4)}(\bar{\alpha}_i)$ is the transform of $\bar{V}^{(4)}(\tau_i)$, which is given by

$$N\, C^{\circ}(14)C^{\circ}(23)\, [D^{\circ}(12)D^{\circ}(34) - D^{\circ}(13)D^{\circ}(24)] \quad ,$$

$$-N\, C^{\circ}(24)C^{\circ}(13)\, [D^{\circ}(12)D^{\circ}(34) + D^{\circ}(14)D^{\circ}(23)] \tag{6.67}$$

The simplified notation $C^{\circ}(14) = C^{\circ}(\tau_1 - \tau_4)$ has been used here for convenience ; the Fourier transform is given by

$$\bar{V}^{(4)}(\bar{\alpha}_1\bar{\alpha}_2\,;\,\bar{\alpha}_3\,\bar{\alpha}_4\,)\,) = \sum_{\nu} N\,\delta(1+2-3-4)\; C^{\circ}(\bar{\alpha}_1 - \bar{\nu})\; D^{\circ}(\bar{\nu}) \;x$$

$$[Z\,(\nu 12;3,4) + Z(\nu 12;4,3)]$$

where ,

$$Z\,(\nu,1,2;3,4\,) = D^{\circ}(\bar{\alpha}_3 - \bar{\alpha}_1 + \bar{\nu})[\,C^{\circ}(\bar{\alpha}_2 + \bar{\nu}\,) - C^{\circ}(\bar{\alpha}_4 - \bar{\nu})\,] \;. \tag{6.68}$$

This is evaluated in the usual manner of converting the sum to an integral over $z = i\bar{\nu}$ involving the Fermi contour, In the low temperature approximation this only picks up the residues at the origin , and those poles which result in f^+ factors - the f^- ones are exponentially small, and can be neglected. Within this approximation

$$\bar{V}^{(4)}(12;34) = -2N\beta\delta(1+2-3-4)[B-i\bar{\alpha}_1+B-i\bar{\alpha}_2]\prod_{j=1}^{4}(B-i\bar{\alpha}_j)^{-1} \qquad (6.69)$$

Again in the low – temperature approximation , the double sum over α and α' picks up only the residues at the respective spin – wave energies $\omega(\underline{k}_j)$ and using : $B-\omega(\underline{k}_j) = \frac{1}{2}. J(\underline{k}_j) \neq 0$

$$\beta^{-2}\sum_{\alpha\alpha'} F(\underline{k},\bar{\alpha})\,F(\underline{k}',\bar{\alpha}')\,V^{(4)}(\bar{\alpha}\,\bar{\alpha}';\bar{\alpha}'\,\bar{\alpha}) = -2^{4}\beta N\, b_{\bar{\underline{k}}}\, b_{\bar{\underline{k}}'}\frac{[J(\underline{k})+J(\underline{k}')]}{J^{2}(\underline{k}).\,J^{2}(\underline{k}')} \qquad (6.70)$$

Thus, the simple 4th order terms result in a contribution :

$$-\beta\,\Delta F^{(4)} = -\frac{\beta}{2N}\sum_{kk'} b_{\bar{\underline{k}}}\, b_{\bar{\underline{k}}'}\,[\,J(\underline{k})+J(\underline{k}')\,] \qquad (6.71)$$

Similarly , one obtains for the 5th order vertex $V^{(5)}$,

$$2^{-5}N^{-1}\,{}^{-2}\sum_{kk'} J^{2}(\underline{k})J^{2}(\underline{k}')[J(\underline{k}-\underline{k}')+J(\underline{0})]F(\underline{k},\bar{\alpha})F(\underline{k}',\bar{\alpha}')\,\bar{V}^{(5)}(\bar{\alpha}\,\bar{\alpha}';\bar{\alpha}'\bar{\alpha}) \qquad (6.72)$$

with

$$\bar{V}^{(5)}(\tau_j) = \int_{0}^{\beta} d\tau_5\; C^{\circ}(15)C^{\circ}(25)C^{\circ}(53)C^{\circ}(54)D^{\circ}(14)D^{\circ}(23) \qquad (6.73)$$

At low temperatures, the Fourier transform of this is ,

$$\bar{V}^{(5)}(\bar{\alpha}_1\bar{\alpha}_2;\bar{\alpha}_3\,\bar{\alpha}_4) = \beta\,\delta(\bar{\alpha}_1+\bar{\alpha}_2-\bar{\alpha}_3-\bar{\alpha}_4)\prod_{j=1}^{4}(B-i\bar{\alpha}_j)^{-1} \qquad (6.74)$$

so

$$\beta^{-2} \sum_{\alpha\alpha'} F(\underline{k}, \bar{\alpha})F(\underline{k}', \bar{\alpha}')\bar{V}^{(5)}(\bar{\alpha}\bar{\alpha}'; \bar{\alpha}'\bar{\alpha}) = \frac{2^4 \beta \bar{b}_{\underline{k}} \bar{b}_{\underline{k}'}}{J^2(\underline{k}).J^2(\underline{k}')} \qquad (6.75)$$

This gives a contribution

$$-\beta \Delta F^{(5)} = \frac{\beta}{2N} \sum_{kk'} \bar{b}_{\underline{k}} \bar{b}_{\underline{k}'} \left(J(\underline{k}-\underline{k}') + J(\underline{0})\right) \qquad (6.76)$$

So to O (T^3) in contributions to ΔF one has

$$\Delta F\ (4+5) = \frac{1}{2N} \sum_{kk'} \bar{b}_{\underline{k}} \bar{b}_{\underline{k}'} \left(J(\underline{k}) + J(\underline{k}') - J(\underline{k}-\underline{k}') - J(\underline{0})\right) \qquad (6.77)$$

This is the well - known result for spin - wave scattering in the first Born approximation at low temperatures obtained by Dyson,[63)] who also showed the cancellation to $O(T^3)$ giving the famous $O(T^4)$ result (or see Mattis.[5)])

If the sum of these two vertices is defined, as V, then all the relevant low - temperature spin - wave results can be derived directly, so

$$V(1,2;3,4,) = V^{(4)}(1,2;3,4) + N\,V^{(5)}(1,2;3,4). \qquad (6.78)$$

In the low temperature region this has the transform

$$V\ (p_1 p_2, p_3 p_4) = \tfrac{1}{2}\beta N\, \delta(p_1+p_2-p_3-p_4)\left[J(\underline{k}_1-\underline{k}_4) - 2B + i\bar{\alpha}_1 + i\,\bar{\alpha}_2\right]$$

$$\cdot \prod_{j=1}^{4} \frac{J(\underline{k}_j)}{(B - i\bar{\alpha}_j)} \qquad (6.79)$$

where the 4 - dimensional notation has been used, $p_j = \underline{k}_j, \bar{\alpha}_j$.

The simple spin - waves $F(\underline{k}, \omega)$ can now be renormalized through the vertex V to the renormalized form $F^r(\underline{k},\omega)$ by means of a Dyson equation directly analogous to the one for C -on renormalization in the molecular field approximation i.e. as illustrated in Fig. (16) . So upon taking into account all possible exit and entry vertex points one obtains for the spin - wave self - energy $\Xi^r(\underline{k}, \omega)$

$$\Xi^r_{qq}(\underline{k}, \alpha) = \frac{N}{(2N)^4} \beta^{-2} \sum_{\underline{k}' \alpha'} F(\underline{k}', \bar{\alpha}')\big(V(pp',pp') + V(pp',p'p) + V(p'p,p'p) + V(p'p,pp')\big) \qquad (6.80)$$

which, in the low temperature approximation becomes

$$\frac{1}{2N} \cdot \frac{J(k)^2}{(B-i\bar{\alpha})^2} \sum_{k'} b_{\underline{k}'}^{-} \big(J(\underline{0}) + J(\underline{k}-\underline{k}') - J(\underline{k}') - 2(B - i\bar{\alpha})\big) \qquad (6.81)$$

Thus, by Eq. (6.44)

$$F^r(\underline{k}, \bar{\alpha}) = (E(\underline{k}) - i\bar{\alpha})^{-1} \qquad (6.82)$$

with

$$E(\underline{k}) = ½(J(\underline{0}) - J(\underline{k})) - 1/N \sum_{k'} b_{\underline{k}'}^{-} \big(J(\underline{0}) + J(\underline{k}-\underline{k}') - J(\underline{k}') - J(\underline{k})\big) \qquad (6.83)$$

This is the usual Hartree - Fock spin - wave renormalization result, in this case obtained by approximating

$\Xi^r_{qq'}(\underline{k}, \bar{\alpha})$ by $\Xi^r_{qq'}(\underline{k}, \omega(\underline{k}))$ or self - consistently by $E(\underline{k})$.

The damping term is introduced into the first self-energy graph which has "dynamic" spin - wave contributions in the intermediate states as in Fig. 23b in distinctionto Fig. 23a , which only has a "static" intermediate spin - wave. The equivalent self - energy diagram corresponding to Fig. 23a gives a self - energy contribution corresponding to Eq. (6.80) of

$$2^{-10} N^{-3} \beta^{-2} \sum_{p_2 p_3 p_4} F(p_2) F(p_3) F(p_4) \delta(p + p_2 - p_3 - p_4) \; . \qquad (6.84)$$

$$Q(p\, p_2;\, p_4) [\, Q(p_3 p_4;\, p) + Q(p_3 p_4;\, p_2)] \frac{J^2(k)}{(B - \bar{\alpha})^2} \prod_{j=2}^{4} \frac{J^2(k_j)}{(B - i\bar{\alpha}_j)^2}$$

where $Q(p_i p_j, p_n) = J(k_i - k_n) + J(k_j - k_n) - 4B + 2i(\alpha_i^{\pm} \alpha_j)$ (6.85)

Instead of evaluating this rigorously the low temperature substitutions $i\bar{\alpha}_j = \omega(\underline{k}_j)$ will be made to exhibit the approximations used in earlier theories,(which, in fact, violates the δ - function on the frequencies $\delta(p_j)$).

Thus

$$\Xi(\underline{k}, \alpha) = \frac{1}{N^3 \beta^2} \sum_{(p_2 p_3)} G(\underline{k}, \underline{k}_2, \underline{k}_3) F(p_2) F(p_3) F(p + p_2 - p_3) \qquad (6.86)$$

where

$$G(\underline{k}, \underline{k}_2, \underline{k}_3) = \tfrac{1}{2}(J(\underline{k}) + J(\underline{k}_2) - J(\underline{k}_3 - \underline{k}_2) - J(\underline{k}_3 - \underline{k})\;) \; x$$

$$.\, (J(\underline{k}_3) + J(\underline{k} + \underline{k}_2 - \underline{k}_3) - J(\underline{k}_3 - \underline{k}) - J(\underline{k}_3 - \underline{k}_2)\;) \qquad (6.87)$$

The final result for the damped spin - wave, in this approximation, is

$$F^{d}(\underline{k},\bar{\alpha}) = [E(\underline{k}) - i\bar{\alpha} - \Xi^{d}(\underline{k},\bar{\alpha})]^{-1} \qquad (6.88)$$

with

$$\Xi^{d}(\underline{k},\alpha) = \frac{1}{N^{2}} \sum_{23} \frac{G(\underline{k};\underline{k}_2,\underline{k}_3)\; M(\underline{k};\underline{k}_2,\underline{k}_3;\beta)}{[E(\underline{k}_3) + E(\underline{k}+\underline{k}_2-\underline{k}_3) - E(\underline{k}_2) - i\bar{\alpha}]} \qquad (6.89)$$

with

$$M(\underline{k};\underline{k},\underline{k};\beta) = b^{-}(\underline{k}_3)(b^{-}(\underline{k}_2) - b^{-}(\underline{k}+\underline{k}_2-\underline{k}_3))\; b^{-}(\underline{k}_2)\,b^{-}(\underline{k}+\underline{k}_2-\underline{k}_3) \qquad (6.90)$$

where the renormalized notation has been used

$$b^{-}(\underline{k}) = (\exp\beta E(\underline{k}) - 1)^{-1} \qquad (6.91)$$

In terms of the analytically continued values $i\bar{\alpha} = \omega \pm is$ for $s \longrightarrow 0^{+}$, the results of Tahir - Kheli and ter Haar,$^{71)}$ for the damping coefficient $\gamma(\underline{k},\omega)$, and the real shift $R(\underline{k},\omega)$ are obtained,

$$\Xi(\underline{k},\omega \pm is) = R(\underline{k},\omega) \pm i\gamma(\underline{k},\omega) \qquad (6.92)$$

The results in this section well illustrate the ideal spin - wave methods of Dyson and others. The T^{4} contribution to the free - energy is obtained from the Dyson form of the Heisenberg model, by considering only the first order terms in the interaction operator.

Thus, in terms of the ideal spin - wave, boson operators $a_{\underline{k}}$ and $a^{+}_{\underline{k}}$ the interaction Hamiltonian is

$$H_1^{\text{Dyson}} = \frac{1}{4N} \sum_{kkq} \Gamma(\underline{kk}'\underline{q})\, a^+_{\underline{k}}\, a^+_{\underline{k}'}\, a_{\underline{k}-\underline{q}}\, a_{\underline{k}'+q} \qquad (6.93)$$

$$\text{with} \quad \Gamma(\underline{kk}'\underline{q}) = J(\underline{k}) + J(\underline{k}') - 2J(\underline{q}) \qquad (6.94)$$

So

$$\Delta F^{\text{Dyson}} = \frac{1}{4N} \sum_{kkq} \Gamma(\underline{kk}'\underline{q}) \langle a^+_{\underline{k}}\, a^+_{\underline{k}'}\, a_{\underline{k}-\underline{q}}\, a_{\underline{k}'+\underline{q}} \rangle \qquad (6.95)$$

or

$$\Delta F^{\text{Dyson}} = \frac{1}{2N} \sum_{kk'} \bar{b}_{\underline{k}}\, \bar{b}_{\underline{k}'}\, (J(\underline{k}) + J(\underline{k}') - J(\underline{k}-\underline{k}') - J(\underline{0})) \qquad (6.96)$$

This is identical with Eq. (6.77). The correspondence occurs because of the method of representing "bose-like" operators S by pairs of fermion operators. This necessitates 4th order graphs (or their equivalent) in the present notation before spin - wave interactions can occur. Consequently one can always identify graphs in the present method with any resulting from spin - wave theory. The advantage of the present method is that it is well - defined throughout the whole temperature regime (in distinction to spin - wave theory, which is strictly valid only at low temperatures, $e^{-\frac{1}{2}\beta J(\underline{0})} << 1$ as Dyson has shown). Moreover, the kinematic restrictions are built directly into the present theory through the dynamical nature (C -ons and D -ons) of the equivalent vertices , and can, in principle, be evaluated at any finite temperature.

Chapter 7.

SUMMARY, CONCLUSIONS, and PROSPECTS.

At the beginning of this thesis the fundamental concepts of the linear response formalism were first introduced , as a natural precursor to the exact (Heisenberg picture) spin - operator averages, and the idea of generalized spin susceptibility functions. The standard methods of Quantum Field Theory cannot be applied to the analysis of these functions, as there is no simple Wick's theorem to decompose products of spin - operators, unlike the usual case for bosons or fermions. Consequently, various fermion representations were analysed, with a view to their possible usefulness in such spin problems.

The 2S fermion spin representation, which was first presented here, has been found useful for converting electronic problems, involving second - quantized electron operators, into an equivalent formulation, involving a Hamiltonian which contains only explicit spin operators. This was demonstrated explicitly for both the Kondo model of isolated localized spins, interacting with the conduction electrons, and for the Heisenberg model of a ferromagnet.

The simplest example of the 2S fermion representation, namely, $S = \frac{1}{2}$, was found by Yolin 9) to give a comparatively simple Wick's theorem for such operators; but the analysis given here indicated that this cannot be easily extended to S = 1, or higher spin values. Abrikosov's 10) method for the 2S+ 1 fermion representation has also been reviewed here and the difficulties associated with this method mentioned.

The representation which has been found to be the most useful in the present work is the drone - fermion representation which has been extended here to all spin values, from the previously known case for S = ½. An investigation of the eigenstates of this representation resulted in two Wick's theorems for spin operators, which were first demonstrated here for S = ½ and S = 1. The Wick theorem for S = ½ has very simple properties, for, unlike that for S = 1 or that of Yolin,9) it involves no normalization factor, and this is important in many - spin problems. As these techniques are immediate extensions of conventional many-body theory, no new elaborate diagrammatic rules need to be formulated - unlike most other attempts at this problem.

The main application of these methods has been to the problem of well - localized magnetic moments, interacting with the spins of the conduction electrons of the host metal. The first example of this Hamiltonian involved only one impurity spin (i.e. the low concentration limit) - the so - called Kondo problem. In the investigation of the static and dynamic magnetic properties of the impurity spins, a log T term was found in the second - order g - shift. This then resulted in the same log T term found in the static susceptibility by several other authors. These particular quantities need to be evaluated in higher orders of the interaction , in order to investigate the low temperature magnetic properties of the impurity, for several authors have indicated that the local moment is quenched by the conduction electrons (for $J< 0$), below the Kondo temperature T_k. Unfortunately most of the work on this point has been carried out on dilute alloys of iron in copper[90-1)] - a better check of the theory might be with rare - earth ions, where the Kondo model is expected to be a better approximation.

The present high - order results for the electron self - energy part M (Eq. (5.75 - 6)) can be compared and contrasted with earlier results of several other authors who have also investigated this Hamiltonian. However, apart from Doniach[11.)], all these authors have calculated M directly, without the aid of V (Eq(5.74)); they have thus included a divergence at T_k for τ_f^{-1} and then restricted their solutions to the high temperature region $T > T_k$. Although the use of V gives a convergent result, it may be invalid to assume that it is the only analytic result below T_k, for a series of terms has been summed in V, beyond its radius of convergence, which occurs at T_k. This may indicate that a possible type of condensation forms around the local moment in this temperature regime; but more sophisticated techniques need to be applied to the present formalism before a definite answer can be given. However, Yosida[48.)], like Nagaoka[41.)] has found anomalies in this region, when he applied conventional perturbation theory to a singlet - correlated ground - state wave - function at 0^oK for $J < 0$. This resulted in an energy approximately k_BT_k lower than the corresponding uncorrelated ground - state. Doniach[11.] has summed a series of self - energy diagrams using his zero - temperature spin - Wick theorem. Although this method results in a resonance, rather than a divergence at T_k, two points must be mentioned. Due to an ansatz extension to finite temperatures, the resulting value of T_k is too small, and because of his method of averaging, the two total spin components ($S = \frac{1}{2}$), $S_T = 1$ and $S_T = 0$ differ from each other, even in zero magnetic field. This latter separation into S_T channels shows up in an instability in the effective potential for $S_T = 0$ but not for $S_T = 1$ - the former having the wrong sign throughout the whole temperature range.

The first successful finite temperature calculation using a perturbational method and treating the spin operators correctly, was that of Abrikosov[10.] who used the method outlined in Chapter 3, and summed a series of "parquet - diagrams" , which , in essence, are similar to most of the self-energy terms treated in the present thesis. The result is quoted in Chapter 5, Eq. (5.58).

Suhl and Wong[42.] have also investigated this problem using Chew - Low scattering theory, but little contact seemed to exist between this approach and those of other authors. However, Silverstein and Duke[92.] have recently shown an exact agreement between Suhl's approach and that of Abrikosov, by imposing the restriction of "on - shell" energies in the scattering amplitude; this also removes any complex poles which have sometimes appeared in recent theories. As a final summary of the basic results of these theories the following parameter "x" , predicted by each theory, is tabulated in Table 2. This parameter is defined for the anti - ferromagnetic case ($J < 0$) by the resonance condition given in equations like Eq. (5.70a) and always converted to the present band - structure and notation, that is

$$1 + x\rho J \quad \ln.\left(\frac{\zeta D}{k_B T_k} \right) = 0$$

Table 2.

Authors.	x
Nagaoka(11)	2
Takano, Ogawa	3/2
Abrikosov	2
Silverstein, Duke	2
Doniach	1
Present calculation	2

It is the exponential dependence of T_k on x which makes its magnitude important if any experimental verification is to be attempted. The damping term τ_k^{-1} (or, equivalently, the spin - impurity resistivity, Eq.(5.78)) is also plotted against the reduced temperature T/T_k for $J < 0$ in Fig. (24)

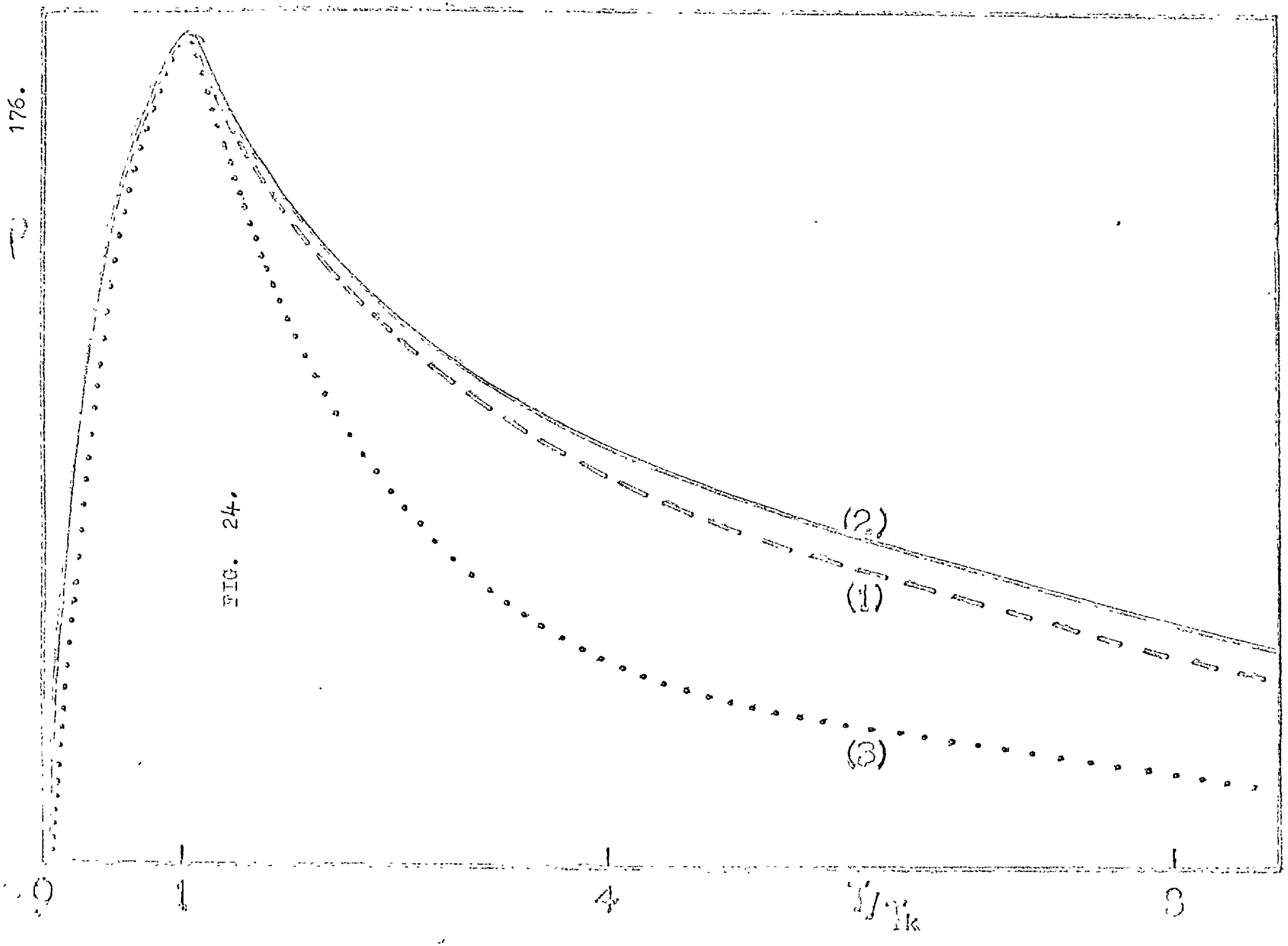


FIG. 24.

The present result is denoted by curve 1, and is contrasted with the modified (high temperature) result of Nagaoka[41.] Eq. (5.84) or Abrikosov[10.], described by curve 2, and also with one of Doniach's[11.] extrapolated results for $S_t = 1$, and illustrated by curve 3 - the latter form is relative to its own T_k. As can be seen, the resonance is not very sharp (this was anticipated by Abrikosov, but was not proved) of width about $3T_k$. This would not seem to indicate a sharp phase transition, as was predicted by Takano and Ogawa[44.]. However, it seems quite likely that all transport properties[22.](like the electrical resistivity) will have smoothly varying properties through T_k, so that experimental investigations should concentrate on properties of the localized spins, for example, the magnetization, where the changes may be more dramatic.

For higher concentrations, the effects of inter - impurity interactions have been shown to be important. When large spin - orbit damping of the conduction electrons exists, it has been shown here , in a microscopic theory, **that** the full first - order Yosida shift appears (section(5.5)) and this needs to be extended to higher orders. The same microscopic theory has also predicted the so - called "bottle - neck" effect, where the local - moment line - width narrows with increasing impurity concentration, and **the** expected Korringa width fails to appear. These techniques are presently being extended to the situation where the local moment is further coupled to the nuclear spin to investigate the effect on the resulting line - shapes.

The rare - earth metals were finally considered, and the ferromagnetic state investigated. A sub - set of diagrams led to Eq. (5.130), which exhibited the coupling of the two spin - wave systems. In the static limit the two spin modes were explicitly demonstrated. These results give a perturbation basis to the decoupling method of Doniach and Wohlfarth 59.), who analysed the dilute Fe in Pd model.

The final example of the new techniques introduced in this thesis was a systematic fermion analysis of the Heisenberg model of ferromagnetism. The usual high - density classification in inverse powers of the correlation - number z , carried out to zeroth and first order, resulted in molecular field theory, and simple spin - wave theory respectively. A low temperature classification, similar to that of Stinchcombe et al 81.) has also been carried out, which extended the validity of these high - density results throughout the whole temperature range, and which systemantically accounted for the kinematical effects of ideal spin - wave theory. Further terms introduced spin - wave scattering effects as the next important contribution to the free - energy at low temperatures. The cancellation of the T^3 term was demonstrated, leaving Dyson's T^4 term in the first Born approximation. Higher order terms, in the interaction, resulted in spin - wave re-normalization and damping - this exhibited the nature of the approximation used by other methods, such as decoupling of the equations of motion of the spin Green's functions. The explicit form of these higher order effects found here suggests that some finite temperature calculations should be considered.

In conclusion, it can be stated that the present techniques for handling spin problems, introduced in this thesis, have a wide range of applications, in many branches of current interest in Solid - State - Physics.

APPENDIX A.

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Standard Many - Body Theory for Fermions or Bosons.

The statistical mechanics of a many - body system is characterized by its Hamiltonian operator H and its total number operator N. For systems where the ground - state energy $E_o(N)$ increases monotonically with the number of particles it is possible to define a chemical potential μ (independent of N) by

$$\mu = E_o(N+1) - E_o(N) \qquad (A.1)$$

The thermodynamics of such a system at temperature T (or $\beta^{-1} = k_B T$, where k_B is Boltzmann's constant) is then described in a grand - canonical ensemble by the combined operator K, where,

$$K = H - \mu N \qquad (A.2)$$

and the density operator,

$$\zeta = e^{-\beta K} \qquad (A.3)$$

The grand-partition function Z is defined in the sum over all states of the density operator, which are simultaneous eigenstates of H and N, that is ,by a trace over such states,

$$Z = \mathrm{Tr.}\,(\zeta) \qquad (A.4)$$

Moreover, the thermodynamic average of any operator which measures some property of the system is given by its weighted average and denoted by

$$< A > \quad = \quad Z^{-1} \; \mathrm{Tr.} \, (\zeta A) \qquad (A.5)$$

This is independent of the picture chosen to represent the time development of the operator. It is the purpose of Many - Body physics to evaluate such averages. The present thesis will use diagrammatic perturbation theory to arrive at approximations to such averages. In the particular case of "free" systems, theaverages can be evaluated exactly in the number representation (second quantization) of the system. If the particles are diagonalized in the p-representation then $N_p = a_p^+ \; a_p$ is the number operator for particles labelled p, where the operators are defined by,

$$[a_p \, , a_{p'}^+]_{-\eta} \quad = a_p \, a_{p'}^+ - \eta \, a_{p'}^+ a_p = \delta_{pp'} \qquad (A.6)$$

The combined notation $\eta = 1$ for bosons and $\eta = -1$ for fermions has been introduced. The eigenvalue spectrum is then defined by

$$K_o \quad = \quad \sum_p \xi_p \; a_p^+ \; a_p$$

$$\text{with} \qquad \xi_p \quad = \quad \varepsilon_p \; - \; \mu \, . \qquad (A.7)$$

The corresponding density operator is $\zeta_o = e^{-\beta K_o}$, so the average number of particles labelled p is given by

$$\bar{n_p} \quad = \quad < a_p^+ \, a_p >_o \; = Z_o^{-1} \, \mathrm{Tr}(\zeta_o \; a_p^+ \; a_p) \qquad (A.8)$$

The corresponding number of holes is given by

$$n_p^+ = < a_p a_p^+ >_o \text{ , so } \quad n_p^+ - \eta\, n_p^- = 1 \qquad (A.9)$$

Since the trace is over all eigenstates of N_p, it is invariant under cyclic permutations of the operators, so using $e^{-x} e^{x} = 1$:

$$\text{Tr.}\,(\zeta_o\, a_p^+ a_p) = \text{Tr.}\,(e^{-\beta K_o} e^{\beta K_o} a_p\, e^{-\beta K_o} a_p^+) \qquad (A.10)$$

The following identity is frequently used; it is obtained by differentiating with respect to λ and then integrating, after evaluating the resulting commutator:

$$a_p\,(\lambda) = e^{\lambda K_o} a_p\, e^{-\lambda K_o} = e^{-\lambda \xi_p} a_p \qquad (A.11)$$

Using this in (A.10) with $\lambda = \beta$ and extracting the scalar exponential, one has,

$$\text{Tr.}(\zeta_o\, a_p^+ a_p) = e^{-\beta \xi_p}\, \text{Tr}\,(\zeta_o a_p\, a_p^+) \qquad (A.12)$$

Dividing by Z_o, using (A.6) and rearranging one obtains the final result,

$$n_p^- = (e^{\beta\xi_p} - \eta)^{-1} \qquad (A.13)$$

So the two fermi functions $f^{\pm}$ and the two bose functions $b^{\pm}$ are defined as

$$f_p^{\pm} = (e^{\mp\beta\xi_p} + 1) \; ; \quad b_p^{\pm} = \mp(e^{\mp\beta\xi_p} - 1) \qquad (A.14)$$

It is now possible to define the temperature - ordered single particle Green's functions by introducing the Wick ordering operator Tw (with $\tau = it$) defined by comparing (A.15) with (A.16).

$$G^{0}_{pp'}(\tau-\tau') = \langle Tw(a_p(\tau), a^{+}_{p'}(\tau'))\rangle_0 \quad (A.15)$$

In the diagonal representation or interaction picture (A.7), this becomes (with $\bar{\tau} = \tau-\tau'$)

$$G^{o}_{pp'}(\bar{\tau}) = \delta_{pp'}\, e^{-\xi_p \bar{\tau}} \left(\theta(\bar{\tau})\, n^{+}_{p} + \eta\theta(-\bar{\tau})\, n^{-}_{p} \right) \quad (A.16)$$

where $\theta(\tau) = 1$ if $\tau > 0$ and 0 if $\tau < 0$;

These results can readily be extended to realistic systems where there are now interactions described by an additional term in the Hamiltonian H_1 (containing more than 2 operators), so

$$H = H_0 + H_1 \quad (A.17)$$

In general, the Heisenberg picture is related to the interaction picture by the following generating function $U(\tau, \tau')$ defined by :

$$U(\tau, \tau') = e^{K_0 \tau}\, e^{-K(\tau-\tau')}\, e^{-K_0 \tau'} \quad (A.18)$$

The two forms of the density operator are related by U for the special case $\tau = \beta$, $\tau' = 0$, denoted $U(\beta)$, so

$$\zeta = \zeta_0 \, U(\beta) \qquad (A.19)$$

Taking the trace of this equation, and multiplying and dividing by Z_0, one has the fundamental equation

$$Z = Z_0 \, \langle U(\beta) \rangle_0 \qquad (A.20)$$

The operator $U(\tau,\tau')$ satisfies the differential equation,

$$\frac{\partial}{\partial\tau} U(\tau,\tau') = -H_1(\tau)\, U(\tau,\tau') \qquad (A.21)$$

this can be iteratively integrated with the boundary condition $U(\tau,\tau) = 1$ to give for the nth term, (A.22)

$$U^n(\tau,\tau') = (-1)^n \int_{\tau'}^{\tau} d\tau_n \, H_1(\tau_n) \int_{\tau'}^{\tau_n} d\tau_{n-1} H_1(\tau_{n-1}) \cdots$$

$$\cdots\cdots \int_{\tau'}^{\tau_2} d\tau_1 H_1(\tau_1)$$

The upper limits can be equated by introducing the Dyson ordering operator P, which orders following operators from right to left in order of their decreasing temperature arguments ; this also produces a degeneracy factor of $(n!)^{-1}$. Formally this can be re-summedto the exponential form:

$$U(\tau,\tau') = P \exp\left(-\int_{\tau'}^{\tau} d\tau_1 \; H_1(\tau_1) \right) \qquad (A.23)$$

The "temperature" -dependence of operators in the Heisenberg picture (denoted $\bar{A}(\tau)$) is given by

$$\bar{A}(\tau) = e^{K\tau} A e^{-K\tau} \tag{A.24}$$

So, using the unity insertion, as in (A.10), one has

$$\bar{A}(\tau)\bar{B}(\tau') = e^{K\tau} A e^{-K_o\tau} U(\tau,\tau') B(\tau') U(\tau',o) \tag{A.25}$$

Introducing Wick ordering of the operators and remembering that U only involves H_1 or P ordering, one can rearrange the operators to use the identity

$$U(\tau,\tau_1) U(\tau_1,\tau') = U(\tau,\tau') \tag{A.26}$$

Finally, on dividing by Z and using Eq. (A.20) one has

$$< Tw\ (\bar{A}(\tau)\bar{B}(\tau')) > = \frac{< Tw\ (A(\tau) B(\tau') U(\beta)) >_0}{< U(\beta) >_0} \tag{A.27}$$

Note that this method does not depend on the adiabatic hypothesis of S - matrix theory.

In the perturbational approach, one expands the operator $U(\beta)$ according to (A.23) and uses Wick's theorem (Appendix B) to expand the ordered products of single particle operators in each term, into all possible conjugate pairs of ordered operators. If each contraction, $G^o_p(\tau - \tau')$, is represented diagrammatically by a directed linefrom τ' to τ, then the usual Linked - Cluster theorem (see Abrikosov et al, P.128.) can be invoked for retaining only those diagrams which are continuously linked to the "external" operators in the average. Only onediagram of each topologically distinct type is to be considered; this removes the factor n! in the denominator; thus

$$< T_W \left(\bar{A}(\tau), \bar{B}(\tau') \right) > \tag{A.28}$$

$$= \sum_{m=0}^{\infty} (-1)^m \int_0^\beta d\tau_1 \ldots d\tau_m < T_W \left(A(\tau)\, B(\tau')\, H_1(\tau_1) \ldots H_1(\tau_m) \right) >_0^{Ld}$$

The free - energy F of the system is given by

$$-\beta F = \log Z \tag{A.29}$$

So by Eq. (A.20) the change in the free - energy ΔF, due to the interaction, is given by

$$-\beta \Delta F = \log < U(\beta) >_0 \tag{A.30}$$

An alternative form of the Linked - Cluster theorem is

$$< U(\beta) >_0 = \exp < U(\beta) >_0^{con.} \tag{A.31}$$

where the superscript denotes that only topologically distinct, connected diagrams are to be considered. Thus one has the important perturbational result,

$$-\beta \Delta F = < U(\beta) >_0^{con.} \tag{A.32}$$

Finally, the periodic nature of the temperature-dependent Green's functions is shown and their Fourier transforms defined. If the exact Green's function defined like (A.15) but in the Heisenberg picture, is written in the form,

$$G_p(\tau) = \Theta(\tau)\, G_p^{>}(\tau) + \Theta(-\tau)\, G_p^{<}(\tau) \qquad (A.33)$$

then

$$G_p^{>}(\tau) = <\bar{a}_p(\tau)\, \bar{a}_p^{+}(o)> = Z^{-1}\mathrm{Tr}(\bar{a}_p(\tau)\bar{a}_p^{+}(o)) \qquad (A.34)$$

If the operator $\bar{a}_p^{+}$ is cyclically transferred around the trace and using the unity identity as in (A.10) for ζ then

$$G_p^{>}(\tau) = <\bar{a}_p^{+}(o-\beta)\, \bar{a}_p(\tau)> = \eta G_p^{<}(\tau-\beta) \qquad (A.35)$$

Now $-\beta < \tau-\tau' < \beta$ so if $\tau > 0$ then

$G_p(\tau) = G_p^{>}(\tau)$ while $G_p(\tau-\beta) = G_p^{<}(\tau-\beta)$

so one has

$$G_p(\tau) = \eta\, G_p(\tau-\beta) \qquad (A.36)$$

Since it is periodic with period β it can be expanded in a Fourier series in terms of a new integral variable ε.
If it is evenly periodic (bose - like) this will be denoted α and ν if it is odd - periodic (fermions), where

$$\bar{\alpha} = 2\alpha\, \Pi\, \beta^{-1} \quad \text{and} \quad \bar{\nu} = (2\nu+1)\, \Pi\, \beta^{-1} \qquad (A.37)$$

and α or ν take all integer values, including zero.

So

$$G_p(\tau) = \frac{1}{\beta}\sum_{\varepsilon} e^{-i\bar{\varepsilon}\tau}\, G_p(\bar{\varepsilon}) \qquad (A.38)$$

The transform is defined by

$$G_p(\varepsilon) = \int_0^{\beta} d\tau\, e^{i\bar{\varepsilon}\tau}\, G_p^{>}(\tau) \qquad (A.39)$$

For the special case of free particles (A.7), one readily finds

$$G_p(\bar{\varepsilon}) = (\xi_p - i\bar{\varepsilon})^{-1} \qquad (A.40)$$

In terms of the analytically continued variable $i\bar{\varepsilon} = \omega$ the function $G_p(\bar{\varepsilon})$ can be continued into the whole of the complex ω - plane. By Carlemann's theorem this is unique if it is bounded as $\omega \longrightarrow \infty$ along any straight line in the upper or lower half - planes, and is <u>analytic</u> off the real - axis (Baym and Mermin)$^{18)}$

The sum over these discrete points can be found from the residues of the following integrand, involving the contour C.

$$G_p(\tau) = \frac{1}{2\pi i}\int_c d\omega\, e^{-\omega\tau}\, G_p(\omega)\, n^+(\omega)\,\left(\Theta(\tau) + \eta\Theta(-\tau)e^{-\beta\omega}\right) \qquad (A.41)$$

where $$n^+(\omega) = (1 - \eta e^{-\beta\omega})^{-1} \qquad (A.42)$$

The contour C encircles the whole of the imaginary ω - axis for $\eta = 1$ (the bose - contour C_b), and encircles the whole of the imaginary ω -axis, except for the origin for $\eta = -1$ (the fermi - contour C_f). The direction is anti - clockwise in both cases.

This technique can be used for any periodic function (e.g. self - energy sums) and if the integrand is convergent at infinity, then either limit in (A.41) will give the same result.

APPENDIX B

Wick's Theorem for Fermions of Bosons.

Gaudin's method for deriving a thermal version of Wick's theorem for bose or fermi particles is presented here.[88)] Consider a set of creation and destruction operators $A_1 \ldots A_m$ written in the temperature interaction picture, and their "free" averages, X. In the notation of Appendix A, one has

$$X = < A_1 A_2 \ldots A_m >_o = Z_o^{-1} \mathrm{Tr} (\zeta_o A_1 \ldots A_m) \quad (B.1)$$

where A_j represents $a_{pj} (\tau j)$ or $a^+_{pj} (\tau j)$. Moreover, for fermions or bosons ($\eta = \pm 1$) one has (A.6)

$$A_i A_j - \eta A_j A_i = [A_i, A_j]_{-\eta} \quad (B.2)$$

The commutator (or anti - commutator) on the R.H.S. of (B.2) will be called an η- commutator and is either a Kronecker delta or zero if both operators are of the same type - in either case it is a c - number; so,

$$X = \eta < A_2 A_1 A_3 \ldots A_m >_o + < A_3 A_4 \ldots A_m >_o [A_1, A_2]_{-\eta} \quad (B.3)$$

Similarly, the operator A_1 can be η-commuted through all the operators, each time adding an η - commutator term as in (B.2), eventually

$$< A_2 \ldots A_1 A_m >_o = \eta < A_2 \ldots A_m A_1 >_o + < A_2 \ldots A_{m-1} >_o [A_1, A_m]_{-\eta}$$

The operator A_1 can now be transferred around the trace as in

Eq.s (A.10 - 12), so

$$\langle A_2 \dots A_m A_1 \rangle_o = e^{\pm\beta\xi p_1} X \qquad (B.4)$$

The plus (minus) sign occurs if A_1 is a creation (destruction) field and denoted by μ, where $\mu = \pm 1$. Transferring this term to the R.H.S. of the final form of (B.3) one has

$$X \; (1 - \eta^{m-1} e^{\mu_1 \beta\xi p_1}) = \sum_j \eta^{j-2} \langle A_2 \dots (A_j) \dots A_m \rangle_o [A_1, A_j]_{-\eta} \qquad (B.5)$$

The notation (A_j) means that this operator is absent from the average. Moveover, since there must be an equal number of creation and destruction operators in any average, then m must be even, so $\eta^m = 1$, thus

$$X = \sum_{(1,j)} \eta^{j-2} \frac{\langle A_2 \dots A_m \rangle_o \; [A_1, A_j]_{-\eta}}{1 - \eta e^{\mu_1 \beta\xi p_1}} \qquad (B.6)$$

where the notation (i, j) in the summation means the two operators A_i and A_j are removed from the average in the form of an η - commutator, and are then summed over the range 1 to m.

However from (A.15 - 16) one has

$$\langle A_1 A_j \rangle_o = [A_1, A_j]_{-\eta} (1 - \eta e^{\mu_1 \beta\xi p_1})^{-1} \qquad (B.7)$$

so $$\langle A_1 A_2 \dots A_m \rangle_o = \sum_{(1,j)} \eta^{j-2} \langle A_2 \dots A_m \rangle_o \langle A_1 A_m \rangle_o \qquad (B.8)$$

The thermal - contraction between two operators is defined as in (A.15) and now written in the short - hand notation:

$$\dot{A}_1\dot{A}_2 = < \mathrm{Tw}(A_1(\tau_1) , A_2(\tau_2)) >_0 \qquad (B.9)$$

Equation (B.8) is now temperature - ordered according to the decreasing temperature arguments of the operators. If the operators are fermions, then a permutation factor $(-1)^P$ for re -ordering under this operator is introduced, but not if they are bosons, so

$$< \mathrm{Tw} \, (A_1A_2\ldots A_m) >_0 = \sum_{(1,j)} \eta^{j-2} \dot{A}_1\dot{A}_j < \mathrm{Tw}(A_2\ldots A_m) >_0 \qquad (B.10)$$

But as $\dot{A}_1 \dot{A}_j$ is just a c-number it can be incorporated into the average, while the factor η^{j-2} is just that for bringing A_1 next to A_j, thus,

$$< \mathrm{Tw} \, (A_1A_2\ldots A_m) >_0 = \sum_{(1,j)} < \mathrm{Tw}(\dot{A}_1A_2\ldots\dot{A}_j\ldots A_m) >_0 \qquad (B.11)$$

This process can be repeated for all the remaining operators inside the average until all operators occur in pair - wise contractions.

Contrary to Quantum Electrodynamics, it is possible to have non - zero contractions between operators at the same temperature, e. g. in $H_1(\tau)$, for in this method, a contraction is not defined as the difference between the T and N -ordered products. Now the contractions take the order in which they occur in $H_1(\tau)$.

APPENDIX C.

Generalized Green's Functions and their Equations of Motion.

In this appendix a slightly different notation from Zubarev[86)] will be used to exhibit the correspondence with the earlier perturbational methods. Using the notation of Appendix A for grand-canonical averages in the Heisenberg picture, one can define the following propagators or Green's functions. In general two operators A and B, which have a non-zero average, will satisfy some commutation rule of the form,

$$[A,B]_{-\eta} = C \qquad (C.1)$$

where $\eta = \pm 1$ corresponding to commutation or anti-commutation rules and C is a further operator. In the case of bosons ($\eta = 1$) or fermions ($\eta = -1$), C is just a δ-function.

In terms of such generalized commutators one can define the retarded Green's function,

$$\langle\langle A(t) \; ; \; B(t') \rangle\rangle_{ret.} = i\Theta(t) < [A(t), \; B(t')]_{-\eta} > \qquad (C.2)$$

and the advanced Green's function,

$$\langle\langle A(t) \; ; \; B(t') \rangle\rangle_{adv.} = -i \; \Theta(-t) < [A(t), B(t')]_{-\eta} > \qquad (c.3)$$

The causal time - dependent Green's function can be defined in terms of the Wick ordering operator (defined in Appendix A),

$$\langle\langle A(t) \; ; \; B(t') \rangle\rangle_{caus.} = i < T_W(A(t), \; B(t')) > \qquad (C.4)$$

A further Green's function, which has properties closely related to the time dependent ones, is the temperature dependent Green's function, denoted by round brackets.

$$((A(\tau) ; B(\tau')))_{\tau} = < T_{\tau} (A(\tau), B(\tau')) > \qquad (C.5)$$

The Green's functions will only depend on the differences of their two arguments, so in future t' will be set equal to zero. Thus, the time - Fourier transforms can be defined,

$$<< A(t) ; B(0) >> \doteq \frac{1}{2\pi}\int_{-\infty}^{\infty} dt e^{-i\omega t} << A ; B(\omega) >> \qquad (C.6)$$

Cyclic rotation of B around the trace leads to the conclusion that the temperature Green's function is periodic over τ with period β so it can be expanded in a Fourier series. (see A. 38)

$$((A(\tau) ; B(0))) = \frac{1}{\beta} \sum_{\varepsilon} e^{-i\bar{\varepsilon}\tau} ((A ; B(\varepsilon))) \qquad (C.7)$$

where, $\varepsilon = \Theta(\eta)\, \alpha + \Theta(-\eta)\, \nu$ as in A. 37 (C.8)

An analysis of the Lehmann spectral representation of all the Green's functions shows that their transforms are related by,

$$<< A ; B(\omega) >>^{*}_{\text{ret}} = << A ; B(\omega) >>_{\text{adv.}} \qquad (C.9)$$

In terms of the analytically continued form ω so that just above or below the real ω -axis, $\omega\pm$ is one has,

$$<< A ; B(\omega) >>_{\substack{\text{ret}\\ \text{adv.}}} = ((A ; B(\omega \pm is))) \qquad (C.10)$$

So the retarded (advanced) Green's function is analytic in the whole upper (lower) half plane of the complex variable ω .

Their difference across the real ω -axis or the discontinuity of the temperature Green's function is i $D_{AB}(\omega)$ and this satisfies the general sum rule,

$$\int_{-\infty}^{\infty} d\omega \; D_{AB}(\omega) \quad = \quad 2\pi < [A,B]_{-\eta} > \tag{C.11}$$

Moreover this function contains all the physical information of the Green's functions and is related to the time-ordered form by,

$$<< A\,(t)\;;\;B(o)>>_{caus.} \quad = \quad \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\, e^{-i\omega t}\; D_{AB}\,(\omega) \tag{C.12}$$
$$x(\;\Theta(t)n^{+}(\omega)+\eta\;\Theta(-t)n^{-}(\omega)\;)$$

where the generalized occupation functions have been used, (A.14).

$$n^{+}(\omega) \quad = \quad (1-\eta e^{-\beta\omega})^{-1} \;\; ; \;\; n^{-}(\omega) = (e^{\beta\omega}-\eta)^{-1} \tag{C.13}$$

In the two limits $t \rightarrow 0^{\pm}$s, one can use (C.12) to find the correlation functions $<AB>$ and $<BA>$.

The equations of motions of all the time-dependent Green's functions are identical and can be obtained using the property that the derivative of the step function is the delta function -

$$\dot{\Theta}\,(t) \quad = \quad -\dot{\Theta}\,(-t) = \quad \delta(t) \tag{C.14}$$

One also has the equation of motion of any operator in the Heisenberg picture,

$$i\dot{A}(t) \quad = \quad [\,A(t),\;K(t)\,]_{-} \tag{C.15}$$

The result of differentiating the Green's functions with respect to the time, t is,

$$<< [A(t),K(t)]_- ; B(o)>> -i \frac{\partial}{\partial t} << A(t) ; B(o)>> = \delta(t) < [A,B]_{-\eta} \qquad (C.16)$$

Using Eq.(C.6) and the identity

$$\delta(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega e^{-i\omega t} \qquad (C.17)$$

this can be transformed to,

$$<<[A,K]_- ; B(\omega)>> - \omega <<A;B(\omega)>> = <[A,B]_{-\eta}> \qquad (C.18)$$

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ADDENDA

The argument leading to the choice of graphs in the high-density expansion presented in the text is in error. The correct form is based on the observation that the $C_k{}^o$ and $D_k{}^o$ propagators are actually independent of their momentum indices, so that only the $\underline{k}$-dependence arising from the $J(\underline{k})$ factors is important. Subsequent summation over $\underline{k}$ introduces a Kronecker delta reduction in the site index summations. So a diagram involving V vertices, L of which appear with explicit $\underline{k}$-dependence, will give V-L independent site summations upon Fourier transforming. This produces a numerical factor of order $(\beta \bar{I})^V Z^{V-L}$, where Z is the number of spins interacting with any other. But from molecular-field theory (as we shall see) the critical temperature is given by $\frac{1}{4}\ \beta_c J(\underline{0}) = 1$ or approximately $Z\bar{I} = kT_c$. So such a diagram will then contribute a factor

$$\left(\frac{T_c}{T}\right)^V \quad Z^{-L}$$

Thus for temperatures above T_c the order of the graph in the high density expansion is Z^{-L}. In general there will be several explicit $\underline{k}$-factors appearing in the interaction terms, i.e. $J(\underline{k})$, due to momentum conservation, so one obtains an expansion in inverse powers of Z.

The actual diagrams chosen in the text still retain the correct 0(Z) dependence and so all the conclusions obtained therein will still be valid.

A further comment is also appropriate with regard to the selection of diagrams in the calculation of the higher order effects in the Kondo model. These diagrams correspond to the generalized T-matrix approximation (in the sense of 3 types of field). This is similar to the electron scattering T-matrix approximation in superconductivity and leads to similar problems. For now the divergence in $Q(\bar{\alpha})$ (as in Eq. 5.64), which first occurs at T_k for $i\bar{\alpha} = 0$, indicates that the radius of convergence has been reached for this particular resummation of such diagrams, see P.173. Consequently one cannot automatically extrapolate the final results, Eqs. (5.68) and (5.78), to temperatures below T_k as extra residues must be included arising from the extra poles. As the temperature is lowered conjugate poles travel outward along the imaginary part of the complex $z = i\bar{\alpha}$ plane in a similar manner to that found by Bloomfield and Hamaan (to be published in the Physical Review). Thus the discussion in chapter 7, including that covering Fig. 24, should be restricted to $T > T_k$. This leads one to expect interesting properties for the longitudinal correlation function between the two spin systems. In this case, given by the following equation

$$\langle \sigma^z S^z \rangle = 1 + \sum_{\lambda} \lambda S^z_{\lambda,-\lambda} (\tau \to 0^-)$$