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ASPECTS OF MAGNETISM AND SUPERCONDUCTIVITY IN METALS

by

J. P. WHITEHEAD

A THESIS

SUBMITTED TO THE FACULTY OF GRADUATE STUDIES AND RESEARCH

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Y. Takahashi

DATE: June 5, 1984

DEDICATION

This work is dedicated to Catherine who, despite having little interest in the content, has nevertheless both sustained and encouraged me in my endeavours and made my lot a truly happy one.

ABSTRACT

In this thesis we consider the application of certain analytical techniques, which have been developed in recent years to examine various problems in magnetism and superconductivity in metals. Wh[illegible] the more formal aspects of these techniques are not without in[illegible] emphasis here is with regard to the calculation and evaluation of experimentally accessible quantities. In the case of magnetism it is shown how the real time quantum field theoretical formulation of quantum statistical mechanics known as thermofield dynamics may be applied, together with the Ward-Takahashi identities, to evaluate the finite temperature effects of the spin fluctuations on various observable quantities, within the itinerant electron model of ferromagnetic metals. Results are obtained in both the ferromagnetic and the paramagnetic domains.

The latter part of the thesis concerns itself with a rather detailed examination of the rather complex and subtle interplay between ferromagnetism and superconductivity that occurs in ferromagnetic superconductors, such as the Chevrel and the $RERh_4B_4$ compounds. A unified treatment of the d-f interaction together with the electromagnetic interaction is presented and applied to the analysis of the mixed state in $ErRh_4B_4$, together with a detailed comparison with some recent experimental results. The method successfully accounts for the first order phase transition to the normal state at H_{c2}, observed experimentally in a very natural way.

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CHAPTER 1

INTRODUCTION

In this work we examine certain theoretical aspects of magnetism and superconductivity in metals. The two main areas of investigation concern firstly, the role of the spin fluctuations in determining the finite temperature properties of metallic ferromagnetic systems, based on the itinerant electron model, in both the ferromagnetic and paramagnetic domains. Secondly, the formulation and application of a unified theory for ferromagnetic superconductors, which considers both the electromagnetic and exchange coupling between the superconducting current and the magnetic ions. In both areas much of the theoretical content is based on analytical methods which have been developed within the last decade or so. In the case of the metallic ferromagnets virtually the entire analysis relies on the technique in real time quantum statistical mechanics referred to as Thermo Field Dynamics (TFD). The TFD formalism, developed in the early seventies[1,2], has the advantage that nearly all the devices of conventional zero temperature field theory can be generalized to the case of finite temperature. This fact of the TFD formalism allows us to investigate, among other things, the important role played by the Ward-Takahashi[3,4] identities (W-T identities) in determining the temperature dependence of various quantities in itinerant electron ferromagnets. In the case of the magnetic superconductors the work presented here is based largely on the approach to the electromagnetic properties of superconductors pioneered by Umezawa and his collaborators, known as the boson method[1,5,6,7]. This method, based on certain structural aspects concerning the operator realization of Quantum Electro Dynamics (QED) in which the phase symmetry of the electron fields is spontaneously broken, has seen widespread application with regard to the magnetic properties of both magnetic and non-magnetic superconductors[7].

While the formal aspects of TFD and the boson method are of considerable interest, and will be touched on in subsequent chapters, the content of this thesis concerns itself mainly with the applicative aspects of these techniques and how they may be used to obtain experimentally relevant results and procedures. In the case of the itinerant electron ferromagnetic system the TFD formalism is used to construct a low temperature expansion in which the various terms appearing in the expansion may be expressed in terms of certain vertices calculated at zero temperature. The practical nature of this expansion scheme is demonstrated by the calculation of the temperature dependence of various measurable quantities, arising from the thermal excitation of the magnons, using only the symmetry requirements of the W-T identities. The role of the W-T identities in ferromagnetic itinerant electron systems are further explored, within the context of the TFD formalism, in the paramagnetic region. Here it is shown how they may be used to obtain an exact expression for the static transverse susceptibility, including vertex corrections, in terms of the electron self energy. The resultant expression is used to examine corrections to the Random Phase Approximation (RPA) arising from spin fluctuations in the local contact interaction model, and a rather elegant and systematic derivation of earlier work (the Paramagnon Approximation[8] and the Self Consistent Renormalization[9] (SCR) scheme) is presented. Such corrections are known to be of crucial importance in the analysis of the magnetic properties of ^3He[8] and a class of materials known as weak itinerant ferromagnets[9].

Similarly the work pertaining to the ferromagnetic superconductors, concerns itself largely with the application of the boson method rather than the more formal, though by no means trivial aspects, surrounding the rather subtle interplay between the diamagnetic nature of the persistent current and the ferromagnetic nature of the magnetic ions. Indeed the formalism presented here was developed in order to provide a precise and realistic analysis of the recently reported[10,11] measurements concerning the magnetic properties of single crystal $ErRh_4B_4$. The application of the formalism to the analysis of the mixed state in $ErRh_4B_4$ successfully accounts for many of the peculiar properties of these results.

The plan of the thesis is as follows. In Chapter 2, we deal with some theoretical preliminaries. Section 2.1 contains a brief outline of the history of real time methods in Quantum Statistical Mechanics, some of the problems that have been encountered and to what extent they have been overcome. This is followed by a fairly detailed discussion of the TFD formalism which, it is hoped, will provide the reader with some insight into the underlying principles together with the various technical and computational devices available. The reason for such a detailed treatment is twofold. First of all, since the TFD formalism is central to much of the work presented in this thesis, it is worthwhile to consider the formalism in some depth. Secondly, while the TFD formalism is finding an increasing number of important applications in both relativistic field theory and non-relativistic many body theory, the method does not, as yet, enjoy widespread application. Indeed some of the calculations presented here were amongst some of the earlier applications of the technique.

In Section 2.2 a discussion of what have come to be known as Ward-Takahashi (W-T) identities is provided. In particular, it is shown how the canonical nature of the TFD formalism provides for an extremely straightforward extension of the identities to finite temperature. Particular emphasis is given to the case of spontaneously broken symmetry and how the arguments should be modified to take into account the features peculiar to this situation. This discussion provides us with not only a number of exact relations, which will prove to be extremely useful, but also provides the conceptual underpinnings for much of our subsequent discussion of the ferromagnetic and superconducting states, both of which correspond to states with spontaneously broken symmetry.

Chapter 3 begins with a brief review of the various theoretical approaches to ferromagnetism in metals and the distinction between the localized model and the itinerant model in Section 3.1. It is shown that while the itinerant model has had remarkable success in the determination of the ground state properties of many ferromagnetic metals, including the familiar 3d transition metals, it has so far failed to account for a wide range of the finite temperature properties. It is argued that this failure must be regarded as a result of the approximation schemes used rather than the basic model itself. We close Section 3.1 with a derivation of the W-T relations arising out of the assumed spin rotational invariance of the system. It is shown how the ferromagnetic state is to be regarded as one in which the spin rotational invariance is spontaneously broken and how Goldstone's theorem is satisfied through the appearance of the magnon excitations in the transverse susceptibility.

In Sections 3.2 and 3.3 we consider the importance to various observable quantities of the effects arising from the spin fluctuations and how they can be calculated in ferromagnetic itinerant electron systems. Particular emphasis is given to the important role played by the W-T relations. Section 3.2, for instance, considers the effect on the low temperature properties of such systems arising from the thermal excitation of the magnon modes. It is shown how an expression for the contribution from the thermal magnon density may be obtained in terms of certain zero temperature vertices following a low temperature expansion. An important aspect of this work is the result that the leading thermal contribution arising from the magnon modes may be computed entirely on the basis of symmetry by means of the W-T relations. From this it is shown how the celebrated Bloch $T^{3/2}$ for the magnetization, together with the result that the magnon corrections to the magnon excitation spectra is of order $T^{5/2}$, may be obtained in an entirely model-independent fashion and as such should be regarded as a strict requirement of the spin rotational invariance.

In Section 3.3 the W-T relations are used to obtain an expression for the static transverse susceptibility in terms of the electron self energy together with the response of the system to some small symmetry breaking terms. The result is used to obtain an expression for the corrections to the RPA arising from the spin fluctuations and it is shown what approximations are required in order to obtain the results of earlier work[8,9]. The analysis is interesting from two points of view. First of all it provides a rather elegant and systematic derivation of previous approximation schemes and secondly it provides a basis from which one may consider higher order corrections as well as a unified treatment of both the ferromagnetic and paramagnetic domains.

In Chapter 4 we turn our attention to the analysis of the magnetic superconductors. In Section 4.1 a brief review of the recent experimental and theoretical developments, following the discovery of the rare earth ternary superconductors[12,13] in the late seventies is given. Due to the relative weakness of the d-f interaction, much of the qualitative nature of these materials may be understood purely in terms of the electromagnetic interaction between the persistent current and the rare earth ions. Perhaps the most important phenomenon arising from the electromagnetic interaction is the screening of the magnetic moments by the persistent current[14]. This can be shown theoretically and gives rise to the existence of a narrow co-existent region just above the re-entrant temperature T_c [14,15,16,17,18]. Furthermore the appearance of the co-existence phase below T_p, the co-existence temperature, is accompanied by the existence of an ordering of the rare earth spins, with a relatively long wavelength modulation[14,15,16,17,18]. Both the screening of the rare earth spins[19,20] and the existence of a modulated spin phase[21,22,23,24,25] above the re-entrant temperature have been confirmed experimentally. While these results illustrate the important role played by the electromagnetic interaction certain features of these compounds do require a unified treatment of both the d-f and the electromagnetic interaction. This is particularly true of the recent measurements on the magnetic properties of single crystal $ErRh_4B_4$[10,11]. Such a formulation of ferromagnetic superconductors is presented in Section 4.2. In this the pair breaking effects induced through the d-f interaction are considered together with the electromagnetic interaction. The pair breaking effects considered include the Zeeman splitting of the electron spins due to the effective field of the rare earth ions together with the scattering of the electrons by the localized spin fluctuations. It will be shown how the effect of the scattering by the localized spin fluctuations can be realized, in the calculation of the various superconducting quantities, by means of a simple scaling law, following the definition of an effective coupling constant. An analysis of the Meissner state properties including the effect of the spin fluctuations is given. The treatment of the electromagnetic field and the persistent current is based on the boson method mentioned earlier, however since the method is widely reported in the literature on both non-magnetic[1,5,6,26] and magnetic[27,28] superconductors a brief outline will suffice in the present context.

In Section 4.3 the formalism presented in Section 4.2 is applied to the analysis of the mixed state in $ErRh_4B_4$. This includes a detailed comparison with the single crystal measurements alluded to previously[10,11]. Good agreement with the observed upper and lower critical field curves is obtained. Furthermore the magnetization curves show the appearance of a first order transition to the normal state at H_{c2} at low temperature. This is consistent with both the measured magnetization curves[11] which show a first order transition to the normal state at H_{c2} and with previous theoretical work which indicates that the slope of the magnetization curve becomes infinite at H_{c2} for some temperature $T > T_{c2}$[29,30]. Unlike the earlier analysis[29,30], the work reported here is able to treat the entire temperature domain, above the co-existence temperature T_p , in an entirely consistent fashion.

Chapter 5 comprises some concluding remarks together with a discussion regarding possible extensions of this work.

We close this introductory chapter with a brief summary of the main results contained in this work.

1) In the case of ferromagnetic itinerant electron systems the leading order contribution arising from the thermal excitation of the magnon modes may be computed at low temperatures, solely on the basis of symmetry, in an exact and model independent fashion. In particular, the Bloch $T^{3/2}$ law is recovered and it is shown that the leading correction to the magnon spectra is of order $T^{5/2}$.

2) By means of certain response identities, generated from the W-T relations, an exact expression for corrections to the RPA paramagnetic susceptibility, due to the spin fluctuations, is obtained and a number of earlier procedures (the Paramagnon Approximation and the SCR method) are recovered in a particularly straightforward fashion.

3) The formulation of the boson method in superconductivity is extended to include the pair breaking effects arising from the d-f interaction.

4) The magnetic properties of $ErRh_4B_4$ are analyzed over the entire temperature range, above T_p the co-existence temperature, including the region where the transition to the normal state at H_{c2} is first order. Good agreement with the recently reported measurements on single crystal $ErRh_4B_4$ is obtained. This is the first time, to our knowledge, that the magnetization curve with a first order transition to the normal state at H_{c2} has been calculated theoretically. Previous theoretical work on this problem has been limited to the temperature domain in which the transition is second order.

CHAPTER 2

WARD-TAKAHASHI IDENTITIES AND FINITE TEMPERATURE FIELD THEORY

2.1 Field Theory at Finite Temperature

In this section I wish to outline recent developments in the application of the techniques of Quantum Field Theory to problems in statistical mechanics. The use of Green's function techniques in statistical mechanics has largely been through the Matsubara method[31]. This method involves the use of imaginary times in the interval 0 to $-i\beta$ and provides a very powerful means whereby the Feynman graph technique in perturbation theory may be applied, suitably modified, to compute various thermodynamic quantities. The method however suffers from a number of inherent limitations. The use of imaginary time restricts the use of the technique to the computation of static quantities although certain dynamical information may be obtained if one is willing to perform a tedious analytical continuation from imaginary to real time. Also the computation of the various diagrammatic contributions involves a complicated summation over discrete frequencies, making the computation of diagrams with overlapping diagrams extremely difficult to calculate even approximately. Furthermore this summation over discrete frequencies mixes both the time and temperature effects making it difficult to identify effects arising from the thermal excitation of quanta. It is also important to note that the technique is limited to the treatment of equilibrium situations.

While many ingenious tricks have been developed to overcome some of the above-mentioned shortcomings, the analytical continuation, mentioned earlier, allows one to calculate certain dynamical quantities while simple deviations from equilibrium may be treated by means of linear response theory, the method is nevertheless cumbersome when applied to dynamical problems and when one wishes to examine the low temperature behaviour of physical systems.

Many of the limitations of the imaginary method in the calculation of real time Green's functions may be seen in the later work of Kadanoff and Baym[32] who, following some earlier work of Martin and Schwinger[33] used the imaginary time method to compute real time Green's functions at finite temperature using the procedures outlined by Baym and Mermin[34]. While this work serves to demonstrate the importance of the real time finite temperature Green's functions, particularly in the analysis of transport properties, the use of the imaginary time procedure limits the authors to rather simple approximation procedures (e.g. Generalized Hartree Fock, Random Phase Approximation, First Born Approximation).

The development of a systematic computational scheme for the evaluation of real time finite temperature was later provided for in the work of Mills[35,36], in the case of equilibrium systems and independently by Keldysh[37] and Craig[38] for non-equilibrium systems. The procedure, often referred to as the path ordering method, allows for the systematic evaluation of real time, finite temperature Green's functions in perturbation theory using the Feynman diagram technique. Significantly the path ordering method while formulated in terms of path in the complex time domain may be realized as a completely real time theory through the correct choice of contour.

In order to appreciate the significance of subsequent developments it is important to realize the distinction between a theory of

Green's functions, which involves purely the spatial and temporal development of expectation values of the quantum field operators, and the full quantum field theory, involving the construction of the appropriate Hilbert space and the realization of the operators in that space. While in principle the construction of the quantum field theory from the Green's functions is in fact possible, provided that the Green's functions satisfy certain axioms[39], such a task is by no means trivial. One may pose the question; given that one can compute the various Finite Temperature many point Green's functions, is it possible to reconstruct from them an operator realization of the original field theory? Turning the problem around a number of authors[1,2] did in fact construct a representation of the Heisenberg operators in the canonical formalism in which the resultant Green's functions are the thermodynamic averages of the time ordered operator products. The formalism known as Thermo Field Dynamics (TFD) involves a doubling of the operator degrees of freedom through the introduction of the so-called tildé fields. The importance of this development is that it allows many of the devices of conventional zero temperature field theory to be extended, in a particularly straightforward manner, to problems at finite temperature. A particularly elegant presentation of the TFD formation together with an analysis of the analytical properties of the single particle propagator was presented by Matsumoto[40] through the introduction of the so-called thermo-doublet $\left(\begin{smallmatrix}\phi \\ \tilde{\phi}\end{smallmatrix}\right)$. An interesting aside on the TFD formalism was presented by Schmutz[41] who, using the so-called superoperator formalism, has shown that the TFD formalism is in fact a particular case of a much wider class of real time finite temperature theories. However it was not realized in this work that the TFD formalism is unique, in that it is the only member of this class of theories in which the Hamiltonian is self adjoint.

A number of recent papers serve to illustrate the close relation between the various approaches. Matsumoto et al[42,43] have examined the relation between the path ordering method of Mills[35,36] and the structure of the Feynman rules in thermo-field dynamics. Niemi and Semenoff[44] have constructed the generating functionals for the thermodynamic average of time ordered products in Minkowski space using the path ordering method of Mills[35,36]. The resultant generating functional is equivalent to that obtained previously by Semenoff and Umezawa[45] from TFD. The effective potential calculated by Niemi and Semenoff agrees with the earlier result of Dolan and Jackiw[46] in the one loop approximation. Ojima[47] on the other hand has shown the equivalence of the TFD formalism with the so-called C^* algebra approaches developed by Haag, Hugenholtz and Winnick[48].

It is therefore the case that there now exists a well established procedure for the evaluation, in real time, of various field theoretic quantities at finite temperature in a wide enough variety of approaches and styles to satisfy the tastes and prejudices of all but the most demanding of physicists. In fact, these recent developments mean that virtually all the devices of conventional zero temperature field theory, the Feynman Diagram technique, the spectral representation, the LSZ formalism, the Ward-Takahashi identities, and so on, may be generalized to finite temperature. Furthermore the practical utility of the real time method has been demonstrated for a number of problems in both relativistic[49,50] and non-relativistic[7] quantum field theory at finite temperature. Indeed much of the content of this thesis concerns itself with an application of these techniques to consider a variety of problems in magnetism and superconductivity.

In what follows we will restrict our attention to problems in equilibrium statistical mechanics and the TFD formalism. Since this formalism is not as widely utilized in the literature as say the Matsubara method, I will briefly describe the method and discuss the derivation of the Feynman rules. The approach I will follow is based on the operator realization of TFD presented in ref. [7]. In order to provide a degree of completeness I have also briefly outlined the path ordering method of Mills[36], as presented by Matsumoto et al[42,43], in Appendix A and give a brief discussion of the relation between the two approaches.

To make our considerations specific we consider an interacting system of bose or fermi particles whose dynamics we assume may be described in terms of certain Heisenberg field operators $\{\psi_i(x)\}$ and their conjugate momenta $\{\Pi_i(x)\}$ obtained from the Lagrangian in the usual way

$$\Pi_i(x) = \frac{\partial \mathcal{L}}{\partial \dot{\psi}_i(x)} \tag{2.1}$$

The equation of motion for the fields and their conjugate momenta is obtained from

$$i\frac{\partial \psi_i(x)}{\partial t} = [\psi(x), H] \quad . \tag{2.2}$$

and

$$i\,\frac{\partial\,\Pi_i(x)}{\partial t} = [\Pi_i(x), H] \quad , \tag{2.3}$$

where H is the Hamiltonian given by

$$H = \int [\sum_i \Pi_i(x)\dot{\psi}_i(x) - \mathcal{L}(x)]\, d^3\vec{x} \tag{2.4}$$

and the fields obey the usual canonical commutation (anti commutation) relations

$$[\psi_i(x),\Pi_j(x')]_\pm\delta(t-t') = i\delta(x-x')\,\delta_{ij} \quad (2.5)$$

$$[\psi_i(x),\psi_j(x)]_\pm\delta(t-t') = [\Pi_i(x),\Pi_j(x')]_\pm\delta(t-t') = 0 \quad . \quad (2.6)$$

We then pose the question is it possible to construct an operator representation of the Heisenberg fields in terms of certain free fields in a Hilbert space which contains some state $|\beta\rangle$ such that the thermal average of an operator product may be realized as an expectation value

$$\mathrm{Tr}\{e^{-\beta H}A_1(x_1)\ldots A_n(x_n)\} = \langle\beta|A_1(x_1)\ldots A_n(x_n)|\beta\rangle \quad . \quad (2.7)$$

To this end we regard $|\beta\rangle$ as a thermal vacuum which reflects the presence of the thermally excited quanta. In distinction to the zero temperature vacuum (or ground state), energy may be absorbed in two ways: it can be absorbed by the excitation of an additional quanta in momentum state $\vec{k}$ or by the annihilation of a thermally excited hole (unoccupied states lying below the fermi energy) in momentum state $\vec{k}$. These processes are denoted by the physical creation and annihilation operators $\alpha_i^\dagger(\vec{k};\beta)$ and $\tilde{\alpha}_i(\vec{k};\beta)$ respectively. These operators obey the usual canonical commutation (anti-commutation) relations

$$[\alpha_i(\vec{k};\beta),\alpha_j^\dagger(k';\beta)]_\pm = \delta_{ij}\,\delta(\vec{k}-\vec{k}') \quad (2.8)$$

$$[\tilde{\alpha}_i(\vec{k};\beta),\tilde{\alpha}_j^\dagger(k;\beta)]_\pm = \delta_{ij}\,\delta(\vec{k}-\vec{k}') \quad (2.9)$$

with all other operators commuting (anti-commuting) and such that both $\alpha_i(k;\beta)$ and $\tilde{\alpha}_i(k;\beta)$ annihilate the thermal vacuum $|\beta\rangle$

$$\alpha_i(\vec{k};\beta)|\beta\rangle = \tilde{\alpha}_i(\vec{k};\beta)|\beta\rangle = 0 \quad . \quad (2.10)$$

They also satisfy the following tilde conjugation laws[7]

$$\widetilde{c\alpha_i(\vec{k};\beta)} = c^*\tilde{\alpha}_i(\vec{k};\beta) \tag{2.11}$$

$$\widetilde{c\alpha_i^\dagger(k;\beta)} = c^*\tilde{\alpha}_i(\vec{k};\beta) \tag{2.12}$$

$$\widetilde{\alpha_i(k;\beta)\alpha_j(k;\beta)} = \tilde{\alpha}_i(k;\beta)\tilde{\alpha}_j(k;\beta) \tag{2.13}$$

and

$$\tilde{\tilde{\alpha}}(\vec{k};\beta) = \rho_F\,\alpha(k;\beta) \tag{2.14}$$

where c is any imaginary C-number and $\rho_F = 1\,(-1)$ for the case of bose (fermi) quanta. From the spectrum of the various elementary excitations, which we have distinguished by the index i, we can construct a set of local free fields $\{\phi_n(x)\}$ which comprise linear combinations of both the tildé and non-tildé fields. While the detailed nature of the relationship between the free fields $\{\phi_n\}$ and the physical creation and annihilation operators depends on the spectrum of the excitations, together with the requirements of locality and causality, contained in the canonical commutation (anti-commutation) relations, the degree of mixing between the tildé and non-tildé fields will be determined by the requirement that the density of the elementary excitations is that obtained by the condition of thermal equilibrium, i.e.

$$\langle\beta|\phi_i^\dagger(x)\phi(x)|\beta\rangle = \int \frac{d^3k}{(2\pi)^3}\,\frac{1}{\exp\,\omega_n(\vec{k}) \pm 1} \tag{2.15}$$

The plus (minus) sign in Eq. (2.15) refers to fermi (bose) quanta and $\omega_n(k)$ corresponds to the energy spectrum of the ϕ_n field.

In order to illustrate the relation between the physical quanta and the free fields $\phi_n(x)$, we consider the example in which the physical quanta consist of fermionic excitations with energy spectrum $\varepsilon(\vec{k})$.

Denoting the physical creation operator of the positive energy quanta (particle states) by $\alpha^{\dagger}(\vec{k};\beta)$ and those of the negative energy states (hole states) by $\beta^{\dagger}(\vec{k};\beta)$ together with the corresponding tildé fields, which we denote as $\tilde{\alpha}^{\dagger}(\vec{k};\beta)$ and $\tilde{\beta}^{\dagger}(\vec{k};\beta)$, we show how the free fermion $\phi(x)$ may be constructed. Writing

$$\phi(x) = \int \frac{d^3k}{(2\pi)^3} \{a(\vec{k})\theta[\varepsilon(\vec{k})] + b^{\dagger}(\vec{k})\theta[-\varepsilon(\vec{k})]\exp\{-i\varepsilon(\vec{k})t + i\vec{k}\cdot\vec{x}\} \quad (2.16)$$

where $\theta[x]=1$ for $x>0$ and $\theta[x]=0$ for $x<0$, we see that $\phi(x)$ and its complex conjugate $\phi^{\dagger}(x)$ are fields which satisfy a free field equation

$$\{i\frac{\partial}{\partial t} - \varepsilon(-i\nabla)\}\,\phi(x) = 0 \quad (2.17)$$

and

$$\{-i\frac{\partial}{\partial t} - \varepsilon(+i\nabla)\}\phi^{\dagger}(x) = 0 \quad (2.18)$$

and which satisfy the usual equal time anti-commutation relation

$$[\phi^{\dagger}(x),\phi(x')]_{+}\,\delta(t-t') = \delta^4(x-x') \quad (2.19)$$

provided the operator $a(k)$; $b(k)$ and their complex conjugate $a^{\dagger}(k)$; $b^{\dagger}(k)$ satisfy the algebra

$$[a(\vec{k}),a^{\dagger}(\vec{k}')]_{+} = \delta(\vec{k}-\vec{k}') \quad (2.20)$$

and

$$[b(\vec{k}),b^{\dagger}(\vec{k}')]_{+} = \delta(\vec{k}-\vec{k}') \quad (2.21)$$

with all other operators anti-commuting. We now express the operator $a(\vec{k})$ $(b(\vec{k}))$ as a linear combination of the physical creation and annihilation operators $\alpha(\vec{k};\beta)$ and $\tilde{\alpha}^{\dagger}(\vec{k};\beta)$ $(\beta(\vec{k};\beta)$ and $\hat{\beta}^{\dagger}(k;\beta))$. Noting that both the operators $a(k)$ and $\alpha(k;\beta)$, together with $\tilde{\alpha}(k;\beta)$, satisfy the equal time anti-commutation relation, they must be related through a canonical transformation. Thus we have that

$$a(\vec{k}) = \cos\theta_{\vec{k}}\,\alpha(\vec{k};\beta) + \sin\theta_{\vec{k}}\,\tilde{\alpha}^{\dagger}(\vec{k};\beta) \tag{2.22}$$

while

$$b(\vec{k}) = \cos\eta_{\vec{k}}\,\beta(\vec{k};\beta) + \sin\eta_{\vec{k}}\,\tilde{\beta}^{\dagger}(\vec{k};\beta)\ . \tag{2.23}$$

It thus remains to determine the transformation functions $\cos\theta_k$ and $\cos\eta_k$ from the requirement of Eq. (2.15) we find that

$$\cos\theta_k = \sqrt{1 - f[\varepsilon(\vec{k})]} \tag{2.24}$$

and

$$\cos\eta_k = \sqrt{1 - f[-\varepsilon(\vec{k})]}\ , \tag{2.25}$$

where f(x) denotes the fermi distribution function

$$f(x) = \frac{1}{e^x + 1}\ . \tag{2.26}$$

Other examples of how the physical creation and annihilation may be used to construct free fields in thermal equilibrium with a heat bath are provided in ref. [7]. In all of these examples the canonical transformation given by Eqs. (2.22) and (2.23) and the corresponding transformation for bose fields plays a central role.

The finite temperature realization of the Heisenberg field operators is therefore achieved by constructing a mapping (often referred to as the dynamical map) between the Heisenberg field operators and some set of free fields constructed out of appropriate combinations of the tildé and non-tildé fields such that equations of motion, Eqs. (2.2) and (2.3), for the Heisenberg fields are satisfied. The thermal average of products of the Heisenberg fields may then be expressed in terms of expectation values with respect to the thermal vacuum exactly as required by Eq. (2.7).

Before going on to demonstrate how the above ideas may be translated into a computational scheme, a number of comments are in order. First of all in the above discussion it is nowhere apparent how elementary excitations and the corresponding free fields are determined a priori. This situation is by no means peculiar to the finite temperature case; even at zero temperature, there is no systematic prescription whereby the nature of the physical fields (the interpolating fields for example) may be determined a priori. The presence of a composite particle (bound state) or the appearance of a spontaneously broken symmetry can give rise to a very rich structure in the spectrum of the elementary excitations, which is by no means apparent from the dynamics of the original Heisenberg fields. A second and not unrelated question is, given that one constructs a particular representation in which the Heisenberg fields are expressed in the correct fashion in terms of certain local free fields, is there any assurance that this representation is unique? Such a situation could arise for example if the free energy of the system contained certain local minima in addition to the global minima. Obviously the presence of such metastable states cannot be ruled out in the case of particularly complex theories. These comments highlight an important distinction between quantum mechanics, in which all representations of the theory are unitarily equivalent, and quantum many body theory, in which different representations of the Heisenberg operators can be constructed which are not unitarily equivalent. This manifests itself in the wide variety of, often quite unexpected, phases that can arise in many body theory.

Returning to more practical concerns we note that the rules for tildé conjugate presented in Eqs. (2.11→2.14) allow us to define, for each of the free fields $\phi_n(x)$, the tildé conjugate fields $\tilde{\phi}_n(x)$ and hence corresponding to any Heisenberg operator $O_H[x;\phi]$, we can construct the corresponding thermal tilde field $\tilde{O}_H[x;\phi]$ as

$$\tilde{O}_H[x;\phi] = O_H^*[x;\tilde{\phi}] \quad . \tag{2.27}$$

The definition of the thermal tilde fields means that, corresponding to any Heisenberg field operator $O_H[x;\phi]$, we can define the thermal doublet[40]

$$\begin{Bmatrix} O_H^1 \\ O_H^2 \end{Bmatrix} = \begin{Bmatrix} O_H \\ \tilde{O}_H^\dagger \end{Bmatrix} \tag{2.28}$$

The introduction of the thermal doublet introduces a considerable elegance into the TFD formalism and as we shall see it provides a useful computational device. Particularly it serves to emphasize the fact that a finite temperature realization of the Heisenberg fields requires a doubling of the field degrees of freedom since at finite temperature every field $\psi(x)$ is replaced by the corresponding thermal doublet $\psi^\alpha(x)$ $(\alpha = 1,2)$

$$\begin{Bmatrix} \psi^1(x) \\ \psi^2(x) \end{Bmatrix} = \begin{Bmatrix} \psi \\ \tilde{\psi}^\dagger \end{Bmatrix} \tag{2.29}$$

the dynamics of which may be obtained from the canonical equations of motion, Eqs. (2.2) and (2.3)

$$i \frac{\partial}{\partial t} \psi_i^{\alpha}(x) = [\psi_i^{\alpha}, \hat{H}] \tag{2.30}$$

and $$i \frac{\partial}{\partial t} \Pi_i^{\alpha}(x) = [\Pi_i^{\alpha}, H] \tag{2.31}$$

where $\hat{H}$ is given by

$$\hat{H} = \sum_a \varepsilon_a H^a \tag{2.32}$$

with $H^1 = H$, $H^2 = \tilde{H}$ and $\varepsilon^1 = 1$, $\varepsilon^2 = -1$. The doublet fields now satisfy the commutation (anti-commutation) relation

$$[\psi_i(x)^{\alpha}, \Pi_j^{\beta}(x')]_{\pm}\delta(t-t') = i\delta_{\alpha\beta}\delta^4(x-x')\delta_{ij}(\rho_A)^{\alpha}, \tag{2.33}$$

where $\rho_A = +1$ for fermions and $\rho_A = -1$ for bosons.

Thus the introduction of the thermal vacuum $|\beta\rangle$ together with the physical creation and annihilation operators and the construction of the tildé fields means that virtually all the ingredients present in the conventional zero temperature field theory have their counterpart in the TFD formalism. The practical consequence of this is that virtually all the calculational techniques and devices of conventional field theory may be extended to finite temperature. Of particular interest is the generalization to finite temperature of the many particle Green's functions

$$G_{i_1 i_2 \ldots i_n; j_1 \ldots j_m}^{\alpha_1 \alpha_2 \ldots \alpha_n; \beta_1 \ldots \beta_m}(x_1 x_2 \ldots x_n | y_1 \ldots y_m)$$
$$= \langle\beta| T[\psi_{i_1}^{\alpha_1}(x_1) \ldots \psi_{i_n}^{\alpha_n}(x_n) \Pi_{j_1}^{\beta_1}(y_1) \ldots \Pi_{j_m}^{\beta_m}(y_m)] |\beta\rangle . \tag{2.34}$$

At zero temperature, expressions such as Eq. (2.34) are evaluated in the interaction representation. The derivation is presented in several books in field theory and many body theory[51,52,53] and may be extended to finite temperature with only minor modifications. Separating the Hamiltonian into a free and an interacting part

$$\hat{H} = \hat{H} + \hat{H}_I$$

we define the operators in the interaction representation as

$$\psi_I^\alpha(x) = e^{i\hat{H}_o t}\,\psi^\alpha(\vec{x},t=0)\,e^{-i\hat{H}_o t} \quad . \tag{2.35}$$

These operators satisfy a free field equation, which may be obtained from the Hamiltonian $\hat{H}_o$ and the usual commutation (anti-commutation) relations:

$$i\frac{\partial}{\partial t}\,\psi_I^\alpha(x) = [\psi_I^\alpha(x),\hat{H}_o] \tag{2.36}$$

$$i\frac{\partial}{\partial t}\,\Pi_I^\alpha(x) = [\Pi_I^\alpha(x),\hat{H}_o] \tag{2.37}$$

and

$$\delta(t-t')[\psi_I^\alpha(x),\Pi^\beta(x')] = i\delta_{\alpha\beta}\delta(x-x')(\rho_A)^\alpha \quad . \tag{2.38}$$

The fields in the interaction representation are then related to the Heisenberg fields through the evolution operator $\hat{U}(t;t_o)$

$$\psi^\alpha(x) = \hat{U}(0,t)\psi_I^\alpha(x)\hat{U}(t;0) \tag{2.39}$$

where $\hat{U}(t;t_o)$ is given by

$$\hat{U}(t;t_o) = e^{i\hat{H}_o t}\,e^{-i\hat{H}(t-t_o)}\,e^{-i\hat{H}t_o} \quad . \tag{2.40}$$

The evolution operator may be computed perturbatively in the usual way to give

$$U(t;t_o) = \sum_n \frac{(-i)^n}{n!} \int_{t_o}^{t} dt_1 \ldots \int_{t_o}^{t} dt_n \, T[\hat{H}_I'(t_1) \ldots \hat{H}_I'(t_n)]$$

$$= T[\exp - i \int_{t_o}^{t} \hat{H}_I'(t)] \qquad (2.41)$$

where $\hat{H}_I'(t)$ is simply $\hat{H}_I[\psi_I^\alpha(t);\pi_I^\alpha(t)]$. Since the fields in the interaction representation are free fields we may construct the physical creation and annihilation $\alpha_I(\vec{k};\beta)$ and $\alpha_I(\vec{k};\beta)$ together with their Hermitean conjugates $\alpha_I^\dagger(\vec{k};\beta)$ and $\tilde{\alpha}_I(\vec{k};\beta)$ in the interaction representation by means of the canonical transformation described previously. From these we define the state $|\beta>_I$

$$\alpha_I(\vec{k};\beta)|\beta>_I = \tilde{\alpha}_I(\vec{k};\beta)|\beta>_I = 0 \qquad (2.42)$$

from which the thermal vacuum $|\beta>$ may be constructed by means of the finite temperature generalization of Gell-Mann Low result

$$\lim_{\varepsilon\to 0} |\beta> = \frac{\hat{U}_\varepsilon(0;-\infty)|\beta>_I}{{}_I<\beta|\hat{U}_\varepsilon(0;-\infty)|\beta>_I} \quad , \qquad (2.43)$$

where ε denotes the adiabatic switching parameter. Equations (2.39), (2.41) and (2.43) may then be combined to give the result, quoted in ref. [40]

$$<\beta|T[\psi_{i_1}^{\alpha_1}(x_1)\ldots\psi_{i_n}^{\alpha_n}(x_n)\pi_{j_1}^{\beta_1}(y_1)\ldots\pi_{j_m}^{\beta_m}(y_m)]|\beta>$$

$$= \frac{{}_I<\beta|T[\psi_{Ii_1}^{\alpha_1}(x_1)\ldots\psi_{Ii_n}^{\alpha_n}(x_n)\pi_{Ij_1}^{\beta_1}(y_1)\ldots\pi_{Ij_m}^{\beta_m}(y_m)S]|\beta>_I}{{}_I<\beta|T[S]|\beta>_I} \qquad (2.44)$$

where

$$S = \exp - i \int_{-\infty}^{+\infty} \hat{H}_I'(\psi_I^\alpha(t);\pi_I^\alpha(t))\,dt \quad . \tag{2.45}$$

Equation (2.44) together with the Wick ordering theorem may be combined in the usual way to permit the many particle Green's functions to be evaluated in the usual way, by means of the Feynman diagram method[51,52,53]. While the contribution to each order in the perturbation series will have the same topological and diagramatic structure as the corresponding zero temperature contribution, there will be two important differences. First of all the interaction term is given by

$$\hat{H}_I'[\psi_I^\alpha(t);\pi_I^\alpha(t)^\dagger] = H_I'[\psi_I(t);\pi_I(t)] - H_I'[\widetilde{\psi_I(t)};\widetilde{\pi_I(t)}] \ , \tag{2.46}$$

which means that in addition to the vertices for the $\psi_I(x)$ fields there will appear a corresponding vertex for the tildé field $\tilde{\psi}_I(x)$ which will appear with a relative minus sign. It should be noted that the structure of $\hat{H}_I'$ is such that no mixing of the tildé and non-tildé fields occurs at the vertex. The second difference arises from the fact that the normal ordering procedure, used in the evaluation of the various perturbative contributions to Eq. (2.44), should be with respect to the physical creation and annihilation operators, $\alpha_I(\vec{k};\beta)$, $\alpha_I(\vec{k};\beta)$ and $\tilde{\alpha}_I^\dagger(\vec{k};\beta)$, $\tilde{\alpha}_I^\dagger(\vec{k};\beta)$, the normal ordering does produce a mixing of the fields $\psi_I(x)$ and the tildé fields $\tilde{\psi}_I(x)$ since the resulting propagator has a matrix structure with non-zero off diagonal components. For example in the case where the fields ψ_I in the interaction representation obey a simple Schrödinger equation

$$\{i\frac{\partial}{\partial t} - \varepsilon(-i\nabla)\}\,\psi_I^\alpha(x) = 0 \ . \tag{2.47}$$

Then the internal line appearing in Feynman diagram corresponding to the fields $\psi_I^\alpha(x)$ will be given by

$$S^{\alpha\beta}(x-y) = {}_I\langle\beta|T[\psi_I^\alpha(x)\psi_I^\beta(y)^\dagger]|\beta\rangle_I \quad (2.48)$$

$$= \frac{i}{(2\pi)^4}\int d^4k\, e^{i[\varepsilon(\vec{k})t-\vec{k}.\vec{x}]}U_F(k_o)[k_o-\varepsilon(\vec{k})+i\delta\tau]^{-1}U_F^\dagger(k_o) \quad (2.49)$$

in the case of fermions and

$$= \frac{i}{(2\pi)^4}\int d^4k\, e^{-i[\varepsilon(\vec{k})t-\vec{k}.\vec{x}]}U_B(k_o)\tau[k_o-\varepsilon(\vec{k})+i\delta\tau]^{-1}U_B(k_o) \quad (2.50)$$

in the case of bosons where

$$U_F(k_o) = \begin{pmatrix} \sqrt{1-f(k_o)} & \sqrt{f(k_o)} \\ -\sqrt{f(k_o)} & \sqrt{1-f(k_o)} \end{pmatrix} \quad (2.51)$$

and

$$U_B(k_o) = \begin{pmatrix} \sqrt{1-f_B(k_o)} & \sqrt{f_B(k_o)} \\ \sqrt{f_B(k_o)} & \sqrt{1-f_B(k_o)} \end{pmatrix} \quad (2.52)$$

with

$$f_B(k_o) = \frac{1}{e^{\beta k_o}-1} \quad . \quad (2.53)$$

Similar results hold for other types of fields (e.g. phonons etc.).

Thus the Green's function of Eq. (2.34) may be computed perturbatively in the interaction representation in real time by means of the Feynman diagram method. The Feynman rules which one obtains for a particular theory will be similar to those of the zero temperature theory.

However, due to the two component nature of the fields at finite temperature, the propagators corresponding to the internal lines have the matrix structure given by Eq. (2.51) in the case of fermi particles and Eq. (2.52) in the case of bose particles. A similar result may be obtained by means of the path ordering method of Mills[46] a brief description of which is presented in Appendix A.

The close formal resemblance between the diagrammatic contributions that one obtains in TFD and the analogous contribution at zero temperature proves very useful, since it allows one to generate from the various terms in the perturbation expansion a low temperature expansion of the various dynamical and static physical quantities. This procedure will be elaborated on in Section 3 together with its application to itinerant electron ferromagnetism.

In addition to the extension of the Feynman diagram technique to finite temperature a number of other devices, familiar from conventional zero temperature field theory, may be generalized to finite temperature in a particularly straightforward manner. For example, it is straightforward to show that the two particle propagator may be written in the spectral representation as[40]

$$G^{\alpha\beta}(x-y) = \langle\beta|T[\psi^{\alpha}(x)\psi^{\beta}(y)^{\dagger}]|\beta\rangle$$

$$= \frac{i}{(2\pi)^4}\int d^4k\; e^{ik\cdot x}\; G^{\alpha\beta}(k) \tag{2.54}$$

with

$$G^{\alpha\beta}(k) = \int d\omega\; \rho(\vec{k};\omega)U_F(k_0)[k_0 - \omega + i\delta\tau]^{-1}\; U_F(k_0) \tag{2.55}$$

in the case of fermions and

$$G^{\alpha\beta}(k) = \int d\omega\; \rho(\vec{k};\omega)U_B(k_0)\tau[k_0 - \omega + i\delta\tau]^{-1}\; U_B(k_0) \tag{2.56}$$

in the case of bosons, where $\rho(\vec{k};\omega)$ is a positive definite quantity usually referred to as the spectral function. The formal similarity between the two particle Green's function, expressed in Eqs. (2.55) and (2.56) and the free particle propagator of Eqs. (2.48) and (2.49), allows us to extend to finite temperature the observation at zero temperature that the two particle Green's function may be written a linear superposition of free particle propagators of energy ω.

Another useful device of zero temperature field theory which may be extended to finite temperature by means of TFD in the so-called Lehman-Symanzik-Zimerman (LSZ) formula for the S matrix in terms of the interpolating fields. This allows for various scattering processes to be evaluated at finite temperature in terms of the time ordered Green's functions of Eq. (2.34). Denoting the asymptotic fields by $\phi_0^\alpha(x)$ and the corresponding interpolating field $\phi^\alpha(x)$ such that

$$\lim_{t\to-\infty} \phi^\alpha(x) \sim Z^{-\frac{1}{2}}(-i\nabla)\phi_0^\alpha(x) \ , \tag{2.57}$$

where Eq. (2.57) is to be interpreted in the sense of a weak relation. Then we obtain

$$\begin{aligned} S = \sum_n \sum_m (-i)^{n+m} \int & d^4x_1 \ldots d^4x_n d^4y_1 \ldots dy_m \sum_{a_1} \ldots \sum_{a_n} \\ & \sum_{b_1} \ldots \sum_{b_m} :[\phi_0^{a}(x_1)\lambda(\vec{\partial}_x^1)] \ldots [\phi_0^{a_n}(x_n)\lambda(\vec{\partial}_x^n)] \\ & \langle\beta|T[\phi^{a_1}(x_1)\ldots\phi^{a_n}(x_n)\phi^{b_1}(y_1)^\dagger \ldots \phi^{b_m}(y_m)^\dagger]|\beta\rangle \\ & [\lambda(-\overleftarrow{\partial}_y^1)\phi_0^{b_1}(y_1)^\dagger \ldots \lambda(-\overleftarrow{\partial}_y^m)\phi_0^{b_m}(y_m)]: \quad , \end{aligned} \tag{2.58}$$

where the asymptotic fields are assumed to satisfy the equation of motion

$$\lambda(\partial_x)\phi_0^{\alpha}(x) = 0 \tag{2.59}$$

and the canonical equal time commutation (anti-commutation) relations

$$[\phi_0^{\alpha}(x),\phi_0^{\beta}(x')^{\dagger}]_{\pm}\,\delta(t-t') = \delta^4(x-x')\delta_{\alpha\beta}(\rho_A)^{\alpha} \quad . \tag{2.60}$$

Yet another computational device of the conventional zero temperature formalism which may be extended to finite temperature in a very straightforward manner are the so-called Ward-Takahashi[3,4] relations whose importance to situations involving spontaneously broken symmetry has long been recognized. These are discussed in some detail in the next section.

2.2 Ward-Takahashi Identities at Finite Temperature

Of considerable importance in the study of quantum fields are the identities generated by means of certain continuous transformations of the Heisenberg fields. These identities were first obtained perturbatively for the zero momentum limit of the electron photon vertex in quantum electrodynamics by Ward[3]. The corresponding finite momentum identity, obtained by means of the Heisenberg equation of motion, was presented by Takahashi[4] and is generally referred to as the Ward-Takahashi (W-T) relation in quantum electrodyanmics. Subsequently, however, the term W-T relation has come to be used in a much wider sense, and now is used to refer to any relation generated through a transformation of the Heisenberg fields.

The W-T relations have found a number of important applications in particle physics low energy pion-pion scattering and the PCAS hypothesis[54], the K-lepton decays and the so-called Callen Treiman relations[55], the infrared problem in quantum electrodynamics[56] and the dynamical rearrangement theory[57] being some of the more notable examples. The W-T relations have also found important application in many areas of non-relativistic many body theory; recent examples may be found in studies related to the density of states close to the mobility edge in disordered metals[58], the analysis of amplitude modes in the superconducting charge density wave compound $NbSe_2$[59], the quantum theory of crystals[60], superfluidity[61,62] as well as to problems related to the ferromagnetic[63,64,65,66] and paramagnetic[67] properties of metallic ferromagnets.

Many of the topics outlined above manifest what is often referred to as spontaneously broken symmetry and it is here that the W-T relations play an essential role in several respects. First of all they may be used to obtain certain exact results, Goldstone's theorem and the low energy theorems regarding the scattering of pions, magnons, phonons, etc. are examples of this. Secondly they provide us with various relations between the many point Green's functions and their corresponding vertices which must be satisfied in any approximate calculation if one wishes to assure the self consistency of the calculation.

The W-T relations may be understood within the context of conventional field theory as an expression of Noether's theorem[68,69]. Denoting the Heisenberg fields by $\psi_i(x)$ Noether's theorem states that the charge in the Lagrangian induced by a continuous transformation of the Heisenberg fields

$$\psi(x) \to \psi'(x') = \psi(x) + \theta\delta\psi(x) , \tag{2.61}$$

$$x \to x' = x_\mu + \delta x_\mu \tag{2.62}$$

in which $\delta\psi$ is a linear transformation i.e.

$$\delta\psi_i(x) = \Lambda_{ij}\psi_j(x) , \tag{2.63}$$

where the change induced in the Lagrangian $\delta\alpha(x)$ is defined by

$$d^4x' \mathcal{L}[\psi'(x'),\partial_\mu\psi'(x')] - d^4x \mathcal{L}[\psi(x),\partial_\mu\psi(x)] = \theta d^4x\, \delta\alpha(x) , \tag{2.64}$$

may be written in the form of a divergence as

$$\delta\mathcal{L}(x) = \nabla\cdot\vec{J}(x) - \frac{\partial}{\partial t} J_0(t) . \tag{2.65a}$$

In Eq. (2.65a) we have defined the current $J_\mu = (J_0;\vec{J})$ as

$$\vec{J}(x) = \frac{\partial\mathcal{L}}{\partial[\nabla\psi]} \delta_L\psi(x) + \delta\vec{x}\mathcal{L} \tag{2.66a}$$

and

$$J_0(x) = \frac{\partial\mathcal{L}}{\partial\dot{\psi}} \delta_L\psi(x) + \delta x_0 \mathcal{L} , \tag{2.67a}$$

where δ_L denotes the Lie derivative defined by

$$\delta_L\psi(x) = \delta\psi(x) - [\delta^{\rightarrow}\cdot\nabla\psi(x) - \delta x_0\psi(x)] . \tag{2.68}$$

An entirely analogous result may be obtained in TFD and is given by

$$\sum_a \varepsilon^a \delta\mathcal{L}^a(x) = \sum_a \varepsilon^a\{\nabla\cdot\vec{J}^a(x) - \frac{\partial}{\partial t} J_0^a(x)\} , \tag{2.65b}$$

where

$$\vec{J}^\alpha(x) = \sum \frac{\partial\mathcal{L}^a}{\partial\nabla\psi^a} \delta_L\psi^a(x) - \delta\vec{x}\mathcal{L}^\alpha \tag{2.66b}$$

and

$$J_0^\alpha(x) = \sum_a \frac{\partial\mathcal{L}^\alpha}{\partial\dot{\psi}^a} \delta\psi^a(x) - \delta x_0\mathcal{L}^\alpha . \tag{2.67b}$$

Noting that $\Pi_i^a(x) = \partial\mathcal{L}/\partial\dot{\psi}_i(x)$ is the canonical momentum of the field $\psi(x)$ we may construct the generator of the transformation $Q(t)$ as

$$\hat{Q}(t) = \int d^3x \sum_a \varepsilon_a J_o^a(x) \tag{2.69}$$

since

$$[\psi_i^\alpha(x), \hat{Q}(t)]\delta(t-t_x) = i\delta(t-t_x)\, \delta\psi_i^\alpha(x) \quad . \tag{2.70}$$

If we now consider the following relation between the time ordered products,

$$\frac{\partial}{\partial t} T[\hat{Q}(t)\psi_{i_1}^{\alpha_1}(x_1)\ldots\psi_{i_n}^{\alpha_n}(x_n)] = \sum_{r=1}^{n} i\delta(t-t_n)T[\psi_{i_1}^{\alpha_1}(x_1)\ldots[\hat{Q}(t),\psi_{i_r}^{\alpha_r}(x_r)]\ldots$$
$$\psi_{i_n}^{\alpha_n}(x_n)] + T[\dot{\hat{Q}}(t)\psi_{i_1}^{\alpha_1}(x_1)\ldots\psi_{i_n}^{\alpha_n}(x_n)] \quad . \tag{2.71}$$

Then by virtue of Eqs. (2.70), (2.69) and (2.68) we obtain the following relation from Eq. (2.71)

$$\frac{\partial}{\partial t} T[\hat{Q}(t)\psi_{i_1}^{\alpha_1}(x_1)\ldots\psi_{i_n}^{\alpha_n}(x_n)] = -\sum_r \delta(t-t_r)iT[\psi_{i_1}^{\alpha_1}(x_1)\ldots[\delta\, \psi_{i_r}^{\alpha_r}]\ldots\psi_{i_n}^{\alpha_n}(x_n)]$$
$$+ \int d^3\vec{x}\; T[\delta\mathcal{L}(x)\psi_{i_1}^{\alpha_1}(x_1)\ldots\psi_{i_n}^{\alpha_n}(x_n)] \quad . \tag{2.72}$$

The relation given in Eq. (2.72) is an operator relation and may be used to obtain exact relations between the various finite temperature many point Green's functions, simply by taking the expectation value with respect to the thermal vacuum $|\beta\rangle$. Thus we obtain

$$\frac{\partial}{\partial t} \langle\beta|T[Q(t)\psi_{i_1}^{\alpha_1}(x_1)\ldots\psi_{i_n}^{\alpha_n}(x_n)]|\beta\rangle$$
$$= -\sum_r \delta(t-t_r)i\langle\beta|T[\psi_{i_1}^{\alpha_1}(x_1)\ldots[\delta\, \psi_{i_r}^{\alpha_r}]\ldots\psi_{i_n}^{\alpha_n}(x_n)]|\beta\rangle$$
$$+ \int d^3\vec{x}\langle\beta|T[\delta\hat{\mathcal{L}}(x)\, \psi_{i_1}^{\alpha_1}(x_1)\ldots\psi_{i_n}^{\alpha_n}(x_n)]|\beta\rangle \quad . \tag{2.73}$$

For our purposes it suffices to consider only the zero frequency limit of Eq. (2.73), hence integrating with respect to t from $+\infty$ to $-\infty$ we obtain

$$\sum_r \langle\beta| T[\psi_{i_1}^{\alpha_1}(x_1)\ldots[\delta^o\psi_{i_r}^{\alpha_r}(x_r)]\ldots\psi_{i_n}^{\alpha_n}(x_n)]|\beta\rangle$$

$$= i\int d^4x \langle\beta| T[\delta\hat{\mathcal{L}}(x)\, \psi_{i_1}^{\alpha_1}(x_1)\ldots\psi_{i_n}^{\alpha_n}(x_n)|\beta\rangle \quad . \tag{2.74}$$

It can arise however that one can have a non-vanishing expectation value

$$\langle\beta|\delta_o O_H^{\alpha}|\beta\rangle \neq 0 \tag{2.75}$$

even although the transformation leaves the Lagrangian invariant i.e.

$$\delta\mathcal{L}(x) = 0 \ . \tag{2.76}$$

This situation is referred to as spontaneously broken symmetry (SBS). Obviously Eqs. (2.75) and (2.76) appear to contradict the result of Eq. (2.74) implying that in the case of spontaneously broken symmetry the preceding argument is at fault. Indeed what one finds is that the generator of the transformation $\hat{Q}$ of Eq. (2.69) does not in fact exist in the case of spontaneously broken symmetry and must instead be re[illegible] ized as the limit of a local transformation[7]. This problem may however be circumvented by introducing an explicit symmetry breaking term in the Lagrangian

$$\hat{\mathcal{L}} \longrightarrow \hat{\mathcal{L}}_h = \hat{\mathcal{L}} + h\,\hat{\mathcal{L}}_{SB} \tag{2.77}$$

such that

$$\delta\hat{\mathcal{L}}_h = h\,\delta\hat{\mathcal{L}}_{SB} \neq 0 \tag{2.78}$$

Now provided h remains finite the arguments in the preceding section are correct and Eq. (2.74) now becomes

$$<\beta|\delta_o O_H^\alpha(y)|\beta>_n = i\int d^4x<\beta|T[\delta\hat{\mathcal{L}}_h(x)\, O_H(y)]|\beta> \tag{2.79}$$

$$= ih\int d^4x<\beta|T[\delta\hat{\mathcal{L}}_{SB}(x) O_H(y)|\beta>_n \tag{2.80}$$

The fact that

$$\lim_{h\to 0} <\beta|\delta_o O_H^\alpha(y)|\beta>_n \neq 0 , \tag{2.81}$$

implies that

$$\lim_{h\to 0} \int d^4x<\beta|T[\delta\hat{\mathcal{L}}_{SB}(x)\, O_H^\alpha(y)]|\beta> \sim \frac{Z}{h} . \tag{2.82}$$

The result of Eq. (2.82) implies that Fourier Transform of the propagator $<\beta|T[\delta\mathcal{L}^\alpha_{SB}(x)O_H^\beta(y)]|\beta>$ defined by

$$<\beta|T[\delta\mathcal{L}^\alpha_{SB}(x)O_H^\beta(y)|\beta> = \frac{i}{(2\pi)^4}\int d^4q\ e^{-iq(x-y)}\ F(q) \tag{2.83}$$

is singular in the lim $q\to 0$ and lim $h\to 0$. In relativistic field theory at zero temperature the singular structure of F(q) in the zero momentum, zero h limit implies the existence of certain massless bose like particles often referred to as Goldstone particles or bosons. In the case of non-relativistic field theories (and even relativistic field theories at finite temperature) while the presence of a singularity in F(q), may be realized in forms other than particle like modes, it is often the case that the appearance of a spontaneously broken symmetry state is accompanied by the appearance of gapless boson particle like states. Magnons in ferromagnets and phonons in crystals provide two important examples. The presence of these Goldstone modes in systems with spontaneously broken symmetry gives rise to a number of important experimentally observable consequences. Since the Goldstone modes are gapless they may be easily excited; this means that they play an important role in determining the low temperature properties of such systems. Another consequence arising from the gapless nature of these modes is that under certain situations it may be possible to locally condense macroscopic densities of such boson particles. Many such local structures can be shown to be stable for certain topological and thermodynamic reasons and give rise to various singular structures in condensed states. Examples of this are dislocations in crystals[60], vortex structure in superconductors[7] and superfluids and domain walls in ferromagnets.

In the next two chapters both these aspects of Goldstone modes will be examined in particular situations. In Chapter 3 we examine the role of magnons in determining the low temperature behaviour of various static and dynamical quantities in itinerant electron ferromagnets. In Chapter 4 we consider the thermodynamical aspects of vortex structures in magnetic superconductors.

CHAPTER 3

FERROMAGNETIC ITINERANT ELECTRON SYSTEMS

3.1 Spin Rotational Invariance and Magnetism in Metals

Magnetism in metals is usually considered from one of two extremes. The first viewpoint considers the electrons as localized with respect to the atomic cores of the magnetic ions comprising the lattice and that the separation between the ions is sufficiently large that the overlap between the electronic wavefunctions on the separate lattice sites is small. The physical description of this localized model is commonly given in terms of a spin operator $\vec{S}_n$ associated with each of the magnetic ions at the n^{th} lattice site. The spin operators obey the familiar spin algebra

$$[S_n^i(t), S_m^j(t)] = i\delta_{nm}\varepsilon_{ijk}S_n^k(t) \tag{3.1}$$

with $\vec{S}$ denoting the vector

$$\vec{S}_n = (S_n^1, S_n^2, S_n^3) \quad . \tag{3.2}$$

A particularly simple example of a Hamiltonian used to describe the dynamics of localized spins systems is the Heisenberg Hamiltonian given by

$$H = -\sum J_{nm}\vec{S}_n\cdot\vec{S}_m \tag{3.3}$$

where J_{nm} denotes the exchange coupling and arises from the exchange interaction between the overlapping electronic wavefunctions on the n and m^{th} lattice sites. While even such a simple model as that described by the Heisenberg Hamiltonian cannot be solved exactly, the solutions one obtains in the mean field approximation indicate that even such a simple model can give rise to quite a wide variety of magnetically ordered states[70], ferromagnetism, antiferromagnetism, helimagnetism and in the case of binary alloys ferrimagnetism depending on the detailed nature of the lattice and the form of the exchange interaction. Furthermore an analysis of the paramagnetic susceptibility shows that the Heisenberg model accounts for, in a perfectly straightforward manner, the Curie-Weiss law observed in many materials. Substances such as CrO_3, EuO, CrTe and MnSb all provide examples of metallic ferromagnets whose observed physical properties are in accord with the mean field predictions of the localized model.

Extensions to the Heisenberg model can be constructed, to account for the effect of the crystal fields on the atomic states and the effect of crystalline anisotropy for example. However since such effects are not a major concern of this thesis a detailed discussion of those effects is not given.

The other viewpoint commonly encountered in the analysis of the magnetic properties of metals is based on the assumption that the electrons giving rise to the magnetic properties are not localized but are best described in terms of extended states rather than the localized states of the Heisenberg model. The band model or itinerant model as it is sometimes referred to was first introduced for the case of non-interacting band electrons by Pauli[71] who considered the net electron spin arising from the Zeeman splitting induced, between the spin up and spin down electron energies, by a uniform applied magnetic field. The resultant susceptibility is referred to as the Pauli susceptibility and is characterized by a relatively weak dependence on the temperature at low temperatures. Later Slater[72] and Stoner[73] considered the itinerant electron model from the point of view of mean field theory and provided an explanation for ferromagnetism within the itinerant electron model. The model, commonly referred to in the literature as the Stoner model, provides the well-known Stoner criteria for ferromagnetism in itinerant systems

$$1 - UN(\varepsilon_F) = 0 \ , \qquad (3.4)$$

where U denotes the electron-electron interaction arising from the Coulomb interaction, for example, while $N(\varepsilon_F)$ denotes the density of states at the fermi surface.

A treatment of the ground state similar in spirit to that offered by the Stoner model but somewhat more sophisticated is based on the Local Spin Density Functional (LSDF) method of Hohenberg, Kohn and Sham[74,75]. This formalism is based on the proof provided by Hohenberg and Kohn[74] that the ground state energy of an itinerant electron system is a functional of the electron density $U[\rho]$ where

$$\rho(\vec{r}) = \sum_{i=1}^{N} |\psi_i(\vec{r})|^2 \qquad (3.5)$$

where the electron wavefunctions $\psi_i(\vec{r})$ are obtained from a Hartree-like self-consistent field equation, in which the effective potential is expressed as a functional of the density $\rho(\vec{r})$. This formalism allows one to consider to some extent effects of exchange and correlation omitted in the Stoner model. This formalism has been relatively successful in obtaining many of the ground state properties of a wide range of itinerant magnets on the basis of a simple band theory of the electrons. For example it correctly predicts that of the first 32 elements only iron, cobalt and nickel provide possible candidates for ferromagnetism[76] as well as providing a very accurate value for the net magnetic moment[76,77,78].

A further development of the band theory model was the model proposed by Hubbard[79] based on the Wannier representation of the electron states[80]. The Hubbard Hamiltonian is expressed as

$$H = \sum_{ij\sigma} t_{ij} a^{\dagger}_{i\sigma} a_{j\sigma} + U_o \sum a^{\dagger}_{i\sigma} a_{i\sigma} a^{\dagger}_{i-\sigma} a_{i-\sigma} \quad , \tag{3.6}$$

where $a^{\dagger}_{i\sigma}$ and $a_{i\sigma}$ denote the creation and annihilation operators of the Wannier states on the i^{th} site, t_{ij} denotes the hopping of the electron from site i to j while U_o represents the intraatomic Coulomb repulsion between electrons on the same lattice site and is given as

$$U_o = \iint d^3\vec{r}\, d^3\vec{r}\,' \; \phi_o^*(\vec{r} - \vec{R}_i)\phi_o^*(\vec{r}\,' - \vec{R}_i) V(\vec{r} - \vec{r}\,')\phi_o(\vec{r}\,' - \vec{R}_i)\phi_o(\vec{r} - \vec{R}_i) \tag{3.7}$$

where $\phi_o(\vec{r} - \vec{R}_i)$ denotes the Wannier wavefunction on i^{th} lattice site. The Hubbard Hamiltonian, while containing much of the same physics as the Stoner model, gives more emphasis to the atomic-like character of the electrons and hence is more applicable to the case of narrow band metals. It is also quite straightforward to extend the basic Hubbard model to include orbital degeneracy. The Hubbard Hamiltonian has been used by a number of authors to examine the effect of strong correlations[81].

While it may be argued that the band model provides a fairly accurate description of the ground state properties of magnetic itinerant electron systems the same cannot be said for the finite temperature behaviour. Indeed considerable controversy surrounds many basic aspects of band model ferromagnetism.

The reason for this state of affairs may be appreciated if we consider the temperature dependence of the magnetization in the context of the Stoner model. In the Stoner model the reduction in the magnetization with increasing temperature, arises solely from the thermal excitation of the quasi-electrons and holes and no account is taken of the effect on the magnetization due to the transverse and longitudinal spin fluctuations. In the case of the localized model the importance of these excitation modes has been appreciated for some time, indeed Bloch[82] pointed out that the transverse spin fluctuations give rise to a $T^{3/2}$ temperature dependence in the low temperature magnetization. This result is commonly referred to as the Bloch $T^{3/2}$ law and is observed in a wide range of magnetic materials notably iron and nickel. This temperature dependence is not obtained in the simple Stoner model. The fact that the Stoner model does not include the effect of the spin fluctuations also accounts for the fact that the value of the transition temperature T_c is about 5 times larger than the observed value for Fe, Co and Ni. A similar situation exists even in the case of the more rigorous LSDF theory, the value of T_c predicted for the transition metal ferromagnets is considerably higher than that observed[83].

Such difficulties persist into the paramagnetic domain where in the case of the transition metal ferromagnets the temperature dependence of the susceptibility is well described in terms of a Curie-Weiss law, suggesting a local moment model, rather than a band model, provides a more accurate description of these materials.

Perhaps even more puzzling are the so-called weak itinerant ferromagnetics such as $ZrZn_2$ and Sc_3In discovered in the early 60s[84,85]. These materials exhibit a relatively low transition temperature 26°K in the case of $ZrZn_2$[86] and 6.1°K in the case of Sc_3In[87]; furthermore both $ZrZn_2$ and $ScIn_3$ show a small non-integer magnetic moment per transition metal atom 0.16 μ_B in the case of $ZrZn_2$[86] and 0.25 μ_B in the case of $ScIn_3$[87] both of which are strongly field dependent. These features can only be accounted for in terms of an itinerant model and indeed a theoretical analysis of the magnetic properties of $ZrZn_2$ below T_c in terms of the Stoner model[88] does appear to account for certain of the observed features. However observations show that above T_c the inverse susceptibility is virtually linear with respect to temperature, a result which is inconsistent with the predictions of the Stoner model. A similar Curie-Weiss type temperature dependence is observed in the paramagnetic susceptibility of $ScIn_3$. In both cases the effective moment calculated from the Curie constant bears no obvious relation to that obtained from the zero temperature magnetization measurement.

It would be wrong to conclude on the basis of the preceding discussion that the itinerant model cannot provide a reliable model of ferromagnetism in metals at finite temperature. Indeed the remarkable success of the band model in analyzing the ground state properties of metallic ferromagnets tells us that the apparent failure of the itinerant model lies not with the model itself but with the absence, in the mean field treatment of the Stoner model (or the LSDF formalism for that matter), of the thermal excitation of modes such as the transverse and longitudinal spin fluctuations. The effect of such modes plays an important role in determining the finite temperature behaviour of these systems. This said however, to extend the Stoner or Hubbard model to include higher order corrections, in a manner which is consistent with the requirements of the broken spin symmetry, manifested by the magnetic state, is by no means straightforward. Such difficulties extend to the paramagnetic domain, if we wish to obtain a consistent treatment of these systems both above and below T_c. It is in this context that the W-T relations and their application to finite temperature problems, by means of the TFD formalism, are of crucial importance. As we will show they can provide us with not only certain exact results which arise purely from considerations of symmetry but also provide a great many exact relations between the various vertices. The W-T relations provide us with both a powerful tool and a useful guide in constructing more realistic approximation schemes, than that afforded us by the mean field treatment of Stoner. We turn our attention therefore to examine the role of the spin symmetry in itinerant electron systems and obtain the resultant W-T relations.

In what follows we assume that the system of electrons we wish to study may be described in terms of the Heisenberg operators $\psi_\uparrow(x)$ and $\psi_\downarrow(x)$, for the spin up and spin down electrons respectively, together with their complex conjugates $\psi_\uparrow^\dagger(x)$ and $\psi_\downarrow^\dagger(x)$. The extension to finite temperature is accomplished through the introduction of the corresponding tilde fields in the manner described in Section 2.1. These fields may, for example, be constructed from the Bloch states in the case of the Stoner model or the Wannier states in the case of the Hubbard model. We further assume that the dynamics of the Heisenberg fields may be obtained from some Lagrangian $\hat{\mathcal{L}}$ given by

$$\hat{\mathcal{L}}[\psi(x);\psi^\dagger(x)] = \mathcal{L}[\psi(x);\psi^\dagger(x)] - \widetilde{\mathcal{L}[\psi(x);\psi^\dagger(x)]} , \qquad (3.8)$$

where $\mathcal{L}$ is given by a free part $\mathcal{L}_0$ and interacting part which we denote as $\mathcal{L}_I$ thus

$$\mathcal{L}[\psi(x);\psi^{\dagger}(x)] = \mathcal{L}_0[\psi(x);\psi^{\dagger}(x)] + \mathcal{L}_I[\psi(x);\psi^{\dagger}(x)] \tag{3.9a}$$

with

$$\mathcal{L}_0(x) = i\psi^{\dagger}\frac{\partial\psi}{\partial t} - \psi^{\dagger}\varepsilon(-i\nabla)\psi(x) . \tag{3.9b}$$

In order to keep the discussion fairly general we do not specify the interaction term $\mathcal{L}_I$; the only restriction on it we require is that it does not contain time derivatives of the electron fields and that it is invariant under the following set of transformations:

1.
$$\psi^{\alpha}_{\uparrow}(x) \longrightarrow \psi^{\alpha}_{\uparrow}(x)' = \psi^{\alpha}_{\uparrow}(x) - i\theta\psi^{\alpha}_{\downarrow}(x) \tag{3.10a}$$

$$\psi^{\alpha}_{\downarrow}(x) \longrightarrow \psi^{\alpha}_{\downarrow}(x)' = \psi^{\alpha}_{\downarrow}(x) - i\theta\psi^{\alpha}_{\uparrow}(x) , \tag{3.10b}$$

2.
$$\psi^{\alpha}_{\uparrow}(x) \longrightarrow \psi^{\alpha}_{\uparrow}(x)' = \psi^{\alpha}_{\uparrow}(x) + \theta\psi^{\alpha}_{\downarrow}(x) \tag{3.11a}$$

$$\psi^{\alpha}_{\downarrow}(x) \longrightarrow \psi^{\alpha}_{\downarrow}(x)' = \psi^{\alpha}_{\downarrow}(x) - \theta\psi_{\uparrow}(x) \tag{3.11b}$$

and

3.
$$\psi^{\alpha}_{\uparrow}(x) \longrightarrow \psi^{\alpha}_{\uparrow}(x)' = \psi^{\alpha}_{\uparrow}(x) - i\theta\psi^{\alpha}_{\uparrow}(x) \tag{3.12a}$$

$$\psi^{\alpha}_{\downarrow}(x) \longrightarrow \psi^{\alpha}_{\downarrow}(x)' = \psi^{\alpha}_{\downarrow}(x) + i\theta\psi^{\alpha}_{\downarrow}(x) \tag{3.12b}$$

together with the corresponding transformations for the conjugate fields.

The assumption that $\mathcal{L}_I$ does not contain the derivatives of the fields allows us to construct the canonical momenta for the fields $\psi^{\alpha}(x)$ as

$$\begin{Bmatrix} \Pi^{\alpha}_{\uparrow}(x) \\ \Pi^{\alpha}_{\downarrow}(x) \end{Bmatrix} = i \begin{Bmatrix} \psi^{\alpha}_{\uparrow}(x)^{\dagger} \\ \psi^{\alpha}_{\downarrow}(x)^{\dagger} \end{Bmatrix} . \tag{3.13}$$

Hence we may write the Heisenberg equations of motion in terms of the

Hamiltonian H given by

$$\hat{H}[\psi(x);\psi^{\dagger}(x)] = H[\psi;\psi^{\dagger}] - \widetilde{H[\psi;\psi^{\dagger}]} \tag{3.14}$$

with

$$H[\psi;\psi^{\dagger}] = \int d^3\vec{x}[\Pi(x)\psi(x) - \mathcal{L}[\psi;\psi^{\dagger}]]$$

$$= \int d^3\vec{x}\{\psi^{\dagger}(x)\varepsilon(-i\nabla)\psi(x) - \mathcal{L}_I[\psi(x);\psi^{\dagger}(x)]\} \tag{3.15}$$

together with the equal time canonical anti-commutation relations of Eq. (2.33) which gives together with Eq. (3.13)

$$[\psi^{\alpha}_{\uparrow}(x),\psi^{\beta}_{\uparrow}(x')^{\dagger}]_{+}\delta(t-t') = \delta_{\alpha\beta}\delta(x-x') \tag{3.16a}$$

$$[\psi^{\alpha}_{\downarrow}(x),\psi^{\beta}_{\downarrow}(x')^{\dagger}]_{+}\delta(t-t') = \delta_{\alpha\beta}\delta(x-x') \tag{3.16b}$$

and

$$[\psi^{\alpha}_{\downarrow}(x),\psi^{\beta}_{\uparrow}(x)^{\dagger}]_{+}\delta(t-t') = 0 \ . \tag{3.16c}$$

Corresponding to each of the three transformations given by Eqs. (3.10→3.12) we may define a charge $Q_i(t)$ $(i = 1,2,3)$ following Eqs. (2.67a) and (2.69) and we obtain the result that

$$\hat{Q}_i(t) = Q(t) - \tilde{Q}(t) \ , \tag{3.17}$$

with

$$Q_i(t) = \int d^3x\,\psi^{\dagger}(x)\sigma_i\psi(x) \ , \tag{3.18}$$

where σ_i denote the Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} ; \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} ; \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} . \tag{3.19}$$

The charges $\hat{Q}_i(t)$ may then be used to generate the transformations according to Eq. (2.70).

$$[\psi^{\alpha}_{\uparrow}(x),\hat{Q}_i(t)]\delta(t-t_x) = i\delta(t-t_x)\delta_i\psi^{\alpha}_{\uparrow}(x) \tag{3.20}$$

and

$$[\psi_{\downarrow}^{\alpha}(x),\hat{Q}_i(x)]\delta(t-t_x) = i\delta(t-t_x)\delta_i\psi_{\downarrow}^{\alpha}(x) \; . \tag{3.21}$$

It should be noted in passing that the operators $\vec{Q} = (Q_1, Q_2, Q_3)$ defined by Eq. (3.18) may be shown by virtue of the canonical anti-commutation relations to obey the algebra

$$[Q_i^{\alpha}(t),Q_j^{\beta}(t)]\delta(t-t') = i\delta(t-t')\delta_{\alpha\beta}\varepsilon_{ijk}Q_k^{\alpha}(t) \; . \tag{3.22}$$

The transformations presented in Eqs. (3.10→3.12) are generally referred to as rotations in spin space, the operators Q_i as the generators of spin rotation and the invariance of the Lagrangian under the transformation as spin rotational invariance.

In the case of ferromagnetic systems we have that

$$\vec{M} = \langle\beta|\vec{\sigma}(x)|\beta\rangle \neq 0 \tag{3.23}$$

where we have used the notation $\vec{\sigma}(x) = (\sigma_1(x),\sigma_2(x),\sigma_3(x))$ with

$$\sigma_i(x) = \psi^{+}(x)\sigma_i\psi(x) \; . \tag{3.24}$$

Condition (3.23) implies that for some i and j we have that

$$\begin{aligned} \langle\beta|\delta_i\sigma_j(x)|\beta\rangle &= \langle\beta|[\sigma_j(x),Q_i]|\beta\rangle \\ &= \varepsilon_{ijk}\langle\beta|\sigma_k(x)|\beta\rangle \\ &\neq 0 \; . \end{aligned} \tag{3.25}$$

From the discussion of Section 2.2 we see that the ferromagnetic state therefore, corresponds to the situation in which the spin rotational invariance of the system is spontaneously broken. As was pointed out in the discussion in Section 2.2, in order to ensure that the generators of spin rotational invariance are well defined and that our analysis of the ferromagnetic state is meaningful then we must add a small symmetry breaking term to the Lagrangian. We therefore consider

$$\mathcal{L} \longrightarrow \mathcal{L}_h[\psi;\psi^\dagger] = \mathcal{L}[\psi;\psi^\dagger] + h\sigma_3(x) \ , \qquad (3.26)$$

where h is some small but finite constant. The condition for the spontaneous breakdown of the spin rotational invariance and the existence of the ferromagnetic state may then be expressed as

$$\lim_{h\to 0} \langle\beta|\sigma_3(x)|\beta\rangle \neq 0 \ , \qquad (3.27a)$$

$$\lim_{h\to 0} \langle\beta|\sigma_1(x)|\beta\rangle = \lim_{h\to 0} \langle\beta|\sigma_2(x)|\beta\rangle = 0 \ . \qquad (3.27b)$$

This above procedure may be interpreted intuitively as applying a small magnetic field along the z direction, for $T < T_c$ the magnetization remains finite in the limit as $h \to 0$.

The assumption of spin rotational invariance means that

$$\delta_i \hat{\mathcal{L}}_h[\psi;\psi^\dagger] = h\,\delta_i\,\hat{\sigma}_3(x) \ . \qquad (3.28)$$

Thus the W-T relations given in Eq. (2.73) assume the form

$$\frac{\partial}{\partial t} \langle\beta|T[\hat{Q}_i(t)A_1^{\alpha_1}(x_1)\ldots A_n(x_n)]|\beta\rangle$$

$$= -\sum_r \delta(t-t_r)\, i\langle\beta|T[A_1^{\alpha_1}(x_1)\ldots[\delta A_r^{\alpha_r}(x_r)]\ldots A_n^{\alpha_n}(x_n)]|\beta\rangle$$

$$+ h\int d^3\vec{x}\,\langle\beta|T[\delta_i\hat{\sigma}_3(x)A_1^{\alpha_1}(x_1)\ldots A_n^{\alpha_n}(x_n)]|\beta\rangle \qquad (3.29)$$

and in Eq. (2.74)

$$\sum_r <\beta|T[A_1^{\alpha_1}(x_1)\ldots[\delta A_r^{\alpha_r}(x_r)]\ldots A_n^{\alpha_n}(x_n)]|\beta>$$

$$= ih\int d^4x <\beta|T[\delta\hat{\sigma}_3(x)\, A_1^{\alpha_1}(x_1)\ldots A_n^{\alpha_n}(x_n)]|\beta> \quad . \qquad (3.30)$$

If we now make the following definitions

$$\sigma_\pm^\alpha(x) = \frac{1}{2}\,[\sigma_1^\alpha(x) \pm i\sigma_2^\alpha(x)] \qquad (3.31)$$

$$\hat{Q}_\pm(t) = \int d^3\vec{x}[\sigma_\pm(x) - \tilde{\sigma}_\pm(x)] \quad , \qquad (3.32)$$

and

$$[A^\alpha(x),\hat{Q}_\pm(t)]\delta(t-t_x) = i\delta(t-t_x)\delta_\pm A^\alpha(x) \qquad (3.33)$$

then Eq. (3.29) yields the following relation between the transverse spin correlation function $<\beta|T[\sigma_+^\alpha(x)\sigma_-^\beta(y)]|\beta>$ and the magnetization $<\beta|\sigma_3(x)|\beta>$

$$\delta(t_x - [illegible](x)|\beta> = \int d^3\vec{x}\sum_a \varepsilon^a \{\frac{\partial}{\partial t} + 2ih\}<\beta|T[\sigma_+^a(x)\sigma_-^\alpha(y)]|\beta> \quad , \qquad (3.34)$$

where [illegible] have used the result that

$$\delta_\pm\sigma_3^\alpha(x) = \mp 2i\sigma_\pm^\alpha(x) \qquad (3.35a)$$

and

$$\delta_\pm\sigma_\mp^\alpha(x) = \pm i\sigma_3^\alpha(x) \quad . \qquad (3.35b)$$

Denoting

$$<\beta|\sigma_3^\alpha(x)|\beta> = M \qquad (3.36)$$

and writing

$$<\beta|T[\sigma_+^\alpha(x)\sigma_-^\beta(y)]|\beta> = \frac{i}{(2\pi)^4}\int d^4q\; e^{-iq(x-y)}\Delta^{\alpha\beta}(q) \quad , \qquad (3.37)$$

Eq. (3.34) yields

$$M = (q_0 - 2h)\sum_a \varepsilon^a \Delta^{a\alpha}(q)_{\vec{q}=0} \quad . \qquad (3.38)$$

The result of Eq. (3.38) implies that when the spin rotational symmetry is spontaneously broken (i.e. $\lim_{h\to 0} M \neq 0$) then the transverse spin susceptibility contains a zero frequency (again in the limit $h\to 0$) pole. This is a particular example of the celebrated Goldstone theorem.

Expressing $\Delta(q)$ in the spectral representation[7, 40] discussed in Section 2.1 (Eq. (2.56))

$$\Delta^{\alpha\beta}(q) = \int d\omega\ \rho(\omega;\vec{q})U_B(q_0)\tau[q_0-\omega+i\delta\tau]^{-1}U_B(q_0)\ , \qquad (3.39)$$

where the matrices $U_B(q_0)$ are those given in Eq. (2.52), the result (3.38) implies that

$$\lim_{\vec{q}\to 0} \rho(q_0;\vec{q}) = M\delta(q_0 - 2h)\ . \qquad (3.40)$$

Goldstone's theorem has important experimental consequences, in that it implies the existence of low energy, long wavelength, particle-like excitations associated with the transverse spin susceptibility, below T_c. Such modes are generally referred to as magnons and have been observed in a number of metallic ferromagnets [89,90,91]. Furthermore the fact that the excitation spectrum of the magnons is gapless (for $h = 0$) means that such modes are easily excited. This together with the manner in which they couple to the electronic degrees of freedom can, as we will show in the next section, give rise to the Bloch $T^{3/2}$ law[82] mentioned earlier.

An analogous argument may be employed in the case of the localized model and the existence of the magnon excitation may also be shown to be an exact requirement of the spontaneously broken spin rotational invariance[7]. A number of authors have considered the effect of such modes on the low temperature behaviour of the localized model using the Heisenberg model[92,93].

The W-T relations given by Eqs. (3.29) and (3.30) may also be used to derive a number of other identities which, as we shall see, prove extremely useful in examining the effect of the spin fluctuations in both the low temperature ferromagnetic domain ($T < T_c$) as well as the high temperature paramagnetic domain ($T > T_c$). Using the relation that

$$\delta_{\pm}\psi^{\alpha}(x) = -i\sigma_{\pm}\psi^{\alpha}(x) \tag{3.41a}$$

and

$$\delta_{\pm}\psi^{\alpha}(x)^{\dagger} = i\psi^{\alpha}(x)^{\dagger}\sigma_{\pm} \tag{3.41b}$$

we obtain, from Eq. (3.30), that

$$<\beta|T[\psi^{\alpha}_{\uparrow}(x)\psi^{\beta}_{\uparrow}(y)^{\dagger}]|\beta> - <\beta|T[\psi^{\alpha}_{\downarrow}(x)\psi^{\beta}_{\downarrow}(y)^{\dagger}]|\beta>$$
$$= 2ih\sum_{\gamma}\varepsilon^{\gamma}\int dz <\beta|T[\sigma^{\gamma}_{+}(z)\psi^{\alpha}_{\uparrow}(x)\psi^{\beta}_{\downarrow}(y)^{\dagger}]|\beta> \quad , \tag{3.42}$$

$$<\beta|T[\psi^{\alpha}_{\uparrow}(x)\psi^{\beta}_{\uparrow}(y)^{\dagger}]|\beta> - <\beta|T[\psi^{\alpha}_{\downarrow}(x)\psi^{\beta}_{\downarrow}(y)^{\dagger}]|\beta>$$
$$= -2ih\sum_{\gamma}\varepsilon^{\gamma}\int d^4z <\beta|T[\psi^{\alpha}_{\uparrow}(x)\psi^{\beta}_{\downarrow}(y)^{\dagger}\sigma^{\gamma}_{-}(z)]|\beta> \quad , \tag{3.43}$$

$$<\beta|T[\psi^{\alpha_1}_{\uparrow}(x_1)\psi^{\alpha_2}_{\uparrow}(x_2)^{\dagger}\sigma^{\beta}_{3}(y)]|\beta> - <\beta|T[\psi^{\alpha_1}_{\downarrow}(x_1)\psi^{\alpha_2}_{\uparrow}(x_2)^{\dagger}\sigma^{\beta}_{-}(y)]|\beta>$$
$$= -2ih\int d^4z\sum_{\gamma}\varepsilon^{\gamma}<\beta|T[\sigma^{\gamma}_{+}(z)\psi^{\alpha_1}_{\uparrow}(x_1)\psi^{\alpha_2}_{\uparrow}(x_2)^{\dagger}\sigma^{\beta}_{-}(y)]|\beta> \tag{3.44}$$

and

$$<\beta|T[\psi^{\alpha_1}_{\downarrow}(x_1)\psi^{\alpha_2}_{\downarrow}(x_2)^{\dagger}\sigma^{\beta}_{3}(y)]|\beta> + <\beta|T[\psi^{\alpha_2}_{\uparrow}(x_1)\psi^{\alpha_2}_{\downarrow}(x_2)^{\dagger}\sigma^{\beta}_{+}(y)]|\beta>$$
$$= -2ih\int d^4z\sum_{\gamma}\varepsilon^{\gamma}<\beta|T[\sigma^{\gamma}_{-}(z)\psi^{\alpha_1}_{\downarrow}(x_1)\psi^{\alpha_2}_{\downarrow}(x_2)^{\dagger}\sigma_{+}(y)]|\beta> \quad . \tag{3.45}$$

We also obtain the following relation between the spin operator

Green's functions

$$<\beta|T[\sigma_3^\alpha(x)\sigma_3^\beta(y)]|\beta> - 2<\beta|T[\sigma_+^\alpha(x)\sigma_-^\beta(y)]|\beta>$$

$$= -2ih\int d^4z \sum_\gamma \varepsilon^\gamma <\beta|T[\sigma_-^\gamma(z)\sigma_+^\alpha(x)\sigma_3^\beta(y)]|\beta> \quad (3.46a)$$

$$= 2ih\int d^4z \sum_\gamma \varepsilon^\gamma <\beta|T[\sigma_+^\gamma(z)\sigma_-^\alpha(x)\sigma_3^\beta(y)]|\beta> \quad (3.46b)$$

and finally

$$<\beta|T[\sigma_+^{\alpha_1}(x_1)\sigma_3^{\alpha_2}(x_2)\sigma_-^{\alpha_3}(x_3)]|\beta> + <\beta|T[\sigma_+^{\alpha_1}(x_1)\sigma_-^{\alpha_2}(x_2)\sigma_3^{\alpha_3}(x_3)]|\beta>$$

$$= -2ih\int d^4z \sum_\gamma \varepsilon^\gamma <\beta|T[\sigma_+^\gamma(z)\sigma_+^{\alpha_1}(x_1)\sigma_-^{\alpha_2}(x_2)\sigma_-^{\alpha_3}(x_3)]|\beta> \quad . \quad (3.47)$$

We close this section by restating the basic assumption underlying our treatment of the itinerant electron ferromagnets namely that the ferromagnetic state in metals may be regarded as the spontaneous polarization of a spin rotationally invariant system of itinerant spin 1/2 fermions, induced through the self-interaction. A number of exact results may be shown to follow from this statement by virtue of the W-T relations outlined in Section 2.2, most important of those is the existence of the low frequency long wavelength particle-like excitations in the transverse spin susceptibility, the magnons (Goldstone's theorem). In the next section we demonstrate how the W-T relations contained in Eqs. (3.42→3.46b) to compute the effect of the magnons on the temperature dependence of various static and dynamic quantities, thus giving flesh to the somewhat formal bones of this section.

3.2 The Thermal Excitations of Magnons at Low Temperatures

In the previous section we outlined the need to consider a more sophisticated treatment of the itinerant electron model of ferromagnetism than that provided by the simple Stoner theory, if we wish to employ such a model to analyze the finite temperature behaviour of metallic ferromagnets. In this section we present a low temperature expansion, using the TFD formalism, which allows us to express the finite temperature corrections to various static and dynamical quantities, arising from the thermal excitation of the magnons, in terms of vertices calculated at zero temperature. It will then be demonstrated how by virtue of the W-T relations an exact expression for the leading finite temperature magnon correction may be obtained, in an entirely model independent fashion, for several experimentally important quantities.

The reason one may obtain certain exact results in this way may be understood as follows: the requirements of spin rotational invariance not only require, for $T < T_c$, the existence of the magnon excitation, as demonstrated in the previous section, but also serves to determine many of its properties through the W-T relations given by Eqs. (3.42→3.47).

We begin by formulating in the real time formalism a low temperature expansion for the ferromagnetic domain of an itinerant electron ferromagnet. A similar expansion has found several applications in finite temperature relativistic field theory[49,50,94] and also by means of the real time formulation of statistical mechanics. As outlined in Section 2.1, the TFD formalism may be used to calculate the statistical average of any time ordered product of the Heisenberg fields in perturbation theory, by means of a Feynman diagram technique, in a manner entirely analogous to that obtained at zero temperature. Thus we may write that

$$\langle\beta|T[A_1^{\alpha_1}(x_1)\ldots A_n^{\alpha_n}(x_n)]|\beta\rangle = F(x_1\alpha_1\ldots x_n\alpha_n|S_+,S_-;\lambda) \qquad (3.48)$$

where $S_{\pm}$ denote the bare electron propagators defined as

$$S_{\pm}(p) = U_F(p_0)\{p_0 - [\varepsilon(\vec{p}) \mp h] + i\delta\tau\}^{-1} U_F^{\dagger}(p_0) \quad , \tag{3.49}$$

where $\varepsilon(\vec{p})$ is the energy spectra of the bare electrons given in Eq.(3.9), λ denotes the bare electron-electron vertex and $U_F(p_0)$ is the thermal transformation matrix defined in Eq. (2.51).

The expansion of the various many point Green's functions in terms of the bare vertex and electron propagators is inappropriate, however, in the analysis of the ordered state, since the spontaneous polarization of the fermion spins may only be realized if an infinite summation of terms in the perturbation series is performed. Instead we therefore consider the following quantities:

$$<\beta|T[\psi_{\uparrow}^{\alpha}(x)\psi_{\uparrow}^{\beta}(y)^{\dagger}]|\beta> = G_{\uparrow}^{\alpha\beta}(x-y|S_{+},S_{-};\lambda) \quad , \tag{3.50}$$

$$<\beta|T[\psi_{\downarrow}^{\alpha}(x)\,\psi_{\downarrow}^{\beta}(y)^{\dagger}]|\beta> = G_{\downarrow}^{\alpha\beta}(x-y|S_{+},S_{-};\lambda) \tag{3.51}$$

and

$$<\beta|T[\sigma_{+}^{\alpha}(x)\sigma_{-}^{\beta}(y)]|\beta> = \Delta^{\alpha\beta}(x-y|S_{+},S_{-};\lambda) \ . \tag{3.52}$$

If we now accumulate all the self-energy diagrams belonging to $G_{\uparrow}$, $G_{\downarrow}$ and Δ, that appear in the diagramatic expansion of Eq. (3.48), then we may re-express it as

$$<\beta|T[A_1^{\alpha_1}(x_1)\ldots A_n^{\alpha_n}(x_n)]|\beta> = F(x_1\alpha_1,\ldots x_n\alpha_n|G_{\uparrow},G_{\downarrow},\Delta;\lambda), \tag{3.53}$$

where F is now constructed in terms of the reduced graphs comprising $G_{\uparrow}$, $G_{\downarrow}$ and Δ as the internal lines. The appearance of the magnon line in the expansion represented by Eq. (3.53) is of essential importance since it is this function which will contain the effect of the magnon pole.

Defining the functions $G_\uparrow(p)$, $G_\downarrow(p)$ and $\Delta(q)$ through the Fourier transforms

$$G_\uparrow^{\alpha\beta}(x-y) = \frac{i}{(2\pi)^4}\int d^4p\; e^{-ip(x-y)}\, G_\uparrow^{\alpha\beta}(p) \quad , \tag{3.54}$$

$$G_\downarrow^{\alpha\beta}(x-y) = \frac{i}{(2\pi)^4}\int d^4p\; e^{-ip(x-y)}\, G_\downarrow^{\alpha\beta}(p) \tag{3.55}$$

and Eq. (3.37)

$$\Delta^{\alpha\beta}(x-y) = \frac{i}{(2\pi)^4}\int d^4q\; e^{-iq(x-y)}\, \Delta^{\alpha\beta}(q) \tag{3.56}$$

and as was pointed out in Section 2.1 $G(p)$ and $\Delta(q)$ may be written in the spectral representation as

$$G_\uparrow(p) = \int d\kappa\; g_\uparrow(\kappa;\vec{p})U_F(p_0)[p_0 - \kappa + i\delta\tau]^{-1}U_F^\dagger(p_0) \quad , \tag{3.57}$$

$$G_\downarrow(p) = \int d\kappa\; g_\downarrow(k;\vec{p})U_F(p_0)[p_0 - \kappa + i\delta\tau]^{-1}U_F^\dagger(p_0) \tag{3.58}$$

and

$$\Delta(q) = \int d\omega\; \rho(\omega;\vec{q})U_B(q_0)\tau[q - \omega + i\delta\tau]^{-1}\, U_B(q_0) \quad . \tag{3.59}$$

The functions $G_\uparrow$, $G_\downarrow$ and Δ depend on temperature in two ways: first of all through the explicit temperature dependence of the thermal transformation matrices U_F and U_B and secondly through the spectral functions $g_\uparrow$, $g_\downarrow$ and ρ. In order to formulate a low temperature expansion we find it convenient to introduce the propagators $\overline{G}_\uparrow$, $\overline{G}_\downarrow$ and $\overline{\Delta}$ which are obtained from $G_\uparrow$, $G_\downarrow$ and Δ by replacing the finite temperature spectral function with the zero temperature spectral function, thus;

$$\overline{G}_\uparrow^{\alpha\beta}(p) = \int d\kappa\; g_\uparrow^0(\kappa;\vec{p})U_F(p_0)[p_0 - \kappa + i\delta\tau]^{-1}\, U_F^\dagger(p_0) \quad , \tag{3.60}$$

$$\overline{G}_\downarrow^{\alpha\beta}(p) = \int d\kappa\; g_\downarrow^0(\kappa;\vec{p})U_F(p_0)[p_0 - \kappa + i\delta\tau]^{-1}\, U_F^\dagger(p_0) \tag{3.61}$$

and

$$\overline{\Delta}^{\alpha\beta}(q) = \int d\omega\, \rho^{o}(\omega;\vec{q}) U_B(q_o)\tau[q_o - \omega + i\delta\tau]^{-1} U_B(q_o) \tag{3.62}$$

where $g^{o}_{\uparrow}$, $g^{o}_{\downarrow}$ and ρ^{o} denote the spectral functions $g_{\uparrow}$, $g_{\downarrow}$ and ρ respectively evaluated at zero temperature. The propagators $\overline{G}_{\uparrow}$, $\overline{G}_{\downarrow}$ and $\overline{\Delta}$ are related through the Dyson equation which is of the following form.

$$G^{\alpha\beta}_{\uparrow}(p) = \overline{G}^{\alpha\beta}_{\uparrow}(p) + \sum_{\gamma} \overline{G}^{\alpha\gamma}_{\uparrow}(p) F^{\gamma\beta}_{\uparrow}(p|G_{\uparrow};G_{\downarrow};\Delta;\lambda) , \tag{3.63}$$

$$G^{\alpha\beta}_{\downarrow}(p) = \overline{G}^{\alpha\beta}_{\downarrow}(p) + \sum_{\gamma} \overline{G}^{\alpha\gamma}_{\downarrow}(p) F^{\gamma\beta}_{\downarrow}(p|G_{\uparrow};G_{\downarrow};\Delta;\lambda) \tag{3.64}$$

and

$$\Delta^{\alpha\beta}(q) = \overline{\Delta}^{\alpha\beta}(q) + \sum_{\gamma} \overline{\Delta}^{\alpha\gamma}(q) F^{\gamma\beta}_{\Delta}(q|G_{\uparrow};G_{\downarrow};\Delta;\lambda) . \tag{3.65}$$

Since $\overline{G}_{\uparrow}$, $\overline{G}_{\downarrow}$ and $\overline{\Delta}$ are defined in such a way that the temperature dependence only appears through the thermal transformation matrices they may be expressed as

$$\overline{G}^{\alpha\beta}_{\uparrow}(p) = G^{o}_{\uparrow}(p)^{\alpha\beta} + \delta G^{\alpha\beta}_{\uparrow}(p) , \tag{3.66}$$

$$\overline{G}^{\alpha\beta}_{\downarrow}(p) = G^{o}_{\downarrow}(p)^{\alpha\beta} + \delta G^{\alpha\beta}_{\downarrow}(p) \tag{3.67}$$

and

$$\overline{\Delta}^{\alpha\beta}(p) = \Delta^{o}(q)^{\alpha\beta} + \delta\Delta^{\alpha\beta}(p) , \tag{3.68}$$

where $G^{o}_{\uparrow}$, $G^{o}_{\downarrow}$ and Δ^{o} are the zero temperature propagators and are given by

$$G^{o}_{\uparrow}(p)^{\alpha\beta} = \int d\kappa\; g^{o}_{\uparrow}(\kappa;\vec{p}) \left(\frac{1}{p_o - \kappa + i\varepsilon(\kappa)\delta\tau}\right)^{\alpha\beta} , \tag{3.69}$$

$$G^{o}_{\downarrow}(p)^{\alpha\beta} = \int d\kappa\; g^{o}_{\downarrow}(\kappa;\vec{p}) \left(\frac{1}{p_o - \kappa + i\varepsilon(\kappa)\delta\tau}\right)^{\alpha\beta} \tag{3.70}$$

and

$$\Delta^{o}(q)^{\alpha\beta} = \int d\omega\; \rho^{o}(\omega;\vec{q}) \left(\frac{\tau}{q_o - \omega + i\varepsilon(\omega)\delta\tau}\right)^{\alpha\beta} . \tag{3.71}$$

While the terms $\delta G_{\uparrow}$, $\delta G_{\downarrow}$ and $\delta\Delta$ represent the finite temperature corrections and are given by

$$\delta G_{\uparrow}^{\alpha\beta}(p) = 2\pi i\ \varepsilon(p_0) g_{\uparrow}^{0}(p_0;\vec{p}) \begin{pmatrix} f_F(|p_0|) & [f_F(p_0)g_F(p_0)]^{\frac{1}{2}} \\ [f_F(p_0)g_F(p_0)]^{\frac{1}{2}} & -f_F(|p_0|) \end{pmatrix} \tag{3.72}$$

and

$$\delta\Delta^{\alpha\beta}(q) = -2\pi i\ \varepsilon(q_0)\rho^{0}(q_0;\vec{q}) \begin{pmatrix} f_B(|q_0|) & [f_B(q_0)g_B(q_0)]^{\frac{1}{2}} \\ [f_B(q_0)g_B(q_0)]^{\frac{1}{2}} & f_B(|q_0|) \end{pmatrix}. \tag{3.73}$$

The low temperature expansion of the many point Green's function of Eq. (3.53) may now be obtained by performing a functional expansion of the function F in powers of $\delta\Delta$ and δG. Thus we have

$$\begin{aligned} <\beta|T[A_1^{\alpha_1}(x_1)\ldots A_n^{\alpha_n}(x_n)]|\beta> &= F(x_1\alpha_1\ldots x_n\alpha_n|G_{\uparrow};G_{\downarrow};\Delta;\lambda) \\ &= \overline{F}(x_1\alpha_1\ldots x_n\alpha_n|\overline{G}_{\uparrow};\overline{G}_{\downarrow};\overline{\Delta};\lambda) \\ &= F^{0}(x_1\alpha_1\ldots x_n\alpha_n|G_{\uparrow}^{0};G_{\downarrow}^{0};\Delta^{0};\lambda) \end{aligned}$$

$$+ \frac{i}{(2\pi)^4}\int d^4q \sum_{ab} \mathcal{F}_{\Delta}(x_1\alpha_1\ldots x_n\alpha_n|q;ab|G_{\uparrow}^{0};G_{\downarrow}^{0};\Delta^{0};\lambda)\delta\Delta^{ab}(q)$$

$$+ \frac{i}{(2\pi)^4}\int d^4p \sum_{ab} \mathcal{F}_{\uparrow}(x_1\alpha_1\ldots x_n\alpha_n|p;ab|G_{\uparrow}^{0};G_{\downarrow}^{0};\Delta^{0};\lambda)\delta G_{\uparrow}^{ab}(p)$$

$$+ \frac{i}{(2\pi)^4}\int d^4p \sum_{ab} \mathcal{F}_{\downarrow}(x_1\alpha_1\ldots x_n\alpha_n|p;ab|G_{\uparrow}^{0};G_{\downarrow}^{0};\Delta^{0};\lambda)\delta G_{\downarrow}^{ab}(p)$$

$$+ \ldots\ldots\ldots\ldots \tag{3.74}$$

The form factors appearing in the above expansion, $\mathcal{F}_{\uparrow}$, $\mathcal{F}_{\downarrow}$ and $\mathcal{F}_{\Delta}$, have an obvious diagramatic interpretation. The first term, for example, simply corresponds to the sum of all the reduced diagrams calculated using the zero temperature propagators and hence may be identified as

$$F^{o}(x_1\alpha_1 \ldots x_n\alpha_n | G^{o}_{\uparrow};G^{o}_{\downarrow};\Delta^{o};\lambda) \tag{3.75}$$

$$= \begin{cases} <0|T[A_1(x_1)\ldots A_n(x_n)]|0> & \text{for } \{\alpha_i\} = \{1\} \text{ or } \{2\} \\ 0 & \text{otherwise} \end{cases}$$

where $|0>$ denotes the zero temperature vacuum. In particular we have that

$$G^{o}_{\uparrow}(x-y)^{\alpha\beta} = \delta_{\alpha\beta}<0|T[\psi_{\uparrow}(x)\psi^{\dagger}_{\uparrow}(y)]|0> \quad , \tag{3.76}$$

$$G^{o}_{\downarrow}(x-y)^{\alpha\beta} = \delta_{\alpha\beta}<0|T[\psi_{\downarrow}(x)\psi^{\dagger}_{\downarrow}(y)]|0> \tag{3.77}$$

and

$$\Delta^{o}(x-y)^{\alpha\beta} = \delta_{\alpha\beta}<0|T[\sigma_{+}(x)\sigma_{-}(y)]|0> \quad . \tag{3.78}$$

The second term $\mathcal{F}_{\Delta}$, for example, corresponds to the sum of all diagrams with (n+2) external lines, n of which correspond to the fields $\{A_i(x_1)\}$; the remaining two corresponding to external magnon lines with the magnon propagators removed. The third (fourth) term $\mathcal{F}_{\uparrow(\downarrow)}$ corresponds to the sum of all the diagrams with (n+2) external lines n of which correspond to the fields $\{A_i(x)\}$, while the remaining two correspond to external spin-up (-down) electron lines with the electron propagators removed.

It is important to realize that while the reduced diagrams constructed in terms of the propagators $\overline{G}_{\uparrow}$, $\overline{G}_{\downarrow}$ and $\overline{\Delta}$ may have had a somewhat different topological structure than those obtained at zero temperature the above considerations show that the coefficients appearing in the low temperature expansion may be calculated in terms of the zero temperature diagrams. Therefore there is no need to calculate any new diagrams since any change in the topological structure will be realized through the summation of the low temperature expansion given by Eq. (3.74).

While the nature of the above discussion may appear to be of a rather formal nature the final result contained in Eq. (3.74) and the diagramatic interpretation of the form factors has an obvious intuitive appeal.

In order to demonstrate the practical merit of the low temperature expansion we consider the correction to the magnetization arising from the thermal excitation of the magnons. From Eq. (3.36) together with Eqs. (3.50) and (3.51) we have that

$$M(T) = -\frac{i}{(2\pi)^4}\int d^4p[G_{\uparrow}^{11}(p) - G_{\downarrow}^{11}(p)] \quad . \tag{3.79}$$

The propagators $G_{\uparrow}(p)$ and $G_{\downarrow}(p)$ may be computed in the low temperature expansion and we write

$$\begin{aligned} G_{\uparrow}^{\alpha\beta}(p) &= G_{\uparrow}^{0}(p)^{\alpha\beta} + \frac{i}{(2\pi)^4}\int d^4q \sum_{ab} \mathcal{F}_{\Delta}^{\uparrow}(p;q)_{ab}^{\alpha\beta}\,\delta\Delta^{ab}(q) \\ &+ \frac{i}{(2\pi)^4}\int d^4p' \sum_{ab} [\mathcal{F}_{\uparrow}^{\uparrow}(p;p)_{ab}^{\alpha\beta}\,\delta G_{\uparrow}(p')^{ab} + \mathcal{F}_{\downarrow}^{\uparrow}(p;p')_{ab}^{\alpha\beta}\delta G_{\downarrow}(p)^{ab}] \\ &+ \ldots\ldots \end{aligned} \tag{3.80}$$

and

$$\begin{aligned} G_{\downarrow}^{\alpha\beta}(p) &= G_{\downarrow}^{0}(p)^{\alpha\beta} + \frac{i}{(2\pi)^4}\int d^4q \sum_{ab} \mathcal{F}_{\Delta}^{\downarrow}(p;q)_{ab}^{\alpha\beta}\delta\Delta(q)^{ab} \\ &+ \frac{i}{(2\pi)^4}\int d^4p' \sum_{ab} [\mathcal{F}_{\downarrow}^{\downarrow}(p;p')_{ab}^{\alpha\beta}\delta G_{\downarrow}(p)^{ab} + \mathcal{F}_{\uparrow}^{\downarrow}(p;p')_{ab}^{\alpha\beta}\,\delta G_{\uparrow}^{ab}(p')] \\ &+ \ldots\ldots\ldots \end{aligned} \tag{3.81}$$

Since the form factors $\mathcal{F}$ appearing in Eqs. (3.80) and (3.81) are constructed using the Green's function $G^{0}(p)^{\alpha\beta}$ which is diagonal in the indices $\alpha\beta$ and since the vertices do not mix the tildé and non-tildé fields then we have that

$$\mathcal{F}^{\alpha\beta}_{\alpha'\beta'} = \mathcal{F}\,\delta_{\alpha\beta}\delta_{\alpha'\beta'}\delta_{\alpha'\alpha} \tag{3.82}$$

Therefore if we consider Eqs. (3.80) and (3.81) in the case $\alpha = \beta = 1$ and, since it is the magnon correction we wish to calculate, we consider only the contribution arising from the $\delta\Delta(q)$ term. Then Eqs. (3.80) and (3.81) reduce to

$$G^{11}_{\uparrow}(p) = G^{o}_{\uparrow}(p) + \frac{1}{(2\pi)^3}\int d^4q\, \mathcal{F}^{\uparrow}_{\Delta}(p;q) f_B(|q_o|)\rho^o(q_o;\vec{q})\varepsilon(q_o) + \dots \tag{3.83}$$

and

$$G^{11}_{\downarrow}(p) = G^{o}_{\downarrow}(p) + \frac{1}{(2\pi)^3}\int d^4q\, \mathcal{F}^{\uparrow}_{\Delta}(p;q) f_B(|q_o|)\rho^o(q_o;\vec{q})\varepsilon(q_o) + \dots \tag{3.84}$$

where we have used Eq. (3.73). Now the spectral function $\rho^o(q_o;\vec{q})$ contains both the magnon pole and the continuum contribution

$$\rho^o(q_o;\vec{q}) = Z^o(\vec{q})\,\delta(q_o - \omega^o_B(\vec{q})) + \rho^o_c(q_o;\vec{q}) \tag{3.85}$$

which, since we are concerned with the magnon contribution, we approximate ρ^o as

$$\rho^o(q_o;\vec{q}) \simeq Z^o(\vec{q})\delta(q_o - \omega^o_B(\vec{q})) + \dots \quad . \tag{3.86}$$

Now from the result of Eq. (3.40) we have that

$$\lim_{\vec{q}\to 0} Z^o(\vec{q}) = M(T=0) \equiv M_o \tag{3.87}$$

and

$$\lim_{\vec{q}\to 0} \omega^o_B(q) = 2h \tag{3.88}$$

from which we can deduce that

$$\omega_B^o(\vec{q}) = 2h + Dq^2 + \ldots\ldots \quad , \tag{3.89}$$

where D is referred to as the spin wave stiffness.

Equations (3.83), (3.84) and (3.86) then lead to the following result

$$G_\uparrow^{11}(p) = G_\uparrow^o(p) + \int \frac{d^3\vec{q}}{(2\pi)^3}\, \mathcal{F}_\Delta^\uparrow(p;q)\Big|_{q_o=\omega_B^o} Z_B^o(\vec{q})\, f_B(\omega_B^o(\vec{q})) + \ldots \tag{3.90}$$

and

$$G_\downarrow^{11}(p) = G_\downarrow^o(p) + \int \frac{d^3\vec{q}}{(2\pi)^3}\, \mathcal{F}_\Delta^\downarrow(p;q)\Big|_{q_o=\omega_B^o} Z_B^o(\vec{q})\, f_B(\omega_B^o(\vec{q})) + \ldots \tag{3.91}$$

The fact that the magnon excitation energy tends to zero (for $h=0$) in the long wavelength limit allows us to expand the above expression in terms of $\vec{q}$. Retaining only the first term in the expression we have

$$G_\uparrow^{11}(p) \simeq G_\uparrow^o(p) + Z_B^o(0)\,\mathcal{F}_\Delta^\uparrow(p;0) \int \frac{d^3\vec{q}}{(2\pi)^3}\, f_B(\omega_B^o(\vec{q})) + \ldots \tag{3.92}$$

and

$$G_\downarrow^{11}(p) \simeq G_\downarrow^o(p) + Z_B^o(0)\,\mathcal{F}_\Delta^\downarrow(p;0) \int \frac{d^3\vec{q}}{(2\pi)^3}\, f_B(\omega_B^o(\vec{q})) + \ldots \tag{3.93}$$

Thus we find that the leading correction to the electron propagators $G_\uparrow$ and $G_\downarrow$ is proportional to the magnon density $\int d^3\vec{q}\, f_B(\omega(\vec{q}))$ which may be calculated to give

$$\int d^3\vec{q}\, f_B(\omega_B^o) = \left(\frac{\pi}{D}\right)^{3/2} \zeta\left(\frac{3}{2}\right) \beta^{-3/2} + O(\beta^{-5/2}) \quad , \tag{3.94}$$

where ζ denotes the Rieman zeta function. The higher order terms in the low momentum expansion will be proportional to

$$\int \frac{d^3\vec{q}}{(2\pi)^3}\, |\vec{q}|^{2N}\, f_B(\omega_B^o(\vec{q})) \propto \beta^{-(3+2N)/2} \quad . \tag{3.95}$$

It remains, therefore, to compute the form factors $\mathcal{F}_\Delta^\uparrow$ and $\mathcal{F}_\Delta^\downarrow$. From the discussion of the previous section the form factors $\mathcal{F}_\Delta^\uparrow$ and $\mathcal{F}_\Delta^\downarrow$ are given by the sum of all graphs containing two external electron lines and two magnon lines with the external magnon lines removed. Thus if we define $\Gamma_{\uparrow M}$ as

$$<0|T[\psi_\uparrow(x_1)\sigma_+(y_1)\sigma_-(y_2)\psi_\uparrow^\dagger(y_2)]|0>_c$$
$$= \left(\frac{i}{(2\pi)^4}\right)^4 \int d^4p_1 d^4p_2 d^4q_1 d^4q_2 \; e^{-i(p_1x_1-p_2x_2+q_1y_1-q_2y_2)} \times$$
$$\delta(p_1+q_1-q_2-p_2)G_\uparrow^0(p_1)\Delta^0(q_1)\Gamma_{\uparrow M}(p_1,q_1;q_2,p_2)\Delta^0(q_2)G_\uparrow^0(p_2), \quad (3.96)$$

where the subscript c means that we consider only the connected diagrams, then we have

$$\mathcal{F}_\Delta^\uparrow(p;q) = \frac{i}{(2\pi)^4} G_\uparrow^0(p)\Gamma_{\uparrow M}(p;q;q;p)G_\uparrow^0(p) \quad . \qquad (3.97)$$

Similarly if we define the vertex $\Gamma_{\downarrow M}$ as

$$<0|T[\psi_\downarrow(x_1)\sigma_+(y_1)\sigma_-(y_2)\psi_\downarrow^\dagger(x_2)]|0>$$
$$= \left(\frac{i}{(2\pi)^4}\right)^4 \int d^4p_1 d^4p_2 d^4q_1 d^4q_2 \; e^{-i(p_1x_1-p_2x_2+q_1y_1-q_2y_2)} \times$$
$$\delta(p_1+q_1-q_2-p_2)G_\downarrow^0(p_1)\Delta^0(q_1)\Gamma_{\downarrow M}(p_1;q_1;q_2;p_2)\Delta^0(q_2)G_\downarrow(p_2) \quad (3.98)$$

then we obtain

$$\mathcal{F}_\Delta^\downarrow(p;q) = \frac{i}{(2\pi)^4} G_\downarrow^0(p)\Gamma_{\downarrow M}(p;q;q;p)G_\downarrow^0(p) \quad . \qquad (3.99)$$

Thus Eqs. (3.92) and (3.93) may be written as

$$G_\uparrow^{11}(p) = G_\uparrow^0(p) + Z_B^0(0)G_\uparrow(p)\frac{i}{(2\pi)^4}\Gamma_{\uparrow M}(p;0;0;p)G_\uparrow(p)\int\frac{d^3\vec{q}}{(2\pi)^3} f_B(\omega_B^0(\vec{q})) + \ldots \quad (3.100)$$

and

$$G^{11}_{\downarrow}(p) = G^{0}_{\downarrow}(p) + Z^{0}_{B}(0)G_{\downarrow}(p)\,\frac{i}{(2\pi)^4}\,\Gamma_{\downarrow M}(p;0;0;p)G_{\downarrow}(p)$$

$$\int \frac{d^3\vec{q}}{(2\pi)^3}\, f_B(\omega_B(\vec{q})) + \ldots. \qquad (3.101)$$

The behaviour of the vertices $\Gamma_{\uparrow M}$ and $\Gamma_{\downarrow M}$ are severely controlled by the requirements of spin rotational invariance as expressed in Eqs. (3.42→3.45). From Eqs. (3.42) and (3.44) we obtain, for T = 0, that

$$4h^2\int d^4y_1 d^4y_2 \langle 0|T[\psi_{\uparrow}(x_1)\sigma_{+}(y_1)\sigma_{-}(y_2)\psi_{\uparrow}(x_2)]|0\rangle$$

$$= 2ih\int d^4y_2 \langle 0|T[\psi_{\uparrow}(x_1)\psi^{\dagger}_{\uparrow}(x_2)\sigma_3(y_2)]|0\rangle$$

$$- 2ih\int d^4y_2 \langle 0|T[\psi_{\downarrow}(x_1)\psi^{\dagger}_{\uparrow}(x_2)\sigma_{-}(y_2)]|0\rangle$$

$$= 2ih\int d^4y_2 \langle 0|T[\psi_{\uparrow}(x_1)\psi^{\dagger}_{\uparrow}(x_2)\sigma_3(y_2)]|0\rangle$$

$$+ \langle 0|T[\psi_{\uparrow}(x_1)\psi^{\dagger}_{\uparrow}(x_2)]|0\rangle - \langle 0|T[\psi_{\downarrow}(x_1)\psi^{\dagger}_{\downarrow}(x_2)]|0\rangle\,. \qquad (3.102)$$

From the definition of $\Gamma_{\uparrow M}$ given by Eq. (3.96), Eq. (3.102) yields

$$\lim_{h\to 0} 4h^2\, G^{0}_{\uparrow}(p)\Delta^{0}(0)\,\frac{i}{(2\pi)^4}\,\Gamma_{\uparrow M}(p;0;0;p)\Delta^{0}(0)G_{\uparrow}(p) = G^{0}_{\downarrow}(p) - G^{0}_{\uparrow}(p) \qquad (3.103)$$

and noting from Eq. (3.38) that in the limit $q_o \to 0$ and $T \to 0$

$$\lim_{h\to 0} 4h^2\, \Delta^{0}(0) = M(T=0)\,. \qquad (3.104)$$

Thus Eq. (3.103) yields

$$G^{0}_{\uparrow}(p)\,\frac{i}{(2\pi)^4}\,\Gamma_{\uparrow M}(p;0;0;p)G^{0}_{\uparrow}(p) = \frac{1}{M^2}\,\{G_{\downarrow}(p) - G_{\uparrow}(p)\}\,. \qquad (3.105)$$

An analogous argument based on Eqs. (3.45) and (3.43) yields

$$G^{0}_{\downarrow}(p)\,\frac{i}{(2\pi)^4}\,\Gamma_{\downarrow M}(p;0;0;p)G^{0}_{\downarrow}(p) = \frac{1}{M^2}\,\{G_{\uparrow}(p) - G_{\downarrow}(p)\} \qquad (3.106)$$

Substituting Eqs. (3.105) and (3.106) together with (3.87) into Eqs. (3.100) and (3.101) we obtain

$$G_{\uparrow}^{11}(p) = G_{\uparrow}^{o}(p) - \frac{1}{M_o}\,[G_{\uparrow}^{o}(p) - G_{\downarrow}^{o}(p)]\int\frac{d^3\vec{q}}{(2\pi)^3}\,f_B(\omega_B^o(\vec{q})) + \ldots \tag{3.107}$$

$$G_{\downarrow}^{11}(p) = G_{\downarrow}^{o}(p) - \frac{1}{M_o}\,[G_{\downarrow}^{o}(p) - G_{\uparrow}^{o}(p)]\int\frac{d^3\vec{q}}{(2\pi)^3}\,f_B(\omega_B^o(\vec{q})) + \ldots \tag{3.108}$$

Subtracting Eq. (3.107) from Eq. (3.108) and integrating with respect to d^4p we obtain

$$M(T) = M_o\left\{1 - \frac{2}{M}\int\frac{d^3\vec{q}}{(2\pi)^3}\,f_B(\omega_B^o(\vec{q}))\right\} + O(T^{5/2}) \tag{3.109}$$

and on adding Eqs. (3.107) and (3.108) we obtain

$$N(T) = N(T=0) + O(T^{5/2}) \;, \tag{3.110}$$

where N(T) is defined as

$$N(T) \equiv \langle\beta|\psi^{\dagger}(x)\psi(x)|\beta\rangle \quad . \tag{3.111}$$

The correction to the magnetization in Eq. (3.109) is of course the Bloch $T^{3/2}$ term predicted by the spin wave theory and is consistent with approximate calculations on the ferromagnetism of itinerant electron systems[95]. Equation (3.110) implies that if we assume the electron density remains constant then the renormalization of the chemical potential is order $T^{5/2}$.

The result contained in Eq. (3.109) and the manner in which it was derived is of interest for a number of reasons. First of all it demonstrates that the Bloch $T^{3/2}$ law may be obtained, in the case of itinerant electron ferromagnets, in an exact and unambiguous fashion purely from considerations of symmetry. This implies that the Bloch

$T^{3/2}$ law may be regarded as an exact requirement of the spin rotational invariance of the system. Secondly the derivation illustrates the practical importance of the W-T relations in determining the effect of the magnons on the low temperature behaviour of such systems. It is important therefore that any approximation scheme used in the analysis of itinerant electron ferromagnets be consistent with the W-T relations if it is to properly represent the low temperature behaviour of such systems. In Appendix B we apply these considerations to the particular case of a system of electrons, interacting via a contact interaction. The approximations employed, satisfy the W-T relations of Eqs. (3.105) and (3.106). In addition to the $T^{3/2}$ contribution arising from the magnons, the $T^{5/2}$ contribution is calculated explicitly in terms of certain band parameters.

A similar analysis may be applied to other experimentally accessible quantities. For example it was mentioned earlier that the magnon excitation may be observed in neutron scattering experiments and the excitation spectra measured. Observations indicate that the magnon spectra is relatively insensitive to temperature around $T = 0$ [91]; we therefore apply the preceding analysis to consider the effect of the thermally excited magnons on two excitation spectra of the magnons.

The arguments proceed much as before, in analogy with Eqs.(3.80) and (3.81) we have that

$$\Delta^{11}(q) = \Delta^{o}(q) + \frac{i}{(2\pi)^4}\int d^4q' \,\mathcal{F}^{\Delta}_{\Delta}(q;q')^{\alpha\beta}_{ab}\, \delta\Delta^{ab}(q') \tag{3.112}$$

where we have neglected to include the corrections δG which are of no interest to us in this discussion. Proceeding exactly as in the calculation of the one electron Green's function we obtain

$$\Delta(q) = \Delta^o(q) + \int \frac{d^3\vec{q}\,'}{(2\pi)^3} \mathcal{F}^{\Delta}_{\Delta}(q;q')_{q'=\omega^o_B(q')} Z^o(\vec{q}) f_B(\omega^o_B(\vec{q})) + \ldots \quad (3.113)$$

$$= \Delta^o(q) + Z^o(0)\, \mathcal{F}^{\Delta}_{\Delta}(q;0) \int \frac{d^3\vec{q}}{(2\pi)^3} f_B(\omega^o_B(\vec{q})) + \ldots \quad (3.114)$$

Following the arguments of the previous Section 3.1 we may identify $\mathcal{F}^{\Delta}_{\Delta}$ as the sum of all connected diagrams with four external magnon lines, two of which are removed. Then if we define Γ_{MM} as

$$<0|T[\sigma_+(x_1)\sigma_+(x_2)\sigma_-(y_1)\sigma_-(y_2)]|0>_c$$

$$= \left(\frac{i}{(2\pi)^4}\right)^4 \int d^4q_1 d^4q_2 d^4q_3 d^4q_4\, e^{-i(q_1x_1+q_2x_2+q_3y_1-q_4y_2)} \times$$

$$\Delta^o(q_1)\Delta^o(q_2)\Gamma_{MM}(q_1;q_2;q_3;q_4)\Delta^o(q_3)\Delta^o(q_4) \, , \quad (3.115)$$

we obtain

$$\mathcal{F}^{\Delta}_{\Delta}(q;q') = \Delta^o(q) \frac{i}{(2\pi)^4} \Gamma_{MM}(q;q';q';q)\Delta^o(q) \quad (3.116)$$

and hence that

$$\Delta^{11}(q) = \Delta^o(q) + \Delta^o(q) \frac{i}{(2\pi)^4} \Gamma_{MM}(q;0;0;q)\Delta^o(q)Z^o(0) \int \frac{d^3\vec{q}}{(2\pi)^3} f_B(\omega_B(\vec{q})) + \ldots \quad (3.117)$$

In order to evaluate the low momentum behaviour of the magnon-magnon vertex Γ_{MM} we refer to the W-T relations given by Eqs. (3.46) and (3.47) from which we obtain, for $T = 0$,

$$4h^2 \int d^4x_2 d^4y_1 <0|T[\sigma_+(x_1)\sigma_+(x_2)\sigma_-(y_1)\sigma_-(y_2)]|0>$$

$$= 2ih \int d^4y_1 <0|T[\sigma_+(x_1)\sigma_3(y_1)\sigma_-(y_2)]|0>$$

$$+ 2ih \int d^4y_1 <0|T[\sigma_+(x_1)\sigma_-(y_1)\sigma_3(y_2)]|0>

$$= 2ih\int d^4y_1 <0|T[\sigma_+(x_1)\sigma_3(y_1)\sigma_-(y_2)]|0>$$

$$+ 2<0|T[\sigma_+(x_1)\sigma_-(y_2)]|0> - <0|T[\sigma_3(x_1)\sigma_3(y_2)]|0> . \qquad (3.118)$$

Substituting the expression of Eq. (3.115) into (3.118) we obtain that

$$\lim_{h\to 0} \Delta^0(q) \frac{i}{(2\pi)^4} \Gamma_{MM}(q;0;0;q)\Delta^0(q) = \frac{1}{M^2} [\Delta_L^0(q) - 2\Delta^0(q)] , \qquad (3.119)$$

where we have defined

$$<0|T[(M_0 - \sigma_3(x))(M_0 - \sigma_3(y))]|0> = \frac{i}{(2\pi)^4} \int d^4q \, e^{-iq(x-y)} \Delta_L^0(q) . \qquad (3.120)$$

Substituting Eq. (3.119) into Eq. (3.117) and noting that $\Delta_L^0(q)$ consists entirely of continuum contribution we obtain to order $T^{3/2}$ that

$$\Delta^{11}(q) = \Delta^0(q)\left\{1 - \frac{2}{M}\int \frac{d^3\vec{q}}{(2\pi)^3} f_B(\omega_B^0(q)) + \ldots\right\}$$
$$+ \text{continuum} \qquad (3.121)$$

where we have used Eq. (3.87). It immediately follows from Eq. (3.121) that, to order $T^{3/2}$, the magnon energy is independent of temperature, while the wavefunction renormalization $Z_B(\vec{q})$ is given by

$$Z_B(q) = Z_B^0(q)\left\{1 - \frac{2}{M}\int \frac{d^3q}{(2\pi)^3} f_B(\omega_B^0(q)) + \ldots\right\} . \qquad (3.122)$$

This means that any contribution to the magnon energy spectra arising from the thermal excitation of the magnons will be of order $T^{5/2}$. A similar result has been obtained by Dyson[93] in the case of the Heisenberg model, although it can be shown[7] that Dyson's result may be obtained from symmetry considerations similar to those presented here.

In the case of the itinerant electron ferromagnetism, however, calculations regarding the temperature dependence of the magnon energy differ[95,96], depending on the approximation scheme used. It does appear to be generally accepted, however, that contributions of order $T^{3/2}$ in the magnon energy are spurious and the result of an inadequate approximation scheme[95,96,97]; similar difficulties arise in the Heisenberg model[98].

The above procedures may be applied to consider the temperature dependence of the electron spectra, however difficulties arise since calculations show[65] that the dispersive part of the electron self-energy correction is non-vanishing even at zero temperature and hence the electron propagator does not have a simple pole structure associated with a particle-like excitation. However one can obtain an operational definition of the electron energy spectra, $\varepsilon_\uparrow(\vec{p})$ and $\varepsilon_\downarrow(\vec{p})$, in terms of the inverse electron propagator as

$$[\mathrm{Re}\ G_\uparrow(p)]^{-1}_{p_0=\varepsilon_\uparrow(p)} = 0 \tag{3.123}$$

and

$$[\mathrm{Re}\ G_\downarrow(p)]^{-1}_{p_0=\varepsilon_\downarrow(p)} = 0 \tag{3.124}$$

while the wavefunction renormalization of the spin up and spin down electrons may be defined as

$$Z_\uparrow(\vec{p}) = [\frac{\partial}{\partial p_0}\ \mathrm{Re}\ G_\uparrow^{-1}(p)]_{p_0=\varepsilon_\uparrow(\vec{p})} \tag{3.125}$$

and

$$Z_\downarrow(\vec{p}) = [\frac{\partial}{\partial p_0}\ \mathrm{Re}\ G_\downarrow^{-1}(p)]_{p_0=\varepsilon_\downarrow(\vec{p})} \tag{3.126}$$

Such definitions will be meaningful when the dispersive part of the electron self-energy is small and hence the spectral function of the electrons will manifest a strong particle-like resonant peak in the neighbourhood of $p_0 = \varepsilon_\uparrow(p)$ in the case of the spin up electrons and

$p_0 = \varepsilon_{\downarrow}(p)$ in the case of the spin down electrons. From the expressions for $G_{\uparrow}(p)$ and $G_{\downarrow}(p)$ given by Eqs. (3.107) and (3.108) and the result that for A we expand in terms of α as

$$A = A_0 + \alpha + \ldots\ldots , \tag{3.127}$$

we may expand A^{-1} as

$$A^{-1} = A_0^{-1} + A_0^{-1}\,\alpha\,A_0^{-1} + \ldots\ldots \tag{3.128}$$

for α small, then we obtain to order $T^{3/2}$

$$G_{\uparrow}^{-1}(p) = G_{\uparrow}^{0}(p)^{-1} - \frac{1}{M}\left[G_{\uparrow}^{0}(p)^{-1} - G_{\uparrow}^{0}(p)^{-1}G_{\downarrow}^{0}(p)G_{\uparrow}^{0}(p)^{-1}\right] \int\frac{d^3\vec{q}}{(2\pi)^3}\, f_B(\omega_B^0(\vec{q})) + \ldots\ldots \tag{3.129}$$

and

$$G_{\downarrow}^{-1}(p) = G_{\downarrow}^{0}(p)^{-1} - \frac{1}{M}\left[G_{\downarrow}^{0}(p)^{-1} - G_{\downarrow}^{0}(p)^{-1}G_{\uparrow}^{0}(p)G_{\downarrow}^{0}(p)^{-1}\right] \int\frac{d^3\vec{q}}{(2\pi)^3}\, f_B(\omega_B^0(q)) + \ldots\ldots \tag{3.130}$$

This result may be obtained in a somewhat more precise manner following the definition of the electron self-energy[66]. From Eqs. (3.129) and (3.130) we immediately see that

$$\left[\mathrm{Re}\; G_{\uparrow}^{-1}(p)\right]_{p_0=\varepsilon_{\uparrow}^0(p)} = 0 \tag{3.131}$$

$$\left[\mathrm{Re}\; G_{\downarrow}^{-1}(p)\right]_{p_0=\varepsilon_{\downarrow}^0(p)} = 0 \tag{3.132}$$

where $\varepsilon_{\uparrow}^0(p)$ and $\varepsilon_{\downarrow}^0(p)$ denote the electron energy spectra at zero temperature and that

$$\left(\frac{\partial}{\partial p_0}\,\mathrm{Re}\; G_{\uparrow}^{-1}(p)\right)_{p_0=\varepsilon_{\uparrow}(p)} = Z^0(\vec{p})\left(1 - \frac{1}{M}\int\frac{d^3\vec{q}}{(2\pi)^3}\, f_B(\omega_B^0(\vec{q})) + \ldots\ldots\right) \tag{3.133}$$

and

$$\left(\frac{\partial}{\partial p_o} \operatorname{Re} G_{\downarrow}^{-1}(p_o)\right)_{p_o=\varepsilon_{\downarrow}(p)} = Z_{\downarrow}^{o}(p) \left[1 - \frac{1}{M}\int \frac{d^3\vec{q}}{(2\pi)^3} f_B(\omega_B^o(q)) + \ldots\right] \quad (3.134)$$

where $Z_{\uparrow}^{o}$ and $Z_{\downarrow}^{o}$ denote the zero temperature electron wave function renormalization constants.

Equations (3.131) and (3.132) yield the result therefore that to order $T^{3/2}$ the quasi-electron spectra are independent of temperature. Again this result appears to be borne out by various approximate calculations although opinions differ as to the exact nature of the cancellation[95,96,99]. However, while the energy spectra of the quasi-electron states is, to order $T^{3/2}$, independent of temperature the wavefunction renormalization constants do exhibit a $T^{3/2}$ dependence.

To summarize we have utilized the real-time formulation of Statistical Mechanics, TFD, to construct a low temperature expansion for the time ordered Green's functions. The coefficients, or form factors, appearing in the expansion may be expressed in terms of the vertices calculated at zero temperature. In this manner we were able to obtain an expression for the leading finite temperature magnon corrections to the magnetization, the transverse spin susceptibility and the one electron Green's function. It was shown how the leading $T^{3/2}$ magnon contribution could be obtained from a low momentum expansion and an explicit evaluation of this term could be accomplished by means of the W-T relations outlined in the previous section.

We were therefore able to obtain the following experimentally relevant results in a completely model indepenent fashion:

i) The Bloch $T^{3/2}$ law

$$M(T) = M_o \left[1 - \frac{2}{M_o}\int \frac{d^3\vec{q}}{(2\pi)^3} f_B(\omega_B^o(\vec{q})) + \ldots\right] \quad (3.135)$$

ii) The temperature dependent quasi-particle spectrum

$$\omega_B(\vec{q}) = \omega_B^0(\vec{q}) + \ldots. \tag{1.136a}$$

$$\varepsilon_\uparrow(\vec{p}) = \varepsilon_\uparrow^0(\vec{p}) + \ldots. \tag{1.136b}$$

and

$$\varepsilon_\downarrow(p) = \varepsilon_\downarrow^0(\vec{p}) + \ldots. \tag{1.136c}$$

iii) The temperature dependent wavefunction renormalization constants

$$Z_B(\vec{q}) = Z_B^0(\vec{q})\left\{1 - \frac{2}{M_0}\int \frac{d^3\vec{q}}{(2\pi)^3} f_B(\omega_B^0(\vec{q})) + \ldots.\right\} \tag{3.137a}$$

$$Z_\uparrow(\vec{p}) = Z^0(\vec{p})\left\{1 - \frac{1}{M_0}\int \frac{d^3\vec{q}}{(2\pi)^3} f_B(\omega_B^0(\vec{q})) + \ldots.\right\} \tag{3.137b}$$

and

$$Z_\downarrow(\vec{p}) = Z_\downarrow^0(\vec{p})\left\{1 - \frac{1}{M_0}\int \frac{d^3\vec{q}}{(2\pi)^3} f_B(\omega_B^0(\vec{q})) + \ldots.\right\} \tag{3.137c}$$

where the dots denote terms with higher order temperature dependence that $T^{3/2}$ (i.e. T^2, $T^{5/2}$ etc.).

The manner in which the above results were derived is such that they may be regarded as exact requirements of the spin rotational invariance of the theory.

3.3 Ward-Takahashi Relations and the Paramagnetic Susceptibility

In this section we turn our attention to the paramagnetic susceptibility of itinerant electron ferromagnets. The approach employed is somewhat novel and is based on an examination of the response of the system to a symmetry breaking term, analogous to that employed in the previous Section 3.2 and given by Eq. (3.26). Since the response of the system is severally controlled by the requirements of spin rotational invariance, we are able to obtain, by means of the W-T relations outlined in Section 3.1, an exact expression for the static susceptibility in terms of the electron self-energy. We use the result of this analysis to consider the effect of spin fluctuations on the static susceptibility and to show what approximations are required in order to make contact with previous works[8,9,100,101,102]. The considerations of this section are based largely on some earlier work by the present author and collaborators reported in the literature[67] but contains some minor modifications.

The importance of the effect of the spin fluctuations in the static susceptibility in itinerant spin systems has been studied by a number of authors. Beal-Monod et al[8] have considered the case of normal ^{3}He while other authors[9,100,101,102] have examined their role in the so-called weak itinerant ferromagnets discussed previously. A notable achievement of this latter work is that it appears to account for the Curie-Weiss type temperature dependence observed in these materials[86,87].

The problem posed is therefore, given the assumptions outlined in Section 3.1 (i.e. that system may be described in terms of the Heisenberg fields $\psi_\uparrow(x)$ and $\psi_\downarrow(x)$ together with their canonical conjugates $\psi_\uparrow^\dagger(x)$ and $\psi_\downarrow^\dagger(x)$ the original dynamics of which may be assumed to be invariant under arbitrary rotations in spin space etc.), can we obtain an expression for the static transverse susceptibility, for $T > T_c$, defined as

$$\tau^{\alpha\beta}\Delta(h) = \lim_{q\to 0} \Delta^{\alpha\beta}(q) \qquad (3.138)$$

where $\Delta^{\alpha\beta}(q)$ was given by Eq. (3.56) as

$$<\beta|T[\sigma_+^\alpha(x)\sigma_-^\beta(y)]|\beta> = \frac{i}{(2\pi)^4}\int d^4q\, e^{-iq(x-y)}\,\Delta^{\alpha\beta}(q)\,. \qquad (3.139)$$

We begin by defining the electron paramagnon vertex[103] as

$$<\beta|T[\sigma_+^\alpha(x)\psi_\uparrow^{\beta_1}(y_1)\psi_\downarrow^{\beta_2}(y_2)^\dagger]|\beta> = \left(\frac{i}{(2\pi)^4}\right)^2\int d^4p_1 d^4p_2 d^4q\, e^{-i(qx+p_1y_1-p_2y_2)} \times$$
$$\delta^4(q+p_1-p_2)[\delta^{\alpha b_1}\delta^{\alpha b_2}\varepsilon^\alpha - \Delta^{\alpha a}(q)\Gamma_a^{b_1b_2}(p_1;q;p_2)]G_\uparrow^{\beta_1 b_1}(p_1)G_\downarrow^{b_2\beta_2}(p_2) \qquad (3.140)$$

where $G_\uparrow$ and $G_\downarrow$ denote the Fourier transform of the one electron Green's function given by Eqs. (3.54) and (3.55) and summation over repeated Latin indices is assumed. Noting that

$$<\beta|T[\sigma_+^\alpha(x)\sigma_-^\beta(y)]|\beta> = -\lim_{\substack{y_1\to y-\delta\\ y_2\to y+\delta}} <\beta|T[\sigma_+^\alpha(x)\psi_\uparrow^{\beta_1}(y_1)\psi_\downarrow^{\beta_2}(y_2)^\dagger]|\beta> \qquad (3.141)$$

we obtain the following expression for the dynamical susceptibility in terms of the one electron Green's functions $G_\uparrow$ and $G_\downarrow$ and the electron paramagnon vertex Γ as

$$\Delta^{\alpha a}(q)\left\{\delta^{\alpha\beta} - \frac{i}{(2\pi)^4}\int d^4p\,\Gamma_a^{b_1b_2}(p+\tfrac{q}{2};q;p-\tfrac{q}{2})\varepsilon^\beta G_\uparrow^{\beta b_1}(p-\tfrac{q}{2})G_\downarrow^{b_2\beta}(p+\tfrac{q}{2})\right\} = D^{\alpha\beta}(q) \qquad (3.142)$$

where $D^{\alpha\beta}(q)$ is given by

$$D^{\alpha\beta}(q) = -\frac{i}{(2\pi)^4}\int d^4p\,\varepsilon^\alpha G_\uparrow^{\alpha\beta}(p-\tfrac{q}{2})G_\downarrow^{\beta\alpha}(p+\tfrac{q}{2})\,\varepsilon^\beta\,. \qquad (3.143)$$

From the spectral representation it is straightforward to show that in the static limit $D^{\alpha\beta}(q)$ is diagonal with respect to the thermal indices $\alpha\beta$ and may be written as

$$\lim_{q\to 0} D^{\alpha\beta}(q) = \tau^{\alpha\beta}D(h)\,. \qquad (3.144)$$

Thus from Eq. (3.142) we obtain the following expression for $\Delta(h)$

$$\Delta(h) = D(h)\left\{1 - \frac{1}{2}\int d^4p \sum_{b,a} \Gamma_a^{b_1b_2}(p;0;p)\varepsilon^b G_\uparrow^{bb_1}(p)G_\downarrow^{b_2b}(p)\right\}^{-1} . \quad (3.145)$$

In order to evaluate the low momentum limit of the electron paramagnon vertex Γ we make use of the W-T relations of Section 3.1. If we use the expression for the electron paramagnon vertex given by Eq. (3.140) together with the result of Eq. (3.42) we obtain the following result

$$G_\uparrow^{\alpha\beta}(p) - G_\downarrow^{\alpha\beta}(p) = -2h\left\{\delta_{ab} - \Delta(h)\sum_g \Gamma_g^{ab}(p;0;p)\right\}G_\uparrow^{\alpha a}(p)G_\downarrow^{b\beta}(p) \quad (3.146)$$

which in terms of the inverse propagators $G_\uparrow^{-1}(p)$ and $G_\downarrow^{-1}(p)$ may be written as

$$\left\{G_\uparrow^{-1}(p) - G_\downarrow^{-1}(p)\right\}_{\alpha\beta} = 2h\left\{\delta_{\alpha\beta} - \Delta(h)\sum_g \Gamma_g^{\alpha\beta}(p;0;p)\right\} \quad (3.147)$$

Thus we see how the W-T relations provide us with an exact expression for the electron paramagnon vertex in terms of the inverse electron propagators.

A somewhat more useful expression for Γ, than that given by Eq. (3.147), may be obtained from the definition of the inverse propagator in terms of the electron self-energies. Writing the equation of motion for the Heisenberg fields as

$$\left\{i\frac{\partial}{\partial t} - \varepsilon(-i\nabla) + h\right\}\psi_\uparrow^\alpha(x) = J_\uparrow^\alpha[\psi;x] \quad (3.148a)$$

and

$$\left\{i\frac{\partial}{\partial t} - \varepsilon(-i\nabla) - h\right\}\psi_\downarrow^\alpha(x) = J_\downarrow^\alpha[\psi;x] \quad (3.148b)$$

where $J[\psi;x]$ is due to the effect of the self-interaction of the electrons. As discussed in Section 2 the analytical structure of the one electron Green's functions in TFD is such that it is possible to define a self-energy term $\sum_{\uparrow(\downarrow)}(p)$, that has similar analytical properties to the propagator $G_{\uparrow(\downarrow)}$ [40], as

$$<\beta|T[J^{\alpha}_{\uparrow}[\psi;x]\psi^{\beta}_{\uparrow}(y)^{\dagger}]|\beta> = \frac{i}{(2\pi)^4}\int d^4p\ e^{-ip(x-y)}\sum\nolimits^{\alpha g}_{\uparrow}(p)G^{g\beta}_{\uparrow}(p) \qquad (3.149a)$$

and

$$<\beta|T[J^{\alpha}_{\downarrow}[\psi;x]\psi^{\beta}_{\downarrow}(y)^{\dagger}]|\beta> = \frac{i}{(2\pi)^4}\int d^4p\ e^{-ip(x-y)}\sum\nolimits^{\alpha g}_{\downarrow}(p)G^{g\beta}_{\downarrow}(p)\ . \qquad (3.149b)$$

The equation of motion for the Heisenberg fields (3.148a,b) then yields the Dyson equation for the one electron Green's function

$$G^{\alpha\beta}_{\uparrow}(p) = S^{\alpha\beta}_{+}(p) + S^{\alpha a}_{+}(p)\sum\nolimits^{ab}_{\uparrow}(p)\ G^{b\beta}_{\uparrow}(p) \qquad (3.150a)$$

and

$$G^{\alpha\beta}_{\downarrow}(p) = S^{\alpha\beta}_{-}(p) + S^{\alpha a}_{-}(p)\sum\nolimits^{ab}_{\downarrow}(p)\ G^{b\beta}_{\downarrow}(p)\ , \qquad (3.150b)$$

where the propagators $S^{\alpha\beta}_{\pm}(p)$ are simply given by

$$S^{\alpha\beta}_{\pm}(p) = U_F(p_0)[p_0 - \varepsilon(p) \pm h + i\delta\tau]^{-1}U_F(p_0)\ , \qquad (3.151)$$

where $U_F(p_0)$ is the fermion thermal transformation matrix defined by Eq. (2.51). The inverse propagators $G^{-1}_{\uparrow}(p)$ and $G^{-1}_{\downarrow}(p)$ may be written in terms of their respective self-energy parts as

$$G^{-1}_{\uparrow}(p)^{\alpha\beta} = [p_0 - \varepsilon(p) + h - \sum\nolimits_{\uparrow}(p)]_{\alpha\beta} \qquad (3.152a)$$

and

$$G^{-1}_{\downarrow}(p)^{\alpha\beta} = [p_0 - \varepsilon(p) - h - \sum\nolimits_{\downarrow}(p)]_{\alpha\beta}\ . \qquad (3.152b)$$

As with the zero temperature case the self-energy part $\sum_{\uparrow(\downarrow)}$ has an obvious diagramatic interpretation, it corresponds to the summation of all the one electron irreducible contributions to the one electron propagator $G_{\uparrow(\downarrow)}$ with the external electron lines removed.

It is important to appreciate that the definition of the inverse propagator and its expression in terms of the self-energy together with the diagramatic interpretation of the self-energy are all made possible, in a practical sense, through the matrix structure of TFD. It is therefore the case that nearly all the important results of this section are a consequence of the computational power afforded us by the TFD formalism.

Equation (3.147) may then be re-expressed in terms of the self-energy Σ as

$$\Sigma_{\uparrow}^{\alpha\beta}(p) - \Sigma_{\downarrow}^{\alpha\beta}(p) = 2h\Delta(h) \sum_{g} \Gamma_{g}^{\alpha\beta}(p;0;p) \ . \tag{3.153}$$

The result of Eq. (3.38) allows us to rewrite Eq. (3.153) as

$$\frac{1}{M} [\Sigma_{\uparrow}^{\alpha\beta}(p) - \Sigma_{\downarrow}^{\alpha\beta}(p)] = -\sum_{g} \Gamma_{g}^{\alpha\beta}(p;0;p) \ . \tag{3.154}$$

In the ferromagnetic regime, $T < T_c$, both the numerator and the denominator of the left hand side of Eq. (3.154) remain finite in the limit $h \to 0$. The role of Eq. (3.154) in analyzing the magnetic properties of itinerant electron systems has been examined in refs. [7] and [65]. In the paramagnetic regime, $T > T_c$, however both the numerator and denominator on the left hand side of Eq. (3.154) tend to zero in the limit $h \to 0$. Thus Eq. (3.154) shows us that, in the zero field case (i.e. $h = 0$), the long wavelength limit of the electron paramagnon vertex Γ may be calculated from the response of the magnetization and the splitting of the spin up and spin down self-energies induced by some infinitesimal symmetry breaking parameter h.

If we now substitute Eq. (3.154) into our expression for the static susceptibility given in Eq. (3.145) we obtain

$$\Delta(h) = D(h)\left\{1 + \frac{i}{(2\pi)^4}\int d^4p\, \frac{1}{2}\, \mathrm{Tr}[\tau G_\uparrow(p)\, \frac{1}{M(h)}\{\Sigma_\uparrow(p) - \Sigma_\downarrow(p)\}G_\downarrow(p)]\right\}^{-1} \tag{3.155}$$

The above expression is exact and model independent and provides us with a useful starting point for our discussions.

In order to see how we may utilize this result in a practical way, we consider the interaction to be given by a local contact interaction, thus

$$\mathcal{L}_I = -\frac{\lambda}{2}\sum_\sigma \psi^\dagger_\sigma(x)\psi^\dagger_{\sigma'}(x)\psi_{\sigma'}(x)\psi_\sigma(x) \quad . \tag{3.156}$$

We then consider the self-energy corrections $\Sigma_\uparrow$ and $\Sigma_\downarrow$, arising from the interaction term, to consist of two parts, the familiar Hartree-Fock or Mean Field (MF) contribution plus a contribution arising from the spin fluctuations. Thus we write

$$\Sigma^{\alpha\beta}_\uparrow(p) = \tau^{\alpha\beta}\lambda\langle n_\downarrow(x)\rangle + \tilde{\Sigma}^{\alpha\beta}_\uparrow(p) \tag{3.157a}$$

and

$$\Sigma^{\alpha\beta}_\downarrow(p) = \tau^{\alpha\beta}\lambda\langle n_\uparrow(x)\rangle + \tilde{\Sigma}^{\alpha\beta}_\downarrow(p) \tag{3.157b}$$

where $\langle n_\uparrow\rangle$ and $\langle n_\downarrow\rangle$ denote the density of the spin up and the spin down electrons respectively and are given by

$$\langle n_\uparrow(x)\rangle = -\frac{i}{(2\pi)^4}\oint_+ d^4k\, G^{11}_\uparrow(k) \tag{3.158a}$$

and

$$\langle n_\downarrow(x)\rangle = -\frac{i}{(2\pi)^4}\oint_+ d^4k\, G^{11}_\downarrow(k) \ , \tag{3.158b}$$

where $\oint_+$ denotes the integration path for dp_0 lies in the upper half of the complex plane. The second terms appearing in Eqs. (3.157a,b) therefore represent corrections to the MF contributions arising from the spin fluctuations. By analogy we define the corresponding MF propagators as

$$G_{\pm}^{\alpha\beta}(p) = U_F(p_o)[p_o - \varepsilon(p) \pm (\frac{\lambda M}{2} + h) + i\delta\tau]^{-1} U_F(p_o) \ . \qquad (3.159)$$

The Dyson Equation, Eq. (3.150a,b), for the one electron Green's function may now be written in terms of the MF propagators $G_{\pm}$ and the self-energy correction $\tilde{\sum}$ as

$$G_{\uparrow}^{\alpha\beta}(p) = G_{+}^{\alpha\beta}(p) + G_{+}^{\alpha a}(p)\tilde{\sum}_{\uparrow}^{ab}(p)\, G_{\uparrow}^{b\beta}(p) \qquad (3.160a)$$

and

$$G_{\downarrow}^{\alpha\beta}(p) = G_{-}^{\alpha\beta}(p) + G_{-}^{\alpha a}(p)\tilde{\sum}_{\downarrow}^{ab}(p)\, G_{\downarrow}^{b\beta}(p) \ . \qquad (3.160b)$$

In order to correlate the result given in Eq. (3.155) with the results of the RPA, we first note the trivial identity, that for any constant A we can rewrite Eq. (3.155) as

$$\Delta(h) = A\left\{1 + \frac{A}{D(h)} \frac{i}{(2\pi)^4} \int d^4p \, \frac{1}{2} \mathrm{Tr}\, [\tau G_{\uparrow}(p) \frac{1}{M} (\sum_{\uparrow}(p) - \sum_{\downarrow}(p)) G_{\downarrow}(p)] - \frac{D(h)-A}{D(h)}\right\}^{-1} \qquad (3.161)$$

If we now let A be given by

$$A = D_o(h)$$

where

$$D_o(h)\tau^{\alpha\beta} = \lim_{q\to 0} D_o^{\alpha\beta}(q)$$

with

$$D_o^{\alpha\beta}(q) = \frac{i}{(2\pi)^4} \int d^4p \, \varepsilon^{\alpha} G_{+}^{\alpha\beta}(p-\frac{q}{2}) G_{-}^{\beta\alpha}(p+\frac{q}{2})\, \varepsilon^{\beta} \ . \qquad (3.162)$$

Then $\Delta(h)$ reduces to

$$\Delta(h) = D_o(h) \{1 + \lambda D_o(h) + \kappa\}^{-1} , \qquad (3.163)$$

where κ represents the corrections to the RPA approximation and may be expressed as

$$\kappa = \frac{D_o(h)}{D(h)} \frac{i}{(2\pi)^4} \int d^4p \frac{1}{2} \mathrm{Tr}[\tau G_{\uparrow}(p) \frac{1}{M} (\tilde{\sum}_{\uparrow}(p) - \tilde{\sum}_{\downarrow}(p)) G_{\downarrow}(p)] - \frac{D(h) - D_o(h)}{D(h)} . \qquad (3.164)$$

The self-energy contributions $\tilde{\sum}_{\uparrow}$ and $\tilde{\sum}_{\downarrow}$ may be calculated using a straightforward perturbation expansion. The lowest order contributions shown diagramatically in Fig. 1 are given by

$$\tilde{\sum}_{\uparrow}^{\alpha\beta}(p) = \lambda^2 \frac{i}{(2\pi)^4} \int d^4k \; G_{\downarrow}^{\alpha\beta}(p+k) \Delta^{\alpha\beta}(k) + \lambda^2 \frac{i}{(2\pi)^4} \int d^4k \; G_{\uparrow}^{\alpha\beta}(p-k) \Delta_{\downarrow}^{\alpha\beta}(k)$$

$$- \lambda^2 \frac{i}{(2\pi)^4} \int d^4k \; G_{\downarrow}^{\alpha\beta}(p+k) D^{\alpha\beta}(k) \qquad \text{[illegible]}$$

and

$$\tilde{\sum}_{\downarrow}^{\alpha\beta}(p) = \lambda^2 \frac{i}{(2\pi)^4} \int d^4k \; G_{\uparrow}^{\alpha\beta}(p-k) \Delta^{\alpha\beta}(k) + \lambda^2 \text{[illegible]} k \; G_{\downarrow}^{\alpha\beta}(p+k) \Delta_{\uparrow}^{\alpha\beta}(k)$$

$$\text{[illegible]} \frac{i}{(2\pi)^4} \int d^4k \; G_{\uparrow}^{\alpha\beta}(p-k) D^{\alpha\beta}(k) , \qquad (3.165b)$$

where $\Delta_{\uparrow}(k)$ and $\Delta_{\downarrow}(k)$ are defined by

$$\langle\beta|T[n_{\uparrow}(x) n_{\uparrow}(x)]|\beta\rangle - \langle\beta|n_{\uparrow}(x)|\beta\rangle \langle\beta|n_{\uparrow}(x)|\beta\rangle$$

$$= \frac{i}{(2\pi)^4} \int d^4k \; \Delta_{\uparrow}(k) \; e^{-ik(x-y)} \qquad (3.166a)$$

and

$$\langle\beta|T[n_{\downarrow}(x) n_{\downarrow}(y)]|\beta\rangle - \langle\beta|n_{\downarrow}(x)|\beta\rangle \langle\beta|n_{\downarrow}(x)|\beta\rangle$$

$$= \frac{i}{(2\pi)^4} \int d^4k \; \Delta_{\downarrow}(k) \; e^{-ik(x-y)} . \qquad (3.166b)$$

The third term appearing in Eqs. (3.165a,b) is included to avoid double counting, and while this term presents no computational difficulties we will neglect it in what follows, in order to simplify the discussion.

Even with the self-energy parts given by Eqs. (3.165a,b) our expression for κ is still of a somewhat formal nature since it involves the as yet undetermined paramagnon propagators[104] $\Delta(k)$, $\Delta_{\uparrow}(k)$ and $\Delta_{\downarrow}(k)$ and there are a variety of ways in which the calculation may proceed depending on how we choose to approximate the paramagnon propagators. We will examine this point in more detail later.

Regardless of how we choose to simplify the internal paramagnon line, the calculation of κ from Eq. (3.164) represents a rather formidable undertaking. One possible approach is to expand κ in terms of the self-energy correction arising from the spin fluctuations $\tilde{\sum}$ and retain only terms up to some finite order. In the case of the weak itinerant ferromagnets it may be adequate to consider only the lowest order terms. Expanding the one electron Green's function in terms of the self-energy corrections $\tilde{\sum}$ and retaining only the lowest order terms we obtain on taking the limit as $h \to 0$ the following expression for κ after some manipulation,

$$\kappa = \frac{i}{(2\pi)^4} \int d^4p \, \frac{1}{2} \, \mathrm{Tr}\left\{\tau G_0^2(p) \lim_{h\to 0} \frac{1}{M(h)} (\tilde{\sum}_{\uparrow}(p) - \tilde{\sum}_{\downarrow}(p)) + \frac{2}{D_0(h)} G_0^3(p)\tilde{\sum}(p)\right\} , \tag{3.167}$$

where we have made use of the following definitions

$$G_0^{\alpha\beta}(p) = \lim_{h\to 0} G_{\pm}^{\alpha\beta}(p) \tag{3.168}$$

and

$$\tilde{\sum}^{\alpha\beta}(p) = \lim_{h\to 0} \tilde{\sum}_{\uparrow}^{\alpha\beta}(p) = \lim_{h\to 0} \tilde{\sum}_{\downarrow}^{\alpha\beta}(p) . \tag{3.169}$$

In the domain of interest, that is in the region above T_c, where we expect the paramagnon contribution to be large and hence the above corrections to be important, the induced effective field experienced by the electrons $H = \lambda M(h)/2 + h$ will be considerably larger than the symmetry breaking parameter h. Hence we obtain the result that

$$\lim_{h\to 0} \frac{1}{M(h)} [\tilde{\Sigma}_{\uparrow}(p) - \tilde{\Sigma}_{\downarrow}(p)] \approx \lambda \frac{\partial}{\partial H} \tilde{\Sigma}(p;H) \tag{3.170}$$

where

$$\tilde{\Sigma}_{\uparrow}(p) = \tilde{\Sigma}(p;H) \tag{3.171}$$

and

$$\Sigma_{\downarrow}(p) = \Sigma(p;-H) \ . \tag{3.172}$$

The fact that we are focussing our attention on the region above T_c means that

$$1 + \lambda D \approx 0$$

and to lowest order in the spin fluctuations

$$\lambda \simeq \frac{1}{D(h)} \simeq \frac{1}{D_o(h)} \ . \tag{3.173}$$

While the approximations contained in Eqs. (3.170) and (3.173) are not essential to the analysis they do allow us to express κ in the following rather compact form

$$\kappa = -\frac{1}{D_o} \frac{i}{(2\pi)^4} \int d^4p \, \frac{1}{2} \frac{d}{dH} \mathrm{Tr}\left[\{\frac{d}{dH} G_+(p)\} \tilde{\Sigma}(p;H)\right]_{H=0} \ . \tag{3.174}$$

In obtaining Eq. (3.174) we have used the result that

$$\frac{d}{dH} G_{\pm}^{\alpha\beta}(p) = \mp\left(G_{\pm}(p)^2\right)_{\alpha\beta} \tag{3.175}$$

$$\frac{d^2}{dH^2} G_{\pm}^{\alpha\beta}(p) = \left(2G_{\pm}(p)^3\right)_{\alpha\beta} \tag{3.176}$$

If we now introduce the expression for $\tilde{\sum}$ given for Eqs.(3.165a,b) then κ given above becomes

$$\kappa = \frac{\lambda^2}{D_o(h)} \left(\frac{i}{(2\pi)^4}\right)^2 \int d^4p\, d^4k\, \frac{d}{dH}\left\{ \frac{1}{2}\sum_\alpha \varepsilon^\alpha [\frac{d}{dH} G_+^{\alpha a}(p)] [G_-^{a\alpha}(p+k)\Delta^{a\alpha}(k) + G_+^{a\alpha}(p+k)\Delta_\downarrow^{a\alpha}(k)]\right\}_{H=0} \quad . \tag{3.177}$$

Now by use of the relations

$$G_+(p) = G_-(p)_{H\to -H} \tag{3.178a}$$

$$\Delta(k) = \Delta(-k)_{H\to -H} \tag{3.178b}$$

and

$$\Delta(k) = \Delta(-k) \ , \tag{3.178c}$$

we arrive at the result

$$\kappa = \frac{\lambda^2}{D_o} \left(\frac{i}{(2\pi)^4}\right)^2 \int d^4p\, d^4k\, \frac{1}{4}\sum_\alpha \varepsilon^\alpha \frac{d}{dH}\left\{ [\frac{d}{dH} G_+^{\alpha a}(p+k) G_-^{a\alpha}(p)] \Delta^{a\alpha}(k) + [\frac{d}{dH} G_+^{\alpha a}(p+k) G_+^{a\alpha}(p)]\Delta_+^{a\alpha}(k)\right\}_{H=0}$$

$$= -\frac{\lambda^2}{4D_o} \frac{i}{(2\pi)^4} \int d^4k\, \frac{d}{dH} \mathrm{Tr}\left\{ [\frac{d}{dH} D_o(k)]\tau\Delta(k) + [\frac{d}{dH} D_\uparrow(k)]\tau\Delta_\downarrow(k)\right\}_{H=0} \quad , \tag{3.179}$$

where $D_o(k)$ is given by Eq. (3.162) and $D_\uparrow(k)$ is given by

$$D_\uparrow^{\alpha\beta}(k) = \frac{i}{(2\pi)^4} \int d^4p\, G_+^{\alpha\beta}(p+k) G_+^{\beta\alpha}(p) \ . \tag{3.180}$$

Using the spectral representation given in Eq. (2.56) we define the following spectral functions

$$D_o^{\alpha\beta}(k) = \int d\omega\, \sigma_H(\omega;\vec{k}) U_B(k_o)\tau[k_o - \omega + i\delta\tau]^{-1}\, U_B(k_o) \ , \tag{3.181a}$$

$$D_{\uparrow}^{\alpha\beta}(k) = \int d\omega\ \sigma_H^{\uparrow}(\omega;\vec{k})U_B(k_0)\tau[k_0 - \omega + i\delta\tau]^{-1}\ U_B(k_0)\ , \tag{3.181b}$$

$$\Delta^{\alpha\beta}(k) = \int d\omega\ \rho_H(\omega;\vec{k})U_B(k_0)\tau[k_0 - \omega + i\delta\tau]^{-1}\ U_B(k_0) \tag{3.181c}$$

and

$$\Delta_{\downarrow}^{\alpha\beta}(k) = \int d\omega\ \rho_H^{\downarrow}(\omega;\vec{k})U_B(k_0)\tau[k_0 - \omega + i\delta\tau]^{-1}\ U_B(k_0)\ . \tag{3.181d}$$

We thus have that

$$\frac{i}{(2\pi)^4}\int d^4k\ \frac{d}{dH}\left[\left(\frac{d}{dH}\ D_0^{\alpha\beta}(k)\right)\varepsilon^{\beta}\Delta^{\beta\alpha}(k)\right]$$
$$= \delta_{\alpha\beta}\ P\int\frac{d^3\vec{k}}{(2\pi)^3}\int\frac{d\omega d\omega'}{\omega - \omega'}\left\{f_B(\omega) - f_B(\omega')\right\}\times$$
$$\left[\rho_H(\omega;\vec{k})\ \frac{d}{dH^2}\ \sigma_H(\omega';\vec{k}) + \frac{d}{dH}\ \rho_H(\omega;\vec{k})\ \frac{d}{dH}\ \sigma_H(\omega';\vec{k})\right] \tag{3.182a}$$

and

$$\frac{i}{(2\pi)^4}\int d^4k\ \frac{d}{dH}\left[\left(\frac{d}{dH}\ D_{\uparrow}^{\alpha\beta}(k)\right)\varepsilon^{\beta}\Delta_{\downarrow}^{\beta\alpha}(k)\right]$$
$$= \delta_{\alpha\beta}P\int\frac{d^3\vec{k}}{(2\pi)^3}\int\frac{d\omega d\omega'}{\omega - \omega'}\left\{f_B(\omega) - f_B(\omega')\right\}\times$$
$$\left[\rho_H^{\downarrow}(\omega;k)\ \frac{d}{dH^2}\ \sigma_H^{\uparrow}(\omega';\vec{k}) + \frac{d}{dH}\ \rho_H^{\downarrow}(\omega:\vec{k})\ \frac{d}{dH}\ \sigma_H^{\uparrow}(\omega';\vec{k})\right] \tag{3.182b}$$

Substituting these results into our expression for κ given by Eq. (3.179) we obtain

$$\kappa = \frac{1}{2\pi}\int_{-\infty}^{+\infty} d\omega\ \coth\frac{\beta\omega}{2}\ [G_1(\omega) + G_2(\omega) + G_3(\omega) + G_4(\omega)]\ , \tag{3.183}$$

where

$$G_1(\omega) = \frac{\lambda^2{}_\pi}{2D_0}\lim_{H\to 0}\ P\int\frac{d^3\vec{k}}{(2\pi)^3}\int\frac{d\omega'}{\omega - \omega'}\left\{\rho_H(\omega;\vec{k})\ \frac{d^2}{dH^2}\ \sigma_H(\omega';\vec{k})\right.$$
$$\left. + \rho_H^{\pm}(\omega';\vec{k})\ \frac{d^2}{dH^2}\ \sigma_H(\omega;\vec{k})\right\}\ , \tag{3.184a}$$

$$G_2(\omega) = \frac{\lambda^2\pi}{2D_o} \lim_{H\to 0} P\int \frac{d^3\vec{k}}{(2\pi)^3}\int \frac{d\omega'}{\omega - \omega'} \left\{ \frac{d}{dH}\rho_H(\omega;\vec{k}) \frac{d}{dH}\sigma_H(\omega';\vec{k}) + \frac{d}{dH}\rho_H(\omega';\vec{k}) \frac{d}{dH}\sigma_H(\omega;\vec{k}) \right\} , \tag{3.184b}$$

$$G_3(\omega) = \frac{\lambda^2\pi}{2D_o} \lim_{H\to 0} P\int \frac{d^3\vec{k}}{(2\pi)^3}\int \frac{d\omega'}{\omega - \omega'} \left\{ \rho_H^{\downarrow}(\omega;\vec{k}) \frac{d^2}{dH^2}\sigma_H^{\uparrow}(\omega';\vec{k}) + \rho_H^{\downarrow}(\omega';\vec{k}) \frac{d^2}{dH^2}\sigma_H^{\uparrow}(\omega;\vec{k}) \right\} \tag{3.184c}$$

and

$$G_4(\omega) = \frac{\lambda^2\pi}{2D_o} \lim_{H\to 0} P\int \frac{d^3\vec{k}}{(2\pi)^3}\int \frac{d\omega'}{\omega - \omega'} \left\{ \frac{d}{dH}\rho_H^{\downarrow}(\omega;\vec{k}) \frac{d}{dH}\sigma_H^{\uparrow}(\omega';\vec{k}) + \frac{d}{dH}\rho_H(\omega';\vec{k}) \frac{d}{dH}\sigma_H(\omega;\vec{k}) \right\} . \tag{3.184d}$$

If we define the complex functions

$$\chi_o(z;\vec{k};H) = \int_{-\infty}^{+\infty} \frac{d\omega}{z - \omega}\sigma_H(\omega;\vec{k}) , \tag{3.185a}$$

$$\chi_o^{\uparrow}(z;\vec{k};H) = \int_{-\infty}^{+\infty} \frac{d\omega}{z - \omega}\sigma_H^{\uparrow}(\omega;\vec{k}) , \tag{3.185b}$$

$$\chi(z;\vec{k};H) = \int_{-\infty}^{+\infty} \frac{d\omega}{z - \omega}\rho_H(\omega;\vec{k}) \tag{3.185c}$$

and

$$\chi^{\uparrow}(z;\vec{k};H) = \int_{-\infty}^{+\infty} \frac{d\omega}{z - \omega}\rho_H^{\downarrow}(\omega;\vec{k}) , \tag{3.185d}$$

then the functions G_i may be written in the somewhat more compact form as

$$G_1(\omega) = \frac{\lambda^2}{2D_o} \lim_{\substack{H\to 0\\ \delta\to 0}} \mathrm{Im} \int \frac{d^3\vec{k}}{(2\pi)^3}\chi(\omega+i\delta;\vec{k};H) \frac{d^2}{dH^2}\chi_o(\omega+i\delta;\vec{k};H) , \tag{3.186a}$$

$$G_2(\omega) = \frac{\lambda^2}{2D_o} \lim_{\substack{H\to 0\\ \delta\to 0}} \mathrm{Im} \int \frac{d^3\vec{k}}{(2\pi)^3} \frac{d}{dH} \chi(\omega+i\delta;\vec{k};H) \frac{d}{dH} \chi_o(\omega+i\delta;\vec{k};H) , \qquad (3.186b)$$

$$G_3(\omega) = \frac{\lambda}{2D_o} \lim_{\substack{H\to 0\\ \delta\to 0}} \mathrm{Im} \int \frac{d^3\vec{k}}{(2\pi)^3} \chi^{\downarrow}(\omega+i\delta;\vec{k};H) \frac{d^2}{dH} \chi_o^{\uparrow}(\omega+i\delta;\vec{k};H) \qquad (3.186c)$$

and

$$G_4(\omega) = \frac{\lambda}{2D_o} \lim_{\substack{H\to 0\\ \delta\to 0}} \mathrm{Im} \int \frac{d^3\vec{k}}{(2\pi)^3} \frac{d}{dH} \chi^{\downarrow}(\omega+i\delta;\vec{k};H) \frac{d}{dH} \chi_o^{\uparrow}(\omega+i\delta;\vec{k};H) . \qquad (3.186d)$$

In order to evaluate the functions $G_i(\omega)$ we must specify how the spectral functions ρ_H and $\rho_H^{\downarrow}$ should be calculated. The simplest approximation is to neglect the effect of the spin fluctuations entirely and to evaluate ρ_H and $\rho_H^{\downarrow}$ using the random phase approximation. This gives

$$\lim_{H\to 0} \chi(z;\vec{k};H) = \frac{\chi_o(z;\vec{k})}{1+\lambda\chi_o(z;\vec{k})} , \qquad (3.187a)$$

$$\lim_{H\to 0} \chi^{\downarrow}(z;\vec{k};H) = \frac{1}{2}\left\{\frac{1}{1+\lambda\chi_o(z;\vec{k})} + \frac{1}{1-\lambda\chi_o(z;\vec{k})}\right\} , \qquad (3.187b)$$

$$\lim_{H\to 0} \frac{d}{dH}\chi(z;\vec{k};H) = \frac{1}{1+\chi_o(z;\vec{k})} \frac{d}{dH}\chi_o(z;\vec{k};H)\Big|_{H=0} \qquad (3.187c)$$

and

$$\lim_{H\to 0} \frac{d}{dH}\chi^{\downarrow}(z;k;H) = \frac{1}{2}\left\{\frac{1}{(1+\lambda\chi_o(z;\vec{k})} + \frac{1}{1-\lambda\chi_o(z;\vec{k})}\right\} \frac{d}{dH}\chi_o^{\downarrow}(z;\vec{k};H)\Big|_{H=0} , \qquad (3.187d)$$

where

$$\chi_o(z;\vec{k}) = \lim_{H\to 0} \chi_o(z;\vec{k};H) = \lim_{H\to 0} \chi_o^{\downarrow}(z;\vec{k};H)$$

$$= \int \frac{d^3\vec{p}}{(2\pi)^3} \frac{1}{z-\varepsilon(\vec{p}+\frac{\vec{k}}{2})+\varepsilon(\vec{p}-\frac{\vec{k}}{2})} \left\{f_F(\varepsilon(\vec{p}+\tfrac{\vec{k}}{2})) - f_F(\varepsilon(\vec{p}-\tfrac{\vec{k}}{2}))\right\} . \qquad (3.188)$$

Using these results in our expression for κ we obtain the results of Beal-Monod et al[8], used in the calculation of magnetic susceptibility of ^3He, which may be regarded as a nearly-ferromagnetic itinerant spin system.

If instead, however, we regard the result of Eq. (3.163) together with the expression for κ given in terms of $\tilde{\sum}$ by Eq. (3.167) as providing us with a self-consistent scheme for the determination of the susceptibility, then the approximations provided by Eqs. (3.187a→d) are inadequate since, at zero momentum, they do not satisfy the requirements of spin rotational invariance provided by Eqs.(3.138),(3.163) and (3.164). The importance of the requirements of self-consistency, in the case of weak itinerant ferromagnets and nearly ferromagnetic itinerant spin systems, has been pointed out by Moriya and Kawabata[9]. Their argument is based on the observation that if the RPA susceptibility is used in the computation of κ then the paramagnons will go soft at the Stoner temperature T_s given by

$$1 + \lambda D_o(h) = 0 \ , \quad h = 0 \ ; \quad T = T_s \tag{3.189}$$

whereas from Eq. (3.163) the thermal instability is seen to occur at a temperature T_c given by

$$1 + \kappa + \lambda D_o(h) = 0 \ , \quad h = 0 \ ; \quad T = T_c \ . \tag{3.190}$$

This inconsistency is resolved if we calculate κ using some renormalized paramagnon, where the renormalization is performed in a manner consistent with the low momentum requirements of the spin rotational invariance. One particularly simple scheme has been proposed by Moriya and Kawabata[9] and consists of making the replacement

$$[1 + \lambda\chi_o(z;\vec{k})]^{-1} \longrightarrow [1 + \kappa + \lambda\chi_o(z;\vec{k})]^{-1} \qquad (3.191)$$

in Eqs. (3.187a-d). The resulting self-consistent equation for κ forms the basis of the so-called self-consistent renormalization (SCR) scheme of Moriya and Kawabata[9]. Despite the simplicity of the SCR scheme it has led to many predictions which are in good agreement with the experimental data for weak ferromagnets[105]. Most notable of its achievements is perhaps the fact that it appears to account for the Curie-Weiss behaviour of the inverse susceptibility observed in the Weak Itinerant Ferromagnets and the fact that the transition temperature T_c is considerably lower than the corresponding Stoner temperature.

The original derivation of the SCR scheme, presented by Moriya and Kawabata[9], was obtained from an examination of an expression for the free energy and was semi-phenomenological. As a consequence, despite the obvious importance of the parameter κ, the physical interpretation and origin was by no means obvious. While later work by Kawabata[102] succeeded in providing a diagrammatic interpretation, by means of the Matsubara technique, the justification for the choice of diagrams and the nature of the approximations employed was not offered. On the other hand, the derivation of the SCR scheme obtained from the general result of Eq. (3.155) together with the approximations presented here, provide us with a rather clear understanding of the nature of and justification for the approximations underlying the SCR scheme, which may be summarized as follows. From the exact expressions for $\Delta(q)$ given by Eq. (3.142) performing an expansion of $G_{\uparrow}$, $G_{\downarrow}$ and Γ in terms of the contributions arising from the spin fluctuations, then following a similar procedure to that used in the static limit to obtain Eq. (3.163) we obtain the rather general expression

$$\Delta(q) = \tau[\tau + \lambda D_0(q) + \kappa(q)]^{-1} D(q) \tag{3.192}$$

where $\kappa(q)$ is now the correction to the dynamical susceptibility arising from the spin fluctuations and hence Eq. (3.192) may be regarded as a self-consistent equation for the dynamical susceptibility. If we now approximate $\kappa(q)$ by its static limit, noting that

$$\lim_{q\to 0} \kappa(q) = \kappa \ , \tag{3.193}$$

then provided the paramagnon correction to the vertex Γ is calculated in a manner that is consistent with the requirements of spin rotational invariance expressed by Eq. (3.154) then the results of the SCR method may be obtained if we consider only the leading paramagnon corrections to the electron self-energy given by Eq. (3.165a,b). Thus the SCR scheme may be interpreted as some kind of temperature dependent mass renormalization of the paramagnon in which the mass is computed to leading order in the spin fluctuations in a manner consistent with the requirements of spin rotational invariance.

In addition to providing us with a rather elegant derivation of such approximation procedures as the SCR scheme, the technique outlined in this section provides us with the framework whereby higher order paramagnon corrections to the static susceptibility may be computed in a systematic way. To see how to extend the SCR scheme to include such higher order corrections in a systematic fashion based on the free energy approach of Moriya and Kawabata is extremely difficult.

Furthermore the close relation between the approximations used in this work and those employed in the zero temperature case[65] suggest that, with appropriate modifications, the considerations presented here could be extended to consider the ferromagnetic domain. It is by no means obvious that the resultant generalization of the SCR scheme to the ferromagnetic domain presented by Moriya and Kawabata[105] would result or whether in fact the mass renormalization scheme of Moriya and Kawabata is the simplest way to proceed.

To summarize in this section the response of an itinerant electron system to some small symmetry breaking term is examined and it is shown, by virtue of the constraints of this response imposed by the spin rotational invariance of the system, how an exact expression for the static susceptibility may be obtained. The results of this analysis are then used to derive an expression for the corrections to the RPA approximation arising from the paramagnon contributions to the electron self-cenergy together with the corresponding vertex corrections required by spin rotational invariance. When the correction term is evaluated in terms of the leading paramagnon contributions to the electron self-energy the result of previous works by other authors is recovered notably the SCR scheme of Moriya and Kawabata[9]. The approach presented here therefore provides for a rather precise diamagnetic interpretation of the SCR method. It also allows for a systematic extension of the procedure to consider higher order paramagnon corrections and to the ferromagnetic domain.

CHAPTER 4

THE d-f INTERACTION IN FERROMAGNETIC SUPERCONDUCTORS

4.1 The Interplay of Magnetism and Superconductivity

In this chapter we focus our attention on the magnetic properties of a somewhat different class of materials than those considered in Chapter 3. In the case of the itinerant systems, studied earlier, the magnetic properties were largely determined from the polarization of the electron spin, either through an applied field, as in the paramagnetic domain, or induced through the self-interactions, as in the ferromagnetic domain. In this section we wish to examine certain aspects of Magnetic Superconductors. These materials may be visualized as consisting of a band of conduction electrons interacting via a phonon induced BCS coupling, together with an array of magnetic ions which reside on particular lattice sites. The interest in such system stems from the fact that, in certain situations, it can arise that as the temperature is lowered the electrons condense into the superconducting state. The magnetic properties of these materials are then determined by the competition between the diamagnetic nature of the persistent current and the ferromagnetic nature of the localized spins. An important feature of these systems therefore is the interplay between superconductivity of the conduction electrons and the magnetism of the magnetic moments, arising from the various interactions between the localized spins and the conduction electrons. This interplay gives rise to a great many features peculiar to these systems.

Of the various interactions in these systems there are two, over and above the BCS interaction mentioned already and the exchange interaction between the localized magnetic moments, which are of interest to us here: the electromagnetic interaction between the magnetic ions and persistent current of the superconducting electrons as well as the indirect exchange interaction between the conduction electron, the d (or s) electrons and the electrons in the unfilled f shell of the magnetic ions. This latter interaction is referred to as the d (or s) f interaction.

Much of the earlier work[106,107,108] on these magnetic superconductors was concerned mainly with the effect of magnetic impurities on the superconducting properties, arising from the d (or s) f interaction. These studies provided a number of important results, they predicted the existence of gapless superconductors and showed that, unlike the situation that pertains for non-magnetic impurities, the presence of a small amount of magnetic impurity could destroy the superconducting state. Experiments on magnetic superconducting alloys confirmed that the presence of magnetic impurities easily quenches the superconductivity[109]. These theoretical and experimental results gave rise to the widespread belief that the prospect of a system exhibiting both superconducting and magnetic order was ruled out, since the two phases tended to destroy one another.

The situation changed dramatically in the late seventies following the discovery of the rare earth ternary and pseudo-ternary superconductors[12,13]. A systematic study has been made on two groups of these compounds, the $ReRh_4B_4$ compounds (RE = Rare Earth) and the Chevrel compounds, $REMo_6X_8$ (X = S or Se). Many of these substances become superconducting for $T \leq T_c$ despite the presence of the rare earth magnetic moments in the crystal lattice. This suggests that the interaction between the d electrons of the Rh or Mo ions giving rise to the superconductivity and the electrons of the unfilled f shell in the rare earth ions is relatively weak. Of these materials $ErRh_4B_4$ and $HoMo_6S_8$ are particularly interesting since, not only do both of these materials exhibit a superconducting phase as the temperature is lowered below the superconducting transition temperature T_{c1}, but as the temperature is lowered further a ferromagnetic normal phase appears at a temperature T_{c2} which persists down to zero temperature[12,13]. This is called the re-entrant phenomenon and T_{c2} is generally referred to as the re-entrant temperature.

The results of these experimental studies led to a renewed interest in the interplay between magnetism and superconductivity and the underlying mechanisms at work in these ternary compounds. Perhaps the most important facet to emerge from the theoretical studies of these compounds was the realization that the relative weakness of the d-f interaction, meant that the electromagnetic interaction between the rare earth spins and the persistent current assumed a major importance in determining their properties. A central feature of the electromagnetic interplay between the diamagnetic nature of the superconducting current and the ferromagnetic nature of the RE spins is the shielding of the RE spins by the persistent current[14]. This effect has been observed in the ultrasonic attenuation experiments[19,20] and predicted the existence of a modulated spin phase[14,15,16,17,18] in a narrow co-existence region above the re-entrant temperature T_{c2}. The existence of this phase has been confirmed by neutron scattering measurements[21,22,23]. In addition to the attenuation experiments and the existence of the spin modulated phase the electromagnetic interplay makes a number of other predictions, the spontaneous surface magnetization[110,111], the oscillatory penetration of the magnetic field[110,111], the superconducting domain wall[112,113], self-induced vortices[114] and the strong shielding of the forward neutron scattering[115].

Calculations have also been done to include the effect of the electromagnetic interaction on the magnetic properties of the mixed state in these compounds[27,28]. In addition to a detailed formulation of the mixed state, including the effect of the electromagnetic interaction, upper and lower critical field curves together with the magnetization curves were presented for a range of parameters. These calculations indicated that the upper critical magnetic induction curve B_{c2} ($= H_{c2} - 4\pi M_{c2}$) behaved in a manner similar to that obtained in the non-magnetic case. The results for the critical field curves can be described qualitatively in terms of the results for the non-magnetic type II superconductors by the replacement $\kappa \to \kappa_{eff} = \kappa(1 + 4\pi\chi)^{\frac{1}{2}}$.[116] The qualitative behaviour of the upper and lower critical field curves is similar to that observed in measurements made on polycrystalline samples[117,118].

While the effect of the d-f interaction is weak and it is possible to obtain a reasonable qualitative explanation for many of the phenomena observed in these ternary compounds solely in terms of the electromagnetic interaction, it does nevertheless give rise to a number of observable features. For example it gives rise to an increase in the superconducting transition temperature with the substitution of magnetic rare earth ions by non-magnetic ones[119] and may account for the deviation of the superconducting gap from the BCS result, observed in tunneling measurements[120,121], and the temperature dependence of the condensation energy measured from the magnetization curves[122]. However perhaps the most compelling argument as to why, that in order to obtain a precise theoretical model of these compounds, one must include not only the electromagnetic interaction but [illegible] the d-f interaction, is provided by the measurements of the [illegible] properties of single crystal $ErRh_4B_4$.[10,11] Calculations [illegible] the electromagnetic interaction cannot, of itself, account for both the hard and easy axis critical field curves by means of a consistent set of parameters. Furthermore the appearance of a first order phase transition around H_{c2} cannot be accounted for solely on the basis of the electromagnetic interaction.

In the light of these considerations there exists a need to provide a unified theory, which embodies the effect of both the d-f and the electromagnetic interactions in a consistent manner, if we wish to obtain a quantitative understanding of these materials. In the remainder of this section we present a theory which aims at such a unified approach and its application to the analysis of the mixed state in $ErRh_4B_4$.

In Section 4.2 we present a detailed derivation of a formalism, for the analysis of magnetic superconductors, which includes in a self-consistent manner, the pair breaking effects, induced through the d-f interaction together with the shielding of the localized magnetic moments by the persistent current. The pair breaking effects describe the modification to the superconducting electron states by the localized moments through their mutual interaction (the d-f interaction). There are two basic mechanisms which are of interest to us here: the scattering of the electrons by the localized spin fluctuations and secondly the

Zeeman splitting of the electron spins due to the effective field of the magnetic ions. Both of these mechanisms tend to destroy the superconductivity. Both of the pair breaking mechanisms are represented in the formalism developed in the next section. It will be shown how the effects of the localized spin fluctuations may be realized by means of a straightforward scaling law, following the definition of an effective coupling constant. While the simplifications afforded us by the scaling law are most evident in the mixed state, their application to the Meissner state is not without interest. In Section 4.2 it is shown how in the Meissner state, the effect of the spin fluctuations on various superconducting quantities, such as the superconducting gap, the condensation energy and the London penetration depth, may be computed from the familiar BCS results by means of the scaling law. Since all of the above quantities are experimentally accessible this provides a useful comparison with experiment.

The treatment of the electromagnetic fields in Section 4.2 is based on the Boson method pioneered by Umezawa and his collaborators[1,5,6,7,27,28]. The technique has found widespread application in the analysis of the mixed state in non-magnetic superconductors[7]. It has also been extended to include the case of magnetic superconductors[27,28]. The method is based on the field theoretic formulation of quantum electrodynamics in the superconducting state, based on the Lagrange multiplier field method of Nakanishi[124] and Lautrap[125]. Due to the spontaneously broken phase symmetry it can be shown that Goldstone's theorem is realized in this case through the appearance of a gapless excitation, the phason, in the positive norm part of the Lagrangian multiplier field. The argument is similar to that presented in Section 3.1 with regard to the appearance of the magnon in the case of the spontaneously broken spin symmetry. The observable properties of the phason are determined by the manner in which it couples to the various gauge invariant operators such as the electron current operator, for example. The nature of this coupling however is strongly governed by the requirements of gauge invariance, since it can be shown, quite generally, that the gauge transformations are realized through a translation of the positive and negative norm parts of the multiplier fields. This would lead one to suppose that, since the effect of the phason may be absorbed by a gauge transformation, its effect on observable quantities would be irrelevant. Such however is not the case if we permit translations of the phason field containing topological singularities. Such transformations cannot be removed simply by a gauge transformation and hence can give rise to observable phenomena. Vortex structures in superconductors provide an example of such singular transformations. Such singular transformations in the phason field belong to a class of transformations known as boson transformations and provide the basis for the so-called boson method in superconductivity.

Since the principles underlying the boson method in superconductivity are not dependent upon the detailed nature of the interactions present and that the effect of the d-f interaction, on the calculation of such quantities as the persisent current, involves only a straightforward extension of previous work[7], we do not include a detailed treatment of the boson method. Instead in Section 4.2 we content ourselves with a rather general outline and statement of the basic results together with the modifications arising from the d-f interaction.

In Section 4.3 the formulation developed in Section 4.2 is used to analyze the mixed state in $ErRh_4B_4$ and a detailed comparison with the recent measurements of the magnetic properties of single crystal $ErRh_4B_4$ is presented. It will be shown how good agreement with both the hard and easy axis magnetization measurements may be obtained from a single value of κ_B. Furthermore the formalism developed in Section 4.2 is applicable to the region in which the transition to the normal state at H_{c2} is first order. Thus the jump in the magnetization may be computed as a function of temperature and compared with experiment. This represents, as far as we know, the first calculation of a magnetization curve that has a first order transition to the normal state at H_{c2}.

4.2 A Formulation of the d-f Interaction in Ferromagnetic Superconductors

In this section we present a formulation for ferromagnetic superconductors which includes in a unified fashion both the d-f and electromagnetic interactions. The dynamics of the system under consideration is assumed to be obtained from the following microscopic Hamiltonian density given by

$$\begin{aligned}\mathcal{H}(x) = {} & \psi^{\dagger}(x)\varepsilon_0\left(-i\left(\vec{\nabla} - \frac{ie}{\hbar c}\vec{A}\right)\right)\psi(x) - V\psi_{\uparrow}^{\dagger}(x)\psi_{\downarrow}^{\dagger}(x)\psi_{\downarrow}(x)\psi_{\uparrow}(x) + \delta\varepsilon_F\psi^{\dagger}(x)\psi(x) \\ & - \frac{1}{2}\vec{M}(x)\gamma_0(-i\nabla)\vec{M}(x) - I\vec{M}(x)\psi^{\dagger}(x)\vec{\sigma}\psi(x) - \vec{M}(x)\cdot\vec{B}(x) \\ & + \mu_B\psi^{\dagger}(x)\vec{\sigma}\psi(x)\vec{B}(x) + \frac{1}{8\pi}\{|\vec{B}(x)|^2 + |\vec{E}(x)|^2\} .\end{aligned} \quad (4.1)$$

In the usual way $\psi(x)$ denotes the electron field, $\vec{A}(x)$ is the vector potential, with the magnetic induction field $\vec{B}(x)$ given by $\vec{B} = \vec{\nabla} \wedge \vec{A}(x)$ and $\vec{M}(x)$ is the density of the localized spin magnetic moment.

The first term corresponds to the gauge invariant expression for the kinetic energy of the electron. The electron energy is denoted by ε_0 and is assumed to be parabolic. The second term corresponds to the phonon induced BCS coupling. The third term is to account for shift of the chemical potential. The fourth term is the interaction between the localized spins other than that mediated by the dipole and the d-f interaction. The fifth term represents the d-f interaction while the sixth and seventh terms denote the interaction between the magnetic induction field $\vec{B}$ and the localized and electron spins respectively. The last term is the electromagnetic energy.

The presence of the d-f interaction term gives rise to two distinct mechanisms both of which serve to suppress the superconductivity. The first concerns the scattering of the electrons by the fluctuations of the localized spins. The second effect is the removal of the electron spin degeneracy caused by the splitting of the electron spectra into two distinct bands due to the polarization induced by the localized spins. It is the purpose of this paper to present a theory in which the above effects may both be incorporated, together with the shielding of the localized spins by the superconducting currents.

It will be shown that, while the splitting of the electron spectra by the internal fields leads to a more complicated functional form for the superconducting quantities such as the gap, condensation energy and the London penetration depth, the scattering of the electrons by the localized spin fluctuations may be realized, in the inelastic limit, by a simple scaling law following the definition of an effective coupling constant.

In addition to considering the effects of the finite field this work includes a somewhat more general treatment of the interactions present in the Hamiltonian than presented hitherto; in particular, the paramagnetic interaction between the electrons and the magnetic field $\vec{B}$ is included together with the self-interaction of the electrons with the electron spin density which arises through the phonon mediated BCS interaction. Such effects are included to provide a degree of completeness to the work and while they do not contribute substantially in the case of $ErRh_4B_4$, for example, they may give rise to important phenomena in other materials. Since such effects may be included simply through a redefinition of the parameters their inclusion does not affect the essence of many of the arguments presented here.

From the Hamiltonian of Eq. (4.1) we obtain the following equation of motion for the electron fields $\psi_\uparrow$ and $\psi_\downarrow$;

$$i\frac{\partial}{\partial t}\,\psi_\uparrow = \varepsilon_o(-i(\vec{\nabla}-\frac{ie}{\hbar c}\vec{A}))\psi_\uparrow - V\psi_\downarrow^\dagger\psi_\downarrow\psi_\uparrow' - \delta\varepsilon_F\psi_\uparrow + (I\vec{M}-\mu_B\vec{B})\cdot(\vec{\sigma}\psi)_\uparrow , \quad (4.2)$$

$$i\frac{\partial}{\partial t}\,\psi_\downarrow = \varepsilon_o(-i(\vec{\nabla}-\frac{ie}{\hbar c}\vec{A}))\psi_\downarrow - V\psi_\uparrow^\dagger\psi_\uparrow\psi_\downarrow - \delta\varepsilon_F\psi_\uparrow + (I\vec{M}-\mu_B\vec{B})\cdot(\vec{\sigma}\psi)_\downarrow . \quad (4.3)$$

The BCS interaction may be treated by the usual Hartree approximation to give

$$V\psi_\downarrow^\dagger\psi_\downarrow\psi_\uparrow = V\langle\psi_\downarrow\psi_\uparrow\rangle\psi_\downarrow^\dagger + V\langle\psi_\downarrow^\dagger\psi_\downarrow\rangle\psi_\uparrow \quad (4.4)$$

and

$$V\psi_\uparrow^\dagger\psi_\uparrow\psi_\downarrow = V\langle\psi_\uparrow\psi_\downarrow\rangle\psi_\uparrow^\dagger + V\langle\psi_\uparrow^\dagger\psi_\uparrow\rangle\psi_\downarrow . \quad (4.5)$$

If we introduce the four component field $\phi(x)$ defined by

$$\phi = \begin{pmatrix} \psi \\ \\ \psi_c \end{pmatrix} \quad (4.6)$$

with

$$\psi_c = i\sigma_2(\psi^\dagger)^t \quad , \tag{4.7}$$

the equation of motion may be written as

$$\{i\frac{\partial}{\partial t} - \epsilon(-i\nabla)\tau_3 + \Delta_o\tau_1 - \mu\sigma_3\}\phi = \{I\vec{M} - \mu_B\vec{B}\}\cdot\vec{\sigma}\phi - \langle I\vec{M} - \mu_B\vec{B}\rangle\cdot\vec{\sigma}\phi \quad , \tag{4.8}$$

where we have neglected the vector potential $\vec{A}$ and have assumed the applied field to point in the z direction. We have designated $\phi^\dagger\sigma_3\phi$ as the electron spin density in the z direction. The parameters μ and Δ_o in Eq. (4.8) are given by

$$\mu = \langle\{I\vec{M} - \mu_B\vec{B} - \frac{V}{2}\vec{\sigma}\}\rangle\cdot\vec{e}_3 \tag{4.9}$$

and

$$\Delta_o = V\langle\psi_\downarrow(x)\psi_\uparrow(x)\rangle \tag{4.10}$$

respectively. The quantity Δ_o may be thought of as the bare unrenormalized gap and μ the effective magnetic field experienced by the conduction electrons. It consists of three terms, the term arising from the d-f interaction due to the polarization of the localized spins, the term arising from the dipole interaction with the magnetic field $\vec{B}$ as well as the self-interaction with the electron spin density arising from the BCS interaction, essentially the last term in Eqs. (4.4) and (4.5).

The spin splitting parameter μ may be calculated in the mean field approximation. We begin with the equation of motion for the operator $S_i(t)$, defined as

$$S_i(t) = \int d^3\vec{x}\ \phi^\dagger\sigma_i\phi \quad , \tag{4.11}$$

which is given by

$$\partial_t S_i(t) = -\varepsilon_{ijk}\int d^3\vec{x}\,(IM_j(x) - \mu_B B_j(x))\sigma_k(x) \quad . \tag{4.12}$$

Thus we have

$$\partial_t \langle R[\sigma_i(x)S_j(t)]\rangle = \delta(t-t_x)\int \langle[\sigma_j(y),\sigma_i(x)]\rangle\Big|_{y_0=t} d^3\vec{y}$$

$$- \varepsilon_{j\ell k}\langle R[\sigma_i(x)\int d^3\vec{y}\,(IM_\ell(y) - \mu_B B_\ell(y))\sigma_k(y)]\rangle \quad . \tag{4.13}$$

Here R denotes the retarded operator product. Integrating with respect to t on both sides, we obtain after some straightforward algebra that

$$\langle\sigma_i(x)\rangle = \frac{1}{2i}\{\delta_{j\ell}\delta_{ik} - \delta_{jk}\delta_{i\ell}\}\int d^4y \langle R[\sigma_j(x)\sigma_k(y)\{IM_\ell(y) - \mu_B B_\ell(y)\}]\rangle. \tag{4.14}$$

Calculating this in the mean field approximation we obtain

$$\langle\sigma_i(x)\rangle = \int d^4y\; \chi_\sigma^{ij}(x-y)\{I\langle M_j(y) - \mu_B B_j(y)\rangle\} \;, \tag{4.15}$$

where χ_σ is a 3×3 matrix

$$\chi_\sigma^{ij}(x-y) = \frac{i}{2}\{\delta_{ij}\sum_k \langle R[\sigma_k(x)\sigma_k(y)]\rangle - \langle R[\sigma_j(x)\sigma_i(y)]\rangle\} \;. \tag{4.16}$$

Thus the expression for μ may be written as

$$\mu = I\langle M_3\rangle - \mu_B\langle B\rangle - \frac{V}{2}\langle\sigma_3\rangle \tag{4.17}$$

$$= \{I - \frac{V}{2}\chi_\sigma^{33}(i\partial)\}\{I\langle M_3\rangle - \mu_B\langle B_j\rangle\} \quad . \tag{4.18}$$

The expression for the magnetic field $\vec{B}$ is obtained from the Maxwell equation

$$\vec{\nabla}\wedge\langle B\rangle = \frac{4\pi}{e}\langle\vec{j}\rangle + 4\pi\nabla\wedge(\langle\vec{M}\rangle - \mu_B\langle\psi^\dagger\vec{\sigma}\psi\rangle) \;. \tag{4.19}$$

The calculation of the macroscopic current $\langle\vec{j}\rangle$ in the superconducting state is by no means straightforward owing to the fact that the appearance of the order parameter means that the phase invariance is spontaneously broken.

The method we employ in this analysis is based on the work of Umezawa and his collaborators and has been used extensively in the analysis of both non-magnetic[1,5,6,7] and magnetic[27,28] superconductors. The technique is based on an operator realization of quantum electrodynamics in the superconducting state using the multiplier field method of Nakanishi[124] and Lautrap[125]. The basic feature of the method, peculiar to the superconducting state, is the appearance of a gapless excitation in the multiplier field. The positive norm part of the multiplier field is referred to as the phason or phase boson while the negative norm part is referred to as the ghost field. The presence of the phase boson in the operator structure of quantum electrodynamics is essential since it can be shown that it is through translations of the phase boson that the gauge transformations are induced. Perhaps the most important consequence of this is that the manner in which the phase boson couples to the observable quantities, such as the electron current operator, is largely determined by the requirements of gauge invariance. This means for example that it always appears in the gauge invariant combination $\{A_\mu - \frac{\hbar c}{e} \partial_\mu f(x)\}$ or as $\{e^{if(x)/2}\, \psi(x)\}$. Thus we find for example that, in the linear approximation we have the following expression for the current operator

$$\vec{j}(x) = - \lambda_L^{-2}\, C(-i\nabla)\{\vec{A}(x) - \frac{\hbar c}{e} \vec{\nabla} f\} + \ldots \tag{4.20}$$

where $C(-i\nabla)$ is a non-local kernel, computed from the photon self-energy including the effect of the collective mode[1,7], and $\vec{A}(x)$ denotes the vector potential. Thus the macroscopic superconducting current may be written as

$$<\vec{j}(x)> = -\lambda_L^{-2} C(-i\nabla)\{<\vec{A}(x)> - \frac{\hbar c}{e}\vec{\nabla}<f(x)>\} + \ldots \quad (4.21)$$

Now due to the gauge invariant nature of the electron field operator, $\psi(x)e^{if(x)/2}$, we may identify $<f(x)>$ as the phase of the order parameter. Thus Eq. (4.21) expresses the superconducting current $<j>$ in terms of the vector potential and the phase of the order parameter.

Due to the fact that the phase boson always couples to the observable quantities in a gauge invariant manner, one would suppose that it would not give rise to any observable phenomena. Indeed if we combine the Maxwell equation Eq. (4.19) together with the constitutive equation for the superconducting current, Eq. (4.21), then we obtain the following expression for the magnetic induction field $<B(x)>$

$$\{\nabla^2 + \lambda_L^{-2} C(-i\nabla)\}<\vec{B}> = \frac{e\hbar}{c}\lambda_L^{-2} C(-i\nabla)\nabla\wedge\nabla<f> + 4\pi\nabla\wedge\{<M> - \mu_B<\psi^\dagger\sigma\psi>\}. \quad (4.22)$$

From Eq. (4.22) we immediately note that the phase boson does not contribute to the macroscopic current unless

$$\nabla\wedge\nabla<f> \neq 0 \quad . \quad (4.23)$$

The condition expressed by Eq. (4.23) cannot be satisfied if the vacuum expectation value $<f>$ (which we will denote simply as f from now on) is Fourier transformable. This implies that the function f must contain certain topological singularities in order that the phase boson contribute to the macroscopic current $<j>$. While a variety of singular solutions to f may be realized, all of them may be constructed by means of a linear superposition of the vortex solutions. The single vortex solution corresponds to the presence of a topological line singularity in the function f of the form:

$$f(x) = \frac{1}{2}\,\theta[\vec{x}-\vec{\xi}] \tag{4.24}$$

where $\theta[\vec{x}-\vec{\xi}]$ corresponds to the cylindrical angle measured with respect to the line singularity at position $\vec{\xi}$. The extension of a single vortex to a vortex array is achieved through a superposition of the single vortex solutions, thus

$$f(x) = \sum_i \frac{1}{2}\,\theta[\vec{x}-\vec{\xi}_i] \tag{4.25}$$

is the phase of the order parameter in a vortex array where $\vec{\xi}_i$ now denotes the position of the i^{th} vortex.

If we then define the vortex density as

$$\vec{n}(x) = \nabla \wedge \nabla f(x) = \vec{e}_3 \sum_i \delta(x-\xi_i) \tag{4.26}$$

then Eq. (4.22) may be written as

$$\{\nabla^2 - \lambda_L^{-2} C(i\nabla)\}\langle B(x)\rangle = \lambda_L^{-2} C(-i\nabla) n(x)\phi + 4\pi\nabla^2\{\langle M\rangle - \mu_B\langle\sigma\rangle\}$$

$$= -\lambda_L^{-2} C(-i\nabla) n(x)\phi + 4\pi\nabla^2\{1 - \mu_B I\chi_\sigma^{33}\}\langle M\rangle + \mu_B^2\chi_\sigma^{33} 4\pi\nabla^2\langle B(x)\rangle \tag{4.27}$$

where we have assumed all the fields are parallel to the z axis and $\vec{n}(x) = \vec{e}_3 n(x)$. Equation (4.15) was used to obtain Eq. (4.27). Thus we obtain the following expression for the induction field $\langle B(x)\rangle$ in terms of the vortex density n(x) and the magnetic moment $\langle M\rangle$ as

$$\langle B(x)\rangle = \{(1 - 4\pi\mu_B^2\chi_\sigma^{33})\nabla^2 - \frac{1}{\lambda_L^2} C(-i\nabla)\}^{-1}\{-\lambda_L^{-2} C(-i\nabla) n(x)\phi + 4\pi\nabla^2(1 - \mu_B I\chi_\sigma^{33})\langle M\rangle\} \tag{4.28}$$

and hence that

$$\mu = -\mu_B\left(1 - \frac{V}{2}\chi_\sigma^{33}\right)\{-(1 - 4\pi\mu_B^2\chi_\sigma^{33})\nabla^2 - \lambda_L^{-2}C(-i\nabla)\}^{-1}\lambda_L^{-2}C(-i\nabla)n(x)\phi$$

$$+\left(1 - \frac{V}{2}\chi_\sigma^{33}\right)\{I - 4\pi\mu_B(1 - I\mu_B\chi_\sigma^{33})(-\nabla^2)(-(1 - 4\pi\mu_B^2\chi_\sigma^{33})\nabla^2 + \lambda_L^{-2}C(-i\nabla))^{-1}\}\langle M\rangle \quad . \tag{4.29}$$

This expression for μ may be written in terms of a renormalized d-f coupling constant $\tilde{I}$ and the bare induction field $\vec{B}_o(x)$ created by the vortices as

$$\mu = \tilde{I}\langle\vec{M}\rangle\cdot\vec{e}_3 - \mu_B\vec{B}_o(x)\cdot\vec{e}_3 \quad , \tag{4.30}$$

where

$$\tilde{I} = \left\{1 - \frac{V}{2}\chi_\sigma\right\}\left\{I - 4\pi\mu_B(1 - I\mu_B\chi_\sigma)\frac{-\nabla^2}{-(1-4\pi\mu_B^2\chi_\sigma)\nabla^2 + \lambda_L^{-2}C(-i\vec{\nabla})}\right\} \tag{4.31}$$

and

$$\vec{B}_o(x) = \frac{\lambda_L^{-2}C(-i\vec{\nabla})}{-(1 - 4\pi\mu_B^2\chi_\sigma)\nabla^2 + \lambda_L^{-2}C(-i\vec{\nabla})}\vec{n}(x)\phi \quad . \tag{4.32}$$

In most situations the contribution to the effective field μ from the self-interaction of the electrons may be safely neglected. As for the paramagnetic interaction it may arise, particularly if the d-f interaction coupling constant I is sufficiently small, that the contribution from the localized spin and the dipole interaction may be of comparable magnitude. This may result in a partial cancellation of the magnetic field by the internal field if I is positive. Such a mechanism was first pointed out by Jaccarino and Peter[126]. This however is not believed to be an important effect in $ErRh_4B_4$ for example, and the paramagnetic interaction may be safely neglected. Thus Eq. (4.30) reduces to

$$\mu = I\langle\vec{M}\rangle\cdot\vec{e}_3 \tag{4.33}$$

or equivalently that

$$\tilde{I} = I \ . \tag{4.34}$$

The term on the right hand side of Eq. (4.8) corresponds to the interaction between the electrons and the spin fluctuations. The fluctuations give rise to self-energy contributions which in general will serve to suppress the superconductivity. Denoting the retarded Green's function S(p) by

$$<R\{\phi(x)\phi^{+}(y)\}> = \frac{i}{(2\pi)^4}\int d^4p\ e^{i\{\vec{p}\cdot(\vec{x}-\vec{y})-p_0(t_x-t_y)\}}\ S(p) \tag{4.35}$$

and the self-energy $\sum(p)$ by

$$S^{-1}(p) = p_0 - \varepsilon(\vec{p})\tau + \Delta_0\tau_1 + \mu\sigma_3 - \sum(p) \ , \tag{4.36}$$

we obtain to lowest order the following expression for $\sum(p)$

$$\sum(p) = \frac{\tilde{I}^2}{(2\pi)^3}\int d^3\vec{k}\int dw\ dv \sum_i \rho_{ij}(w;k)\sigma_i\, \mathcal{S}(v;\vec{p}-\vec{k})\sigma_j \frac{e^{\beta(w+v)}}{(e^{\beta w}-1)(e^{\beta v}+1)}\ \frac{1}{(p_0-v-w+i\varepsilon)} \ , \tag{4.37}$$

where $\mathcal{S}(p)$ is the spectral function of the electron propagator S(p), that is

$$S(p) = \int dV\ \mathcal{S}(v;\vec{p})\ \frac{1}{p_0 - v + i\varepsilon} \tag{4.38}$$

so that

$$\mathcal{S}(p_0;\vec{p}) = -\frac{1}{\pi}\ \mathrm{Im}\ S(p) \ , \tag{4.39}$$

and where $\rho_{ij}(k)$ is the spectral function of the spin spin correlation function

$$<R\{M_i(x)M_j(y)\}> = \frac{i}{(2\pi)^4}\int d^4k\ e^{i\vec{k}(\vec{x}-\vec{y})-ik_0(t_x-t_y)}\ \chi_{ij}(k) \tag{4.40}$$

so that

$$\chi_{ij}(k) = \int dw\, \rho_{ij}(w;k) \frac{1}{k_0 - w + i\varepsilon} \quad . \tag{4.41}$$

The derivation of Eq. (4.37) is tedious but relatively straightforward and is presented in Appendix C.

To Evaluate Eq. (4.37) we assume that the spectral density $\rho_{ij}(k)$ may be written in the hydrodynamical form as

$$\rho_{ij}(w;k) = \frac{1}{\pi} \frac{w\Gamma}{w^2 + \Gamma^2} \chi_{ij}(\vec{k}) \tag{4.42}$$

and expand the thermal weight in a low frequency expansion;

$$\frac{e^{\beta(w+v)} + 1}{(e^{\beta w} - 1)(e^{\beta v} + 1)} = \frac{(e^{\beta v} + 1) + \beta w e^{\beta v} + \ldots}{\beta w(1 - \frac{1}{2}\beta w + \ldots)(e^{\beta v} + 1)}$$

$$= \left\{\frac{1}{\beta w} + \frac{e^{\beta v} - 1}{2(e^{\beta v} + 1)} + 0(w)\right\} \quad . \tag{4.43}$$

The self-energy $\sum(p)$ may then be evaluated to give

$$\sum(p) = \frac{\tilde{I}^2}{(2\pi)^3} \int d^3\vec{k} \int dv\, \mathcal{J}(v;\vec{p}-\vec{k}) \sum_i \chi_{ii}(\vec{k}) \left\{\beta^{-1} \frac{1}{p_0 - v + i\Gamma} - \frac{e^{\beta v} - 1}{2(e^{\beta v} + 1)} \frac{i\Gamma}{p_0 - v + i\Gamma}\right\}. \tag{4.44}$$

There are two limiting cases where the self-energy $\sum(p)$ assumes a rather familiar form. In the extreme elastic limit $\Gamma \to 0$, the gap equation reduces to the result for the impurity case, while in the extreme inelastic limit $\Gamma \to \infty$ the expression for the self-energy reduces to

$$\sum(p) = -\frac{\tilde{I}^2}{(2\pi)^3} \int d^3\vec{k} \int dv\, \mathcal{J}(v;\vec{p}-\vec{k}) \sum_i \chi_{ii}(\vec{k}) \frac{e^{\beta v} - 1}{2(e^{\beta v} + 1)} \quad , \tag{4.45}$$

which was first considered in ref. [127] and further analyzed in ref. [128] and provides the starting point for our discussion.

Defining the renormalized gap $\Delta(p)$ as

$$[\tau_3, S^{-1}(p)] = 2i\,\tau_2\,\Delta(p) \ , \tag{4.46a}$$

then using the approximations outlined, we obtain the following equation for the gap in the extreme inelastic limit

$$\Delta(\vec{p}) = \int \frac{d^3\vec{k}}{(2\pi)^3}\{V - \tilde{I}^2 \sum_i \chi_{ii}(\vec{p}-\vec{k})\}\frac{\Delta(\vec{k})}{2E(\vec{k})}\,\frac{1}{2}\left\{\tanh\frac{\beta(E(k)+\mu)}{2} + \tanh\frac{\beta(E(k)-\mu)}{2}\right\} \tag{4.46b}$$

In order to simplify the above equation we approximate $\Delta(\vec{p})$ by its average value on the Fermi surface and use the effective coupling constant approximation. Thus Eq. (4.46b) reduces to

$$1 = g(T;H)N(0)\int_0^{\omega_D} d\varepsilon\,\frac{1}{E}\{1 - f_F(E+\mu) - f_F(E-\mu)\} \tag{4.47}$$

with

$$E = \sqrt{\varepsilon^2 + \Delta^2} \ , \tag{4.48}$$

where the effective coupling constant $g(T;H)$ is given by

$$g(T;H) = \frac{1}{(4\pi)^2}\int_{|\vec{p}|=|\vec{k}|=k_F} d\Omega_p\, d\Omega_k\,\{V - \tilde{I}^2 \sum_i \chi_{ii}(\vec{p}-\vec{k})\} \ , \tag{4.49}$$

with the H dependence of $g(T;H)$ arising from the H dependence of χ_{ii}.

The equation

$$1 = gN(0)\int_0^{\omega_D} d\varepsilon\,\frac{1}{E}\{1 - f(E+\mu) - f(E-\mu)\} \tag{4.50}$$

has been studied in detail by Sarma[129]. The resultant gap can be written in terms of a two parameter function which we will denote by $\mathcal{D}(t;\tilde{\mu})$

$$\frac{\Delta(T;\mu;gN)}{\Delta_o(gN)} = \mathcal{B}(t;\tilde{\mu}) \tag{4.51}$$

and which is given as the solution of

$$\log \mathcal{B}(t;\tilde{\mu}) = -\Phi_1\left\{\frac{\pi e^{-\gamma}}{t}\mathcal{B}(t;\tilde{\mu})\,;\,\frac{\pi e^{-\gamma}}{t}\tilde{\mu}\right\} \tag{4.52}$$

with

$$\Phi_1\{x;y\} = \frac{x}{4}\,\mathrm{Re}\int_{-\infty}^{+\infty} dz\,\ln\{z+\sqrt{z^2-1}\}\cosh^{-2}\frac{1}{2}\{xz+y\}\ . \tag{4.53}$$

The integrand is calculated along the contour shown in figure 2 with the branch line running between z = -1 and with

$$\lim_{v\to 0}\ \ln\{z+\sqrt{z^2+1}\} = \ln\{u+\sqrt{u^2-1}\}\quad \text{for } u>1 \tag{4.54}$$

where $z = u + iv$. $\Delta_o(gN(0);\omega_D)$ is given by

$$\Delta_o(gN(0);\omega_D) = 2\tilde{\omega}_D\exp-\frac{1}{gN(0)}\ , \tag{4.55}$$

$\tilde{\mu}$ is given by

$$\tilde{\mu} = \frac{\mu}{\Delta_o(gN(0);\omega_D)} \tag{4.56}$$

and t is the reduced temperature

$$t = T/T_c\ . \tag{4.57}$$

We then find therefore that the solution to Eq. (4.47) may be obtained simply by scaling the solution of Eq. (4.50), i.e.

$$\frac{\Delta(T;\mu;g(T;H)N(0))}{\Delta_o(g(T_c;0))} = s(t;H)\,\mathcal{B}(t/s(t;H);\tilde{\mu}/s(t;H))\ , \tag{4.58}$$

where

$$s(t;H) = \exp\left\{\frac{1}{g(T_c;0)N(0)} - \frac{1}{g(T;H)N(0)}\right\} , \tag{4.59}$$

$$\bar{\mu} = \mu/\Delta_0(g(T_c)N(0);\omega_D) \tag{4.60}$$

and we have normalized the gap by $\Delta_0(g(T_c),0)$. The calculation of the scale factor together with an illustration of the resultant temperature dependent gap will be presented later in this section.

Similar approximations may also be used in the calculation of the free energy, however in the case of the free energy particular care must be taken to ensure that certain contributions are not double counted. For example, the localized spins renormalize the superconducting electrons while in turn the superconducting electrons modify the behaviour of the localized spins. Now while both effects must be included in the calculation of the free energy, they both originate from the same term in the Hamiltonian and thus care must be taken not to include such terms twice. The approach used in this work is to separate the Hamiltonian into an electronic magnetic and electromagnetic contribution,

$$\mathcal{H}(x) = \mathcal{H}_{el}(x) + \mathcal{H}_M(x) + \mathcal{H}_{EM}(x) , \tag{4.61}$$

where

$$\mathcal{H}_{el} \equiv \psi^\dagger\varepsilon_0(-i\nabla)\psi - V\psi_\uparrow^\dagger\psi_\downarrow^\dagger\psi_\downarrow\psi_\uparrow - \frac{1}{2}\{I\vec{M} - g_J\mu_B\vec{B}\}\cdot\psi^\dagger\vec{\sigma}\psi \tag{4.62}$$

$$\mathcal{H}_M \equiv -\frac{1}{2}\vec{M}\gamma_0(-i\nabla)\vec{M} - \frac{1}{2}\{I\psi^\dagger\vec{\sigma}\psi + \vec{B}\}\cdot\vec{M} \tag{4.63}$$

and

$$\mathcal{H}_{EM} \equiv \frac{1}{8\pi}\{|\vec{E}|^2 + |\vec{B}|^2\} + \vec{J}\cdot\{\vec{A} - \frac{\hbar c}{e}\vec{\nabla}f\} - \frac{1}{2}\{\vec{M} - g_J\mu_B\psi^\dagger\vec{\sigma}\psi\}\cdot\vec{B} , \tag{4.64}$$

where we have divided the mutual interaction terms equally between the three contributions (e.g. $\frac{1}{2}\vec{M}\cdot\psi^\dagger\vec{\sigma}\psi$ is included in $\mathcal{H}_{el}$ and $\frac{1}{2}\vec{M}\cdot\psi^\dagger\vec{\sigma}\psi$ is included in $\mathcal{H}_M$). The expression for $\mathcal{H}_{EM}$, given in Eq. (4.64), contains the contribution from the phase boson. This arises from the gauge invariant substitution $A_\mu \to A_\mu - \frac{\hbar c}{e}\,\partial_\mu f(x)$ in the expression given in Eq. (4.1). Correspondingly we define U_{el}, U_M and U_{EM} as

$$\frac{1}{V}\int d^3x \, \langle \mathcal{H}_{el} \rangle \equiv U_{el} \quad , \tag{4.65}$$

$$\frac{1}{V}\int d^3x \, \langle \mathcal{H}_{M} \rangle = U_{M} \quad , \tag{4.66}$$

and

$$\frac{1}{V}\int d^3x \, \langle \mathcal{H}_{EM} \rangle = U_{EM} \quad . \tag{4.67}$$

Each of the above terms, U_{el}, U_M and U_{EM}, may then be evaluated using the renormalized quantities making the appropriate subtractions.

In the case of the electronic degrees of freedom this is best achieved if we rewrite the equation of motion Eq. (4.8) in terms of the renormalized or subtracted quantities

$$\{i \frac{\partial}{\partial t} - \varepsilon(-i\nabla)\tau_3 + \Delta\tau_1 + \mu\sigma_3\}\phi = F_\phi \quad , \tag{4.68}$$

where Δ is the renormalized gap obtained from the solution of Eq. (4.47) and F_ϕ is given by

$$F_\phi = -\begin{Bmatrix} V\psi_\downarrow^\dagger\psi_\downarrow\psi_\uparrow + (IM_3 - g_J\mu_B B_3 - \mu)\psi_\uparrow + 2(IM_- - g\mu_B B_-)\psi_\downarrow - \Delta\psi_\downarrow^\dagger \\ V\psi_\uparrow^\dagger\psi_\uparrow\psi_\downarrow - (IM_3 - g_J\mu_B B_3 - \mu)\psi_\downarrow + 2(IM_+ - g\mu_B B_+)\psi_\uparrow + \Delta\psi_\uparrow^\dagger \\ -V\psi_\downarrow^\dagger\psi_\uparrow^\dagger\psi_\uparrow + (IM_3 - g_J\mu_B B_3 - \partial)\psi_\downarrow^\dagger - 2(IM_- - g\mu_B B_-)\psi_\uparrow^\dagger - \Delta\psi_\uparrow \\ V\psi_\uparrow^\dagger\psi_\downarrow^\dagger\psi_\downarrow + (IM_3 - g_J\mu_B B_3 - \mu)\psi_\uparrow^\dagger + 2(IM_+ - g\mu_B B_+)\psi_\downarrow^\dagger - \Delta\psi_\downarrow \end{Bmatrix} \tag{4.69}$$

This allows us to write $\mathcal{H}_{el}$, given by Eq. (4.62) in terms of the renormalized quantities as

$$\int d^3x\, \mathcal{H}_{el} = V\int \frac{d^3k}{(2\pi)^3}(\varepsilon + \mu) + \int d^3\vec{x}\; \phi^\dagger\{\varepsilon(-i\nabla)\tau_3 - \Delta\tau_1 - \mu\sigma_3\}\phi + \frac{\mu}{2}\int d^3\vec{x}\;\phi^\dagger\sigma_3\phi$$
$$+ \frac{\Delta}{2}\int d^3\vec{x}\,\phi^\dagger\tau_1\phi + \frac{1}{4}\int d^3\vec{x}\;\{\phi_1^\dagger F_{\phi_1} + \phi_2 F^\dagger_{\phi_2} - \phi_3 F^\dagger_{\phi_3} - \phi_4 F^\dagger_{\phi_4}\} \quad . \qquad (4.70)$$

Taking the thermal expectation value we obtain

$$\frac{1}{V}\, d^3x\, \langle\mathcal{H}_{el}\rangle = \int \frac{d^3k}{(2\pi)^3}(\varepsilon + \mu) - \frac{i}{(2\pi)^4}\oint_+ d^4k\; \mathrm{Tr}\Big\{S(k)\{\varepsilon(\vec{k}) - \Delta\tau_1 - \mu\sigma_3\}\Big\}$$
$$+ \frac{1}{2}\int d^3k\; \mathrm{Tr}\{(\mu\sigma_3 + \Delta\tau_1)S(k)\} + \frac{1}{2V}\int d^3\vec{x}\; \mathrm{Re}\langle\phi\, F_\phi\rangle \quad . \qquad (4.71)$$

The last term in this expression represents the contributions to the internal energy arising from the renormalized electron self-energy correction. If we now calculate the electron self-energy and the corresponding propagator in the manner outlined in Appendix C, then this term will not contribute since the self-energy and the counter terms Δ and μ will exactly cancel this contribution. The resultant expression for the electronic contribution to the internal energy is

$$\frac{1}{V}\int d^3x\, \langle\mathcal{H}_{el}\rangle = \int \frac{d^3\vec{k}}{(2\pi)^3}\Big\{(\varepsilon - E) + \frac{\Delta^2}{2E}\{1 - f_F(E-\mu) - f_F(E+\mu)\} + (E-\mu)f(E-\mu)$$
$$- (E+\mu)f_F(E+\mu) + \frac{\mu}{2}\{f_F(E-\mu) - f_F(E+\mu)\}\Big\} \quad . \qquad (4.72)$$

The entropy of the electronic states may be computed to give

$$\beta^{-1}S_{el} = \beta^{-1}\int \frac{d^3k}{(2\pi)^3}[f(E+\mu)\log f_F(E+\mu) + \{1 - f_F(E+\mu)\}\log(1 - f_F(E+\mu))]$$
$$+ \beta^{-1}\int \frac{d^3k}{(2\pi)^3}[f(E-\mu)\log f_F(E-\mu) + \{1 - f_F(E-\mu)\}\log(1 - f_F(E-\mu))] \quad . \qquad (4.73)$$

Thus we obtain an expression for the electronic free energy F_{el}, defined as

$$F_{el} = U_{el} - \beta^{-1} S_{el} \quad , \tag{4.74}$$

to be given by

$$F^s_{el} = \int \frac{d^3\vec{k}}{(2\pi)^3} [\varepsilon - E + \frac{\Delta^2}{2E} (1 - f(E-\mu) - f(E+\mu)) + $$
$$+ \beta^{-1}\{\log(1 - f_F(E-\mu)) + \log(1 - f(E+\mu))\} + \frac{\mu}{2}\{f(E-\mu) - f(E+\mu)\}], \tag{4.75}$$

where the superscript s denotes the superconducting state (i.e. $\Delta \neq 0$). A similar calculation in the normal state (i.e. $\Delta = 0$) yields

$$F^N_{el} = \int \frac{d^3\vec{k}}{(2\pi)^3} [\beta^{-1}\{\log(1 - f_F(\varepsilon + \mu))\} + \{\log(1 - f_F(\varepsilon - \mu))\}$$
$$+ \frac{\mu}{2} \{ f_F(\varepsilon - \mu) - f_F(\varepsilon + \mu)\}] \quad . \tag{4.76}$$

We now obtain an expression for the field dependent condensation energy $\frac{H_c^2}{8\pi}(T;H)$, defined by

$$\begin{aligned}
\frac{H_c^2(T;H)}{8\pi} &\equiv F^N_{el}(T;H) - F^s_{el}(T;H) \\
&= 2N(0) \int_0^{\omega_D} d\varepsilon [\varepsilon - E - \frac{\Delta^2}{2E} - \frac{E^2+\varepsilon^2}{2E} \{ f_F(E-\mu) + f_F(E+\mu) \} \\
&\quad + 2\varepsilon f_F(\varepsilon) + \frac{\mu}{2} \{ f_F(E-\mu) - f_F(E+\mu)\}] \\
&= 2N(0) [\frac{1}{4} \Delta^2 - \frac{\pi^2}{6} \beta^{-2} + \int_0^{\infty} d\varepsilon \frac{E^2+\varepsilon^2}{2E} \{f_F(E-\mu) + f_F(E+\mu)\} \\
&\quad - \frac{\mu}{2} \int_0^{\infty} d\varepsilon \{ f_F(E-\mu) - f_F(E+\mu)\}] \quad .
\end{aligned} \tag{4.77}$$

The above condensation energy reduces to the BCS result in the limit $H \to 0$ and $\mu \to 0$.

As in the discussion of the renormalized gap Δ, the effect of the temperature and field dependent effective coupling constant may be realized through the scaling of a two parameter function

$$\frac{H_c(T;H)}{H_{co}} = s(t;H)\,\mathcal{H}(t/s(t;H);\bar{\mu}/s(t;H)) \,, \qquad (4.78)$$

where

$$\mathcal{H}^2(t;\bar{\mu}) = \mathcal{B}^2(t;\bar{\mu}) - \frac{2\pi^2}{3}\left\{\frac{t^2}{\pi e^{-\gamma}} - \frac{3\mathcal{B}^2(t;\bar{\mu})}{\pi^2}\,\Phi_3\{\frac{\pi e^{-\gamma}}{t}\mathcal{B}(t;\bar{\mu});\ \frac{\pi e^{-\gamma}}{t}\bar{\mu}\}\right.$$

$$\left. - \frac{3\bar{\mu}\,\mathcal{B}(t;\bar{\mu})}{\pi^2}\,\Phi_4\{\frac{\pi e^{-\gamma}}{t}\mathcal{B}(t;\bar{\mu});\ \frac{\pi e^{-\gamma}}{t}\bar{\mu}\}\right\} \,. \qquad (4.79)$$

Here the functions $\mathcal{B}(t;\bar{\mu})$ and $s(t;H)$ are those defined previously in Eqs. (4.52) and (4.59). The functions $\Phi_3(x;y)$ and $\Phi_4(x;y)$ are given by

$$\Phi_3(x;y) = \frac{x}{4}\,\mathrm{Re}\int_{-\infty}^{+\infty} dz\; z\sqrt{z^2-1}\,\cosh^{-2}\frac{1}{2}\{xz+y\} \qquad (4.80)$$

and

$$\Phi_4(x;y) = \frac{x}{4}\,\mathrm{Re}\int_{-\infty}^{+\infty} dz\,\sqrt{z^2-1}\,\cosh^{-2}\frac{1}{2}\{xz+y\} \,, \qquad (4.81)$$

while the normalization factor H_{co} is given by

$$H_{co} = \sqrt{4\pi N(0)\Delta_o^2(g(T_c;0))} \qquad (4.82)$$

where Δ_o is given by Eq. (4.55) with g replaced by $g(T_c;0)$. The integrand in Φ_3 and Φ_4 is defined in a manner analogous to Φ_1.

The contribution to the internal energy from the localized spins, U_M, may be easily calculated in the mean field approximation as

$$U_M = -\frac{1}{2}\langle\vec{M}\rangle\gamma_o(-i\nabla)\langle\vec{M}\rangle - \frac{1}{2}\{I\langle\psi^\dagger\vec{\sigma}\psi\rangle - \langle\vec{B}\rangle\}\cdot\langle\vec{M}\rangle \,, \qquad (4.83)$$

while the entropy may be calculated to give

$$\beta^{-1}S_M = -\beta^{-1}N \log Z_J\{g_J J\mu_B|\vec{H}_{MF}|\} - \vec{H}_{MF}\cdot\langle\vec{M}\rangle \ , \tag{4.84}$$

where J is the spin of the localized spin, g_J the Lande's g-factor,

$$Z_J(x) = \frac{\sinh \frac{1}{2J}\, x}{\sinh \frac{1}{2J+1}\, x}$$

and H_{MF} denotes the mean field experienced by the localized spin and is given by

$$\vec{H}_{MF} = \gamma_o(-i\nabla)\langle\vec{M}\rangle + \langle\vec{B}\rangle + I\langle\psi^{\dagger}\vec{\sigma}\psi\rangle \ . \tag{4.85}$$

The contribution to the free energy from the localized spins is therefore given by

$$F_M \equiv U_M - \beta^{-1}S_M = \frac{1}{2}\langle\vec{M}\rangle\cdot\vec{H}_{MF} - \beta^{-1}N \log Z_J(g_J J\mu_B B|\vec{H}_{MF}|) \ . \tag{4.86}$$

Details regarding the calculation of $\langle M\rangle$, $\langle\sigma\rangle$ and H_{MF} will be presented later in the discussion.

The contribution to the ground state energy from the electromagnetic field may be calculated by replacing the fields by their thermal average. Thus we obtain

$$U_{EM} = \frac{1}{8\pi}\frac{1}{V}\int d^3\vec{x}\,(|\langle\vec{E}\rangle|^2 + |\langle\vec{B}\rangle|^2) - \frac{1}{2}\langle\vec{j}\rangle\cdot(\langle\vec{A}\rangle - \frac{\hbar c}{e}\vec{\nabla}f) - \frac{1}{2}(\langle\vec{M}\rangle - g\mu_B\langle\psi^{\dagger}\vec{\sigma}\psi\rangle)\cdot\langle\vec{B}\rangle \ , \tag{4.87}$$

which, after some manipulation involving the Maxwell equations, may be written as[7]

$$U_{EM} = \int_V d^3\vec{x}\,\langle H\rangle\cdot\frac{\hbar c}{e}\,\vec{\nabla}\wedge\vec{\nabla}f \tag{4.88}$$

$$= \frac{1}{V}\int_V d^3\vec{x}\,\langle\vec{H}\rangle\cdot\vec{n}\phi \tag{4.89}$$

in the case of the superconducting state, where $\vec{n}$ denotes the vortex density, $\Phi = \hbar c/2e$ and $\vec{H}$ is the internal magnetic field defined by $\vec{H} = \vec{B} - 4\pi(\vec{M} - \mu_B \psi^{\dagger}\vec{\sigma}\psi)$. This above expression illustrates the well known statement that the vortex interaction is simply given by the vortex magnetic field.

In the normal state we obtain

$$U_{EM} = \frac{1}{V}\int_V d^3\vec{x} < \vec{H} > \cdot < \vec{B} > \quad . \tag{4.90}$$

Combining the preceding expressions, we obtain the complete expression for the free energy in the mixed state to be

$$F_s = -\frac{H_c^2}{8\pi} + \frac{1}{8\pi} < \vec{H} > \cdot \vec{n}\phi + \frac{1}{2} < \vec{H}_{MF} > \cdot < \vec{M} > - \beta^{-1} N \log\{g_J J \mu_B B |\vec{H}_{MF}|\} + E_{core} . \tag{4.91}$$

The last term in Eq. (4.91), E_{core}, corresponds to the effect of the vortices on the energy spectra of the superconducting electrons. It is calculated in the manner outlined in ref. [7]. It should be noted that the above expression has an identical form to that presented in ref. [28], although the calculation of the individual terms is somewhat more complicated due to the effects of the finite fields and magnetization arising from the d-f interaction.

Before going on to evaluate the magnetization and the magnetic susceptibilities, we discuss the calculation of the London penetration depth λ_L and the non-local kernel $C(-i\nabla)$ introduced in Eq. (4.20). In the case of the London penetration the calculation is reasonably straightforward, since using the approximations introduced in the analysis of the renormalized gap and the condensation energy, we may obtain, by a procedure similar to that presented in ref. [1], the following expression

$$\frac{\lambda_L^{-2}(T;H)}{\lambda_{Lo}^{-2}} = \left\{1 + \int_0^\infty d\varepsilon \, \{\frac{\partial}{\partial E} f(E+\mu) + \frac{\partial}{\partial E} f(E-\mu)\}\right\} \tag{4.92}$$

where the normalization factor λ_{Lo} is defined as

$$\lambda_{Lo}^{-2} = \frac{8\pi e^2 v_f^2 N(\varepsilon_f)}{3\hbar\sigma^2} \tag{4.93}$$

where v_f denotes the Fermi velocity and $N(\varepsilon_f)$ the density of states at the Fermi surface.

As with the preceding calculations the effect of the temperature dependent coupling may be realized through the scaling of a two parameter function. Specifically we have

$$\frac{\lambda_L^{-2}(T;H)}{\lambda_{Lo}^{-2}} = \mathcal{L}^{-2}(t/s(t;H);\bar{\mu}/s(t;H)) \ , \tag{4.94}$$

where

$$\mathcal{L}^{-2}(t;\bar{\mu}) = 1 - \Phi_2\left\{\frac{\pi e^{-\gamma}}{t}\vartheta(t;\bar{\mu});\ \frac{\pi e^{-\gamma}}{t}\bar{\mu}\right\} \tag{4.95}$$

with

$$\Phi_2(x;y) = \frac{x}{4}\,\mathrm{Re}\int_{-\infty}^{+\infty} dz\,\frac{z}{\sqrt{z^2-1}}\cosh^{-2}\frac{1}{2}(xz+y) \ . \tag{4.96}$$

Here the integrand in Φ_2 is defined in a manner analogous to Φ_1.

The evaluation of the non-local kernel $C(-i\nabla)$ is somewhat complicated since, as pointed out earlier, it involves the calculation of the photon self-energy including the effect of the collective mode or phason[1,7,26]. While the calculation up to one loop, in the manner presented in[7,26], is possible using similar approximations to those introduced in the calculation of the renormalized gap and condensation energy the resultant expression is of such a complicated form as to be of little practical value. However the results of the calculation shows that, while the effect of the spin fluctuations included in the coupling constant renormalization may be realized by means of a simple scaling of the non-magnetic result, in a manner entirely analogous to the procedure given for the calculation of the renormalized gap Δ and the condensation energy H_c^2, complications arise due to the presence of the effective splitting parameter μ in the thermal distribution functions. However since the thermal distribution functions do not contribute at zero temperature, the result for the non-local kernel $C(-i\nabla)$ at zero temperature may be obtained simply by scaling the results for the non-magnetic case presented in ref. [26] in a manner entirely analogous to the scaling presented in the calculation of the gap and the condensation energy.

However, since we expect the effect of the d-f interaction to be most pronounced at lower temperatures, it is reasonable to suppose that such complications may be avoided simply by extending the scaling argument at zero temperature to finite temperature. In essence we are assuming that the correlation length ξ is related to the inverse of the superconducting gap Δ, which is at least qualitatively correct. Therefore based on the results of ref. [26], we can write

$$C(\vec{k}) = \exp - \nu\{|\vec{k}|\xi(T;H)\}^{\eta} \quad , \tag{4.97}$$

where

$$\nu = -0.4527\ g(T;H)N(0) + 0.559 \tag{4.98}$$

$$\eta = -0.7857\ g(T;H)N(0) + 2.207 \tag{4.99}$$

and

$$\xi(T;H) \simeq \frac{v_F}{\pi\Delta(T;H)} \quad . \tag{4.100}$$

We now turn our attention to the evaluation of the magnetization $\vec{M}$, the splitting parameter $\vec{\mu}$ and the transverse and longitudinal susceptibilities in the case of a finite field. The magnetization $\vec{M}$ is easily calculated in the mean field approximation as

$$<\vec{M}> = g_J\mu_B JNB_J\{\beta g_J\mu_B|\vec{H}_{MF}|\} \quad , \tag{4.101}$$

where J is the spin of the localized spin, g_J the Lande g factor, N the density of magnetic ions, B_J the Brillouin function and $\vec{H}_{MF}$ is given by

$$\vec{H}_{MF} = <\vec{B}> + \gamma_o(-i\nabla)<\vec{M}> + I<\psi^{\dagger}\vec{\sigma}\psi> \quad . \tag{4.102}$$

The thermal average of the electron spin density may be obtained, even in the case of finite polarization, from Eq. (4.14)

$$<\psi^{\dagger}(x)\vec{\sigma}\psi(x)> = \int d^4y \; \chi_\sigma(x-y)(I<\vec{M}(y)> - \mu_B<\vec{B}(y)>) \quad , \tag{4.103}$$

where $\chi_\sigma(x-y)$ is a 3×3 matrix given by Eq. (4.15)

$$\chi_\sigma(x-y)_{ij} = \frac{i}{2}\{<R[\sum_k \sigma_k(x)\sigma_k(y)]>\delta_{ij} - <R[\sigma_j(x)\sigma_i(y)]>\} \quad , \tag{4.104}$$

where R[ ] denotes the retarded product. Since the quantities $<\vec{M}>$ and $<\vec{B}>$ are independent of time, then Eq.(4.103) reduces to

$$<\psi^{\dagger}\vec{\sigma}\psi> = \chi_\sigma\{I<\vec{M}> - \mu_B<\vec{B}>\} \quad , \tag{4.105}$$

where χ_σ denotes the static spin-susceptibility of the electron calculated in the presence of the finite field. The expression for the mean field, Eq. (4.102) may then be written as

$$\vec{H}_{MF} = \{1 - I\chi_\sigma\mu_B\}<\vec{B}> + \{\gamma_o(-i\nabla) + I^2\chi_\sigma\}<\vec{M}> \quad . \tag{4.106}$$

Since $\langle\vec{B}\rangle$, $\langle\vec{H}\rangle$, $\langle\vec{M}\rangle$ and $\langle\psi^\dagger\vec{\sigma}\psi\rangle$ are related through

$$\langle\vec{B}\rangle = \langle\vec{H}\rangle + 4\pi\{\langle\vec{M}\rangle - \mu_B\langle\psi^\dagger\vec{\sigma}\psi\rangle\} \quad , \tag{4.107}$$

the expression for the mean field may be written in terms of $\vec{H}$ and $\vec{M}$ as

$$\vec{H}_{MF} = \frac{1 - \mu_B I \chi_\sigma}{1 - 4\pi\mu_B^2\chi_\sigma}\langle\vec{H}\rangle + \{\gamma_0 + I^2\chi_\sigma + \frac{4\pi(1 - \mu_B I\chi_\sigma)^2}{1 - 4\pi\mu_B^2\chi_\sigma}\}\langle\vec{M}\rangle \quad . \tag{4.108}$$

If we neglect the paramagnetic interaction, then the above expression simplifies to give

$$\vec{H}_{MF} = \langle\vec{H}\rangle + \{\gamma_0 + I^2\chi_\sigma + 4\pi\} \langle\vec{M}\rangle \quad . \tag{4.109}$$

In the case of $ErRh_4B_4$ we assume that Eq.(4.101) together with Eq. (4.109) determine the magnetization as a function of the field $\langle\vec{H}\rangle$ once χ_σ is specified.

To evaluate χ_σ we will assume that the difference between χ_σ calculated in the superconducting state and the normal state is insignificant and may therefore be neglected. This assumption is based on the results of the Knight shift measurements and is generally attributed to the effects of the spin orbit scattering. Furthermore when μ is small compared to ω_D the variation in the density of states may be ignored and hence

$$\chi_\sigma^S \simeq \chi_\sigma^N \simeq \chi_\sigma^N\Big|_{\mu=0} \quad . \tag{4.110}$$

The calculation for the susceptibility of the localized spins is somewhat more complicated and is best achieved by means of a linear response type argument. To this end we modify the original Hamiltonian by including a small perturbing field $\delta h_{ext}(x)$ acting on the localized spins. This will produce a change in the fields $<\vec{B}>$, $<\vec{M}>$ and $<\psi^{\dagger}\vec{\sigma}\psi>$, which we denote by $\delta\vec{b}(x)$, $\delta\vec{m}(x)$ and $\delta\vec{\sigma}(x)$ respectively. The quantities $\delta\vec{b}$, $\delta\vec{m}$ and $\delta\vec{\sigma}$ are not however independent but are instead related through the following equations;

$$\{-\nabla^2 + \lambda_L^{-2}C(-i\vec{\nabla})\}\delta\vec{b} = -4\pi\nabla^2\{\delta\vec{m} - \mu_B\delta\vec{\sigma}\} \quad , \tag{4.111}$$

$$\delta\vec{m}_3 = \frac{C}{T}\alpha_J(\delta\vec{h}_{MF}\cdot\vec{e}_3) \quad , \tag{4.112}$$

$$\delta\vec{m} \wedge \vec{H}_{MF} = <\vec{M}> \wedge \delta\vec{h}_{MF} \tag{4.113}$$

and

$$\delta\vec{\sigma} = \chi_\sigma\{I\delta\vec{m} - \mu_B\delta\vec{b}\} \quad , \tag{4.114}$$

where C denotes the Curie constant, $\delta\vec{h}_{MF}$ denotes the change in the mean field induced by the external field $\delta\vec{h}_{ext}(x)$ given by

$$\delta\vec{h}_{MF} = \delta\vec{b} + \gamma_0(-i\nabla)\delta\vec{m} + I\delta\vec{\sigma} + \delta\vec{h}_{ext} \tag{4.115}$$

and where α_J is given by

$$\alpha_J = \frac{3J}{J+1} B_J'\{\frac{g_J\mu_B J}{k_B T}|\vec{H}_{MF}|\} \quad . \tag{4.116}$$

From Eqs. (4.111) and Eq. (4.114), $\delta\vec{b}$ and $\delta\vec{\sigma}$ may be eliminated from Eq. (4.115) to give

$$\delta\vec{h}_{MF} = \tilde{\gamma}(-i\nabla)\delta\vec{m} + \delta\vec{h}_{ext} \quad , \tag{4.117}$$

with $\tilde{\gamma}$ given by

$$\tilde{\gamma}(\vec{k}) = \gamma(\vec{k}) - 4\pi\frac{(1-\mu_B I\chi_\sigma)^2}{(1-\mu_B^2 4\pi\chi_\sigma)}\frac{C(\vec{k})}{(1-4\pi\mu_B^2\chi_\sigma)\lambda_L^2|\vec{k}|^2 + C(\vec{k})} \quad , \tag{4.118}$$

and $\gamma(\vec{k})$ given by

$$\gamma(\vec{k}) = \gamma_o(\vec{k}) + I^2\chi_\sigma + 4\pi \frac{(1-\mu_B I\chi_\sigma)^2}{1-4\pi\mu_B^2\chi_\sigma} \quad . \tag{4.119}$$

The second term in Eq. (4.118) corresponds to the effect on the effective coupling arising from the persistent current. Thus we see that the shielding of the localized spins by the persistent current is contained in our calculation. Equation (4.117) together with Eq. (4.112) and Eq. (4.113) yield

$$\delta\vec{m} = \chi(-i\nabla)\delta\vec{h}_{ext} \quad , \tag{4.120}$$

with

$$\chi^{-1}(\vec{k}) = \begin{Bmatrix} \frac{H_{MF}}{\langle M\rangle} & & \\ & \frac{H_{MF}}{\langle M\rangle} & \\ & & \frac{T}{\alpha_J C} \end{Bmatrix} - \gamma(\vec{k}) \quad , \tag{4.121}$$

which may be inverted to give

$$\chi_{33}(\vec{k}) = \frac{C\alpha_J}{T - \alpha_J C\gamma_{33}(\vec{k})} \tag{4.122}$$

and

$$\chi_{ii}(\vec{k}) = \frac{1}{\frac{H_{MF}}{\langle M\rangle} - \gamma_{ii}(\vec{k})} \quad \text{for} \quad i = 1,2 \ . \tag{4.123}$$

Parameterizing $\gamma_{ii}(k)$ as

$$\gamma_{ii}(\vec{k}) = \frac{T_m^{(i)}}{C} - \frac{D}{C}|\vec{k}|^2 \quad , \tag{4.124}$$

we obtain

$$\chi_{33}(\vec{k}) = \frac{C}{\frac{T}{\alpha_J} - T_m^{(3)} + D|\vec{k}|^2 + 4\pi C \frac{1 - \mu_B I \chi_\sigma}{1 - 4\pi\mu_B^2\chi_\sigma} \frac{C(\vec{k})}{(1 - 4\pi\mu_B^2\chi_\sigma)|\vec{k}|^2\lambda_L^2 + C(\vec{k})}} \tag{4.125}$$

and

$$\chi_{ii}(\vec{k}) = \frac{C}{\frac{1-\mu_B I\chi_\sigma}{1-4\pi\mu_B^2\chi_\sigma} \frac{C\langle H_3\rangle}{\langle M_3\rangle} + \{T_m^{(3)} - T_m^{(i)}\} + D|\vec{k}|^2 + 4\pi C \frac{1 - \mu_B I\chi_\sigma}{1-4\pi\mu_B^2\chi_\sigma} \frac{C(\vec{k})}{(1-4\pi\mu_B^2\chi_\sigma)|\vec{k}|^2\lambda_L^2 + C(\vec{k})}}$$

for $i = 1,2$. (4.126)

When we neglect the paramagnetic contribution the analysis simplifies somewhat and we obtain

$$\chi_{33}(\vec{k}) \doteq \frac{C}{\frac{T}{\alpha_J} - T_m^{(3)} - D|\vec{k}|^2 - 4\pi C \frac{C(\vec{k})}{|\vec{k}|^2\lambda_L^2 + C(\vec{k})}} \tag{4.127}$$

and

$$\chi_{ii}(\vec{k}) = \frac{C}{\frac{C\langle H_3\rangle}{\langle M_3\rangle} + \{T_m^{(3)} - T_m^{(i)}\} + D|\vec{k}|^2 + 4\pi C \frac{C(\vec{k})}{|\vec{k}|^2\lambda_L^2 + C(\vec{k})}} \quad \text{for } i = 1,2 \tag{4.128}$$

respectively.

Equations (4.125) and (4.126) together with the limiting cases Eq. (4.127) and (4.128) illustrates how the effect of the finite field modifies the calculation of the spin susceptibility.

The expressions given by Eqs. (4.127) and (4.128) represent the generalization of the result of ref. [14] to the finite field case. The last term in the denominator represents the effect of the shielding of the ~~l~~ocalized magnetic moments by the persistent current. As was shown in ref. [14], in the zero field limit, the susceptibility given by Eqs.

(4.127) and (4.128) will diverge at some finite momentum $\vec{k} = \vec{Q}$ at some temperature $T_p < T_m$, giving rise to the appearance of the spin spiral or sinusoidal phase. The divergence at $T = T_p$ results in an infrared divergence in the calculation of the coupling constant and the quenching of the superconductivity at some temperature $T > T_p$. In order to avoid such a catastrophe, we modify our expression for the function $\gamma(k)$ given in Eq. (4.124) to include the effect of the anisotropy in the momentum dependence. We therefore replace Eq. (4.124) with

$$\gamma_{ii}(\vec{k}) = \frac{T_m^{(i)}}{C} - \frac{D}{C}\{1 + \frac{3}{2}\alpha(1 - \cos^2\theta)\}|\vec{k}|^2 , \qquad (4.129)$$

where θ denotes the angle between the vector $\vec{Q}$ and the momentum $\vec{k}$. Equations (4.127) and (4.128) then become

$$\chi_{33}(\vec{k}) = \frac{C}{\frac{T}{\alpha_J} - T_m^{(3)} + D\{1 + \frac{3}{2}\alpha(1 - \cos^2\theta)\}|\vec{k}|^2 + 4\pi C \frac{C(\vec{k})}{|\vec{k}|^2\lambda_L^2 + C(\vec{k})}} \qquad (4.130)$$

$$\chi_{ii}(\vec{k}) = \frac{C}{\frac{C\langle H_3\rangle}{\langle M_3\rangle} + \{T_m^{(3)} - T_m^{(i)}\} + D\{1 + \frac{3}{2}\alpha(1 - \cos^2\theta)\}|\vec{k}|^2 + 4\pi C \frac{C(\vec{k})}{|\vec{k}|^2\lambda_L^2 + C(\vec{k})}} \qquad (4.131)$$

for $i = 1,2$, respectively.

With the finite field susceptibilities given by Eqs. (4.130) and (4.131), we can calculate the coupling constant $g(T;h)$ using Eq. (4.49) in the London limit (i.e. $C(k) = 1$) as

$$g(T;h) = \frac{1}{4k_F^2}\int_0^{4k_F^2} d\ell^2 \int_0^1 d\cos\theta \Bigg[V - \tilde{I}^2 \Bigg\{ \frac{C}{\frac{T}{\alpha_J} - T_m^{(3)} + D(1 + \alpha\frac{3}{2}(1 - \cos^2\theta))\ell^2 + \frac{4\pi C}{\ell^2\lambda_L^2 + 1}} \Bigg\}$$
$$- \sum_{i=1}^{2} \tilde{I}^2 \Bigg\{ \frac{C}{\frac{C\langle H_3\rangle}{\langle M_3\rangle} + \{T_m^{(3)} - T_m^{(i)}\} + D(1 + \frac{3}{2}\alpha(1 - \cos^2\theta))\ell^2 + \frac{4\pi C}{\ell^2\lambda_L^2 + 1}} \Bigg\} \Bigg] \qquad (4.132)$$

The presence of the anisotropy term ensures that for $T \geq T_p$, the coupling constant $g(T;h) > 0$ for a certain range of parameters and hence that Δ remains finite at $T = T_p$. Furthermore calculations show that for $T > T_p$ little error results in the calculation of the coupling constant if the anisotropy term $\frac{3}{2}\alpha(1 - \cos^2\theta)$ is replaced by its angular average, i.e.

$$\frac{3}{2}\,\alpha\,\{1 - \cos^2\theta\} \approx \alpha\,, \tag{4.133}$$

and thus Eq. (4.132) reduces to give

$$g(T;H) = \frac{1}{4k_F^2}\int_0^{4k_F^2} d\ell^2 \left[V - I^2 \left\{ \frac{C}{\frac{T}{\alpha_J} - T_m^{(3)} + D(1+\alpha)\ell^2 + \frac{4\pi C}{\ell^2\lambda_L^2 + 1}} \right.\right.$$

$$\left.\left. - \sum_i \tilde{I}^2 \frac{C}{\frac{C\langle H_3\rangle}{\langle M_3\rangle} + T_m^{(3)} - T_m^{(i)} + D(1+\alpha)\ell^2 + \frac{4\pi C}{\ell^2\lambda_L^2 + 1}} \right\} \right] . \tag{4.134}$$

This may be integrated to give an analytical expression for the effective coupling constant at finite field as

$$g(T;H) = V - \tilde{I}^2 \left\{ G_3\,\{\varepsilon_{||}^{(3)}(t;H)\} + \sum_{i=1,2} G_i\{\varepsilon_{\perp}^{(i)}(t;H)\} \right\} , \tag{4.135}$$

where

$$G_{(i)}(\varepsilon) = \frac{C^{(i)}}{8\pi d_f^{(i)}(1+\alpha)} \left\{ \log\left(\frac{d_f^{(i)2}(1+\alpha) + d_f^{(i)}(\varepsilon + d^{(i)}(1+\alpha)) + d^{(i)}(\varepsilon + C^{(i)})}{d^{(i)}(\varepsilon + C^{(i)})} \right) \right.$$

$$\left. + \,(d^{(i)}(1+\alpha) - \varepsilon)\, I^{(i)}(\varepsilon) \right\} \tag{4.136}$$

with

$$I^{(i)}(\varepsilon) = \frac{1}{\sqrt{\Omega_{(i)}(\varepsilon)}} \log\left\{ \frac{2d_f^{(i)}(1+\alpha) + (d^{(i)}(1+\alpha)+\varepsilon) - \sqrt{\Omega_{(i)}(\varepsilon)}}{2d_f^{(i)}(1+\alpha) + (d^{(i)}(1+\alpha)+\varepsilon) + \sqrt{\Omega_{(i)}(\varepsilon)}}\; \frac{d^{(i)}(1+\alpha)+\varepsilon+\sqrt{\Omega_{(i)}(\varepsilon)}}{d^{(i)}(1+\alpha)+\varepsilon-\sqrt{\Omega_{(i)}(\varepsilon)}} \right\}$$

for $\Omega_{(i)}(\varepsilon) > 0$ (4.137)

and

$$I^{(i)}(\varepsilon) = \frac{1}{\sqrt{-\Omega_{(i)}(\varepsilon)}} \left\{ \tan^{-1} \frac{2d_F^{(i)}(1+\alpha)+d^{(i)}(1+\alpha)+\varepsilon}{\sqrt{-\Omega_{(i)}(\varepsilon)}} - \tan^{-1} \frac{\varepsilon+d^{(i)}(1+\alpha)}{\sqrt{-\Omega_{(i)}(\varepsilon)}} \right\}$$

$$\text{for } \Omega_{(i)}(\varepsilon) < 0 \qquad (4.138)$$

with

$$\Omega_{(i)}(\varepsilon) = (\varepsilon+d^{(i)}(1+\alpha)+2\sqrt{d^{(i)}(1+\alpha)C^{(i)}})(\varepsilon-d^{(i)}(1+\alpha)+\sqrt{d^{(i)}(1+\alpha)C^{(i)}}) \; . \qquad (4.139)$$

The parameters $d^{(i)}$, $d_F^{(i)}$ and $C^{(i)}$ are defined as

$$C^{(i)} = \frac{4\pi C}{T_m^{(i)}} \quad ; \quad d^{(i)} = \frac{D}{T_m^{(i)}\lambda_L^2} \; ; \quad d_F^{(i)} = \frac{4Dk_F^2}{T_m^{(i)}} \; ,$$

and $\varepsilon_\perp^{(i)}(t;H)$ and $\varepsilon_{||}^{(3)}(t;H)$ are given by

$$\varepsilon_{||}^{(3)}(t;H) = \frac{t}{t_m^{(3)}\alpha_J} - 1 \qquad (4.140)$$

and

$$\varepsilon_\perp^{(i)}(t;H) = \frac{C}{T_m^{(i)}} \frac{H}{\langle M_3 \rangle} - 1 + T_m^{(3)} - T_m^{(i)} \; . \qquad (4.141)$$

We rewrite $g(t;H)$ in terms of the renormalized coupling constant $g(1;0)$ which is defined at $T = T_c$ and $H = 0$. Equation (4.135) then becomes

$$g(T;H) = g(1;0)\left\{ 1 - \frac{I^2}{g(1)} \{G_{(3)}\{\varepsilon_{||}^{(3)}(t;H)\} - G_{(3)}\{\varepsilon_{||}^{(3)}(1;H=0)\}\} \right.$$
$$\left. - \sum_{i=1,2} \frac{\tilde{I}^2}{g(1)} \left\{ \{G_{(i)}\{\varepsilon_\perp^{(i)}(t;H)\} - G_{(i)}\{\varepsilon_\perp^{(i)}(1;H=0)\}\} \right\} \right\}. \qquad (4.142)$$

We note that

$$\varepsilon_{||}^{(i)}(t;0) = \varepsilon_\perp^{(i)}(t;0) \equiv \varepsilon^{(i)}(t) = \{ \frac{t}{t_m^{(i)}} - 1\} \quad : \qquad (4.143)$$

The renormalized coupling constant g(1;0) is given by

$$g(1;0) = V - \tilde{I}^2 \sum_i G_{(i)}\{\varepsilon^{(i)}(1)\} , \tag{4.144}$$

where

$$G_{(i)}\{\varepsilon^{(i)}(1)\} = \frac{C}{4\pi d_F} \log \left\{ \frac{\xi^{(i)}(1) + d_F^{(i)}(1+\alpha)}{\varepsilon^{(i)}(1)} \right\} . \tag{4.145}$$

Here we used the fact that $\lambda_L \to \infty$ and at $T = T_c$.

With the effective coupling constant given by Eq. (4.142), the scale factor s(t;H) may be computed from Eq. (4.59) and the superconducting quantities calculated from the scaling laws presented earlier. In the discussion so far we have shown in some detail how the effect of the d-f interaction on the superconducting properties such as Δ, λ_L and H_c may be calculated. In particular it has been shown how the effect of the spin fluctuations may be realized through a simple rescaling of certain two parameter functions. It is perhaps worthwhile summarizing the basic results before going on to present some numerical results which serve to illustrate the effects of the d-f interaction.

From Eq. (4.58) the renormalized gap was found to be given by

$$\frac{\Delta(T;H)}{\Delta_0} = s(t;H)\mathscr{D}(t/s(t;H);\bar{\mu}/s(t;H)) . \tag{4.146}$$

From Eq. (4.78) the field dependent condensation energy was found to be given by

$$\frac{H_c(T;H)}{H_{co}} = s(t;H)\mathscr{H}(t/s(t;H);\bar{\mu}/s(t;H)) . \tag{4.147}$$

From Eq. (4.94) the London penetration depth λ_L was found to be given by

$$\frac{\lambda_L(T;H)}{\lambda_{Lo}} = \mathscr{L}(t/s(t;H);\bar{\mu}/s(t;H)) . \tag{4.148}$$

The normalization parameters Δ_o, H_{co} and λ_{Lo} are given by

$$\Delta_o = 2\omega_D \exp \frac{-1}{g(T_c;0)N(0)} , \tag{4.149}$$

$$H_{co}^2 = 4\pi\Delta_o^2 N(0) \tag{4.150}$$

and

$$\lambda_{Lo}^{-2} = \frac{8\pi}{3c^2} e^2 v_F^2 N(0) . \tag{4.151}$$

We wish to emphasize that the above normalization constants do not correspond to the observable gap and critical field at $T = 0^oK$. They are instead related simply to the quantities for non-magnetic superconductors with similar structure.

The spin splitting parameter $\bar{\mu}$ is also a function of t and H and is given by

$$\bar{\mu}(t;H) = \frac{\tilde{I}\langle M_3(t;H)\rangle}{\Delta_o} , \tag{4.152}$$

where $M_3(t;H)$ is determined from Eqs. (4.101) and (4.109).

The two parameter functions $\mathcal{D}(t;\mu)$, $\mathcal{H}(t;\mu)$ and $\mathcal{L}(t;\mu)$ are given by

$$\log \mathcal{D}\{t;\bar{\mu}\} = -\Phi_1\left\{\frac{\pi e^{-\gamma}}{t}\mathcal{D}(t;\bar{\mu});\ \frac{\pi e^{-\gamma}}{t}\bar{\mu}\right\} \tag{4.153}$$

$$\mathcal{H}^2(t;\bar{\mu}) = \mathcal{D}^2(t;\bar{\mu}) - \frac{2\pi^2}{3}\left\{\frac{t^2}{\pi e^{-\gamma}} - \frac{3\mathcal{D}^2(t;\bar{\mu})}{\pi^2}\Phi_3\left\{\frac{\pi e^{-\gamma}}{t}\mathcal{D}(t;\bar{\mu});\ \frac{\pi e^{-\gamma}}{t}\bar{\mu}\right\}\right.$$
$$\left. - \frac{3\bar{\mu}\mathcal{D}(t;\bar{\mu})}{\pi^2}\Phi_4\left\{\frac{\pi e^{-\gamma}}{t}\mathcal{D}(t;\bar{\mu});\ \frac{\pi e^{-\gamma}}{t}\bar{\mu}\right\}\right\} \tag{4.154}$$

and

$$\mathcal{L}^{-2}(t;\bar{\mu}) = 1 - \Phi_2\left\{\frac{\pi e^{-\gamma}}{t}\mathcal{D}(t;\bar{\mu});\ \frac{\pi e^{-\gamma}}{t}\bar{\mu}\right\} , \tag{4.155}$$

where the functions $\{\Phi_i\}$ may be written as

$$\phi_i(x;y) = \frac{x}{4} \operatorname{Re} \int_{-\infty}^{+\infty} dz \; T_i(z) \cosh^{-2} \frac{1}{2}\{xz + y\} \quad . \tag{4.156}$$

The functions $\{T_i(z)\}$ are complex functions and all are defined on the Rieman sheet with the branch line running between $z = \pm 1$ shown in figure 2 with

$$\lim_{\operatorname{Im} z \to 0} T_i(z) = T_i(\operatorname{Re} z) \qquad \text{for} \qquad \operatorname{Re} z > 1 \ , \tag{4.157}$$

where

$$T_1(z) = \ln\{z + \sqrt{z^2 - 1}\} \tag{4.158}$$

$$T_2(z) = \frac{z}{\sqrt{z^2 - 1}} \tag{4.159}$$

$$T_3(z) = z\sqrt{z^2 - 1} \tag{4.160}$$

$$T_4(z) = \sqrt{z^2 - 1} \quad . \tag{4.161}$$

The scale factor $s(t;H)$ is given by

$$s(t;H) = \exp\left\{\frac{1}{g(1;0)N(0)} - \frac{1}{g(t;H)N(0)}\right\} \tag{4.162}$$

where $g(t;H)$ is the effective coupling constant given by Eq. (4.142).

We now wish to present the results of certain numerical calculations illustrating the temperature and field dependence of these fundamental physical quantities. We first consider the limit where $H = 0$. In this limit the functions $\mathcal{D}$, $\mathcal{H}$ and $\mathcal{L}$ reduce to those obtained in the familiar BCS theory. Thus we find that the properties of the Meissner state (in which the field $\vec{B}$ is excluded) may be obtained from the BCS results by means of a simple scaling law. In order to illustrate the effect of the spin fluctuations on the effective coupling constant figure 3 shows the temperature dependence ($t = t/t_c$) of the effective coupling constant for various values of the field h ($h = H/\phi\lambda_{Lo}^{-2}$). The parameters used in the calculation are given in table 4 and are chosen in order to emphasize the effect of the spin fluctuations.

In figures 4, 5 and 6 we present the temperature dependence of the gap, the condensation energy and the London penetration depth. Here the parameters used are those shown in table 2 and are felt to be appropriate to the case of $ErRh_4B_4$. (A detailed discussion of the particular choice of the parameters will be given together with a detailed analysis of the mixed state in $ErRh_4B_4$ in the next section.) These results clearly show the suppression of the superconductivity at low temperatures, due to the increase in the strength of the localized spin fluctuations.

Estimates of the condensation energy have been made in the case of polycrystalline $ErRh_4B_4$ samples from both bulk and thin film measurements. While these results do indicate a substantial deviation from the BCS result at low temperature, certain difficulties inherent in the various measurements prevent them from providing us with any precise conclusions regarding the temperature dependence of the condensation energy. More recent measurements based on the magnetization curves of single crystal $ErRh_4B_4$ [122] have been made and give more reliable results although the uncertainties arising from pinning effects are still considerable. The single crystal results are in reasonable agreement with the curve shown in figure 5 if we choose a value of $H_{co} \simeq 1.4$ KG a value consistent with similar measurements on $LuRh_4B_4$ obtained from specific heat measurements which give $H_{co} \simeq 1.85$ KG.[130] An accurate determination of the condensation energy for various temperatures would be extremely useful in that it would provide information regarding the strength and the role of the spin fluctuations in modifying the superconducting state as we approach the co-existence regime at $T = T_p$.

The temperature dependence of the superconducting gap also shows a reduction from the BCS value at low temperature, in particular we find that $2\Delta_{max}/k_BT_c$ has a value of 3.03 in contrast to the BCS value of 3.52. Since the effective coupling constant g(T) is always smaller than $g(T_c)$, because of the suppression due to the spin fluctuation, $\Delta(t)$ is always less than $\Delta_{BCS}(t)$.

Tunneling measurements have been performed for both polycrystalline[120] and single crystal $ErRh_4B_4$.[121] The results show that the value of the superconducting gap inferred from the dI/dV vs V curve does in fact differ markedly from the predictions of the BCS theory, in particular it is found to be flat with respect to temperature at low temperature. However, the observed ratio $2\Delta_{max}/k_BT_c$ appears to be in the region 3.8 to 4.2 in contrast to the results presented here.

The London penetration depth shown in figure 6 does not show a dramatic change. While it is the case that the London penetration depth may be obtained from surface impedance measurements, the exact nature of the relationship is complicated by the possible appearance of surface magnetization states[110,111]. A more detailed discussion of the penetration depth is presented in Appendix D.

We can also discuss the effect of an internal field on the superconducting quantities, Δ, H_c and λ_L. From the preceding analysis we see that the presence of an internal field H will lead to two quite distinct effects; namely

(1) it will suppress the spin fluctuation, leading to an increase in the effective coupling constant g(T;H) and therefore enhancing the superconductivity,

(2) it will polarize the localized spins which will result in a finite value for the spin splitting parameter μ which tends to suppress the superconductivity.

Thus we see that the application of an internal magnetic field may result in an increase or decrease in the superconducting quantities depending on which mechanism dominates.

In figures 7, 8 and 9 we present graphs showing the temperature dependence of the gap, the field dependent condensation energy and the London penetration depth in the presence of an internal field. It would appear from the graphs that Δ, H_c^2 and λ_L are in fact insensitive to the internal field until a particular temperature is reached, where there is a rapid decrease as the temperature is lowered further. This arises from the increase in the spin splitting parameter μ due to the increased ordering of the magnetic ions.

Figures 10, 11 and 12 present graphs showing the field dependence of the gap; the field dependent condensation energy and the London penetration depth for various values of the reduced temperature t. Again it would appear that Δ, H_c^2 and λ_L are insensitive to the internal field h until some critical value is reached after which there is a rapid decrease as the field is increased. Again this may be attributed to the increase in μ as the field is increased.

A closer examination of the numerical results however reveals that as h is increased for a given temperature, the field dependent condensation energy is seen first to rise, due to the increase in the effective coupling constant g(T;H), before decreasing rapidly at higher values of the field due to the induced effective field μ. While the actual increase is very small for the present choice of parameters (see table 5) and is not in fact discernable from the graph presented in figure 11, such an increase at low field values may be important when one comes to consider the nature of the transition around the lower critical field H_{c1} in a type II superconductor.

To summarize, there are several results which are of interest here. First we find that, in the effective coupling constant approximation, the effect of the localized spin fluctuations and the spin splitting of the conduction electrons, arising from the d-f interaction, on the superconducting gap factorize. As a result the gap equation can be expressed in terms of a certain two parameter function by means of a simple scaling law involving the temperature and field dependent coupling constant g(T;H). A similar result was also obtained for the field dependent critical field and the London penetration depth. These results provide a somewhat straightforward method, whereby the effect of the localized magnetic moments and the induction field on the superconducting properties of the conduction electrons may be considered. In particular, the method may be applied to consider the properites of the Meissner state. In the Meissner state (i.e. $\mu = 0$) the temperature dependence of the superconducting gap, the condensation energy and the London penetration depth may be obtained from the BCS result by means of a simple scaling rule. Such quantities are in fact experimentally accessible and should provide us with information regarding the nature of the localized spin fluctuations.

Secondly it is both interesting and somewhat surprising that the resultant expression for the free energy given in Eq. (4.91) has the same form as that present in ref. [28], although the expression for the various terms involved is somewhat more complicated due to the d-f and the paramagnetic interactions. The close analogy that exists between the two expressions means that the results presented in this section can be used to extend work presented in ref. [28] to include the effects of the d-f interaction on the magnetic properties of the mixed state in ferromagnetic superconductors in a perfectly straightforward manner.

The third rather interesting feature is the effect of the finite internal field H on the superconducting quantities. Specifically we see that the reduction in the localized spin fluctuation and the increase in the spin splitting parameter μ with the application of an internal field H tends to enhance and suppress, respectively, the superconducting nature of the conduction electrons. The resultant competition between these two mechanisms manifests itself in the slight increase in the field dependent condensation energy $\frac{H_{co}^2(H;T)}{8\pi}$ with increasing H, for low values of the field proceeded by the rapid decrease for high values of H, shown in figure 11. This suggests that the response of the localized spin fluctuations to an applied field will be of importance in determining the behaviour of the system as it makes the transition from the Meissner state to the mixed state, at H_{c1}, while the polarization effect will be of importance at higher field values in particular as the system makes the transition from the mixed state to the normal state at H_{c2}.

In conclusion therefore we have presented a method whereby the effects of the d-f and the paramagnetic interactions together with the electromagnetic interaction may be included in the analysis of magnetic superconductors.

The results obtained show several interesting and important features and allow for the extension of previous work on the mixed state to include both the d-f as well as the electromagnetic interactions. The application of the formalism presented here, to the analysis of the mixed state in $ErRh_4B_4$ is presented in the next section.

4.3 An Analysis of the Mixed State in $ErRh_4B_4$

In this section we apply the formalism developed in the previous section 4.2 to an analysis of the mixed state in $ErRh_4B_4$. In particular we wish to compare the results of our analysis with the results of the recent measurements on single crystal $ErRh_4B_4$.[10,11] Due to the quite pronounced anisotropy in the spin-spin interaction, arising from the effects of the crystalline field, the magnetic properties differ significantly if measured relative to the easy axis (a-axis) or the hard axis (c-axis). For example when the applied field lies along the hard axis, the polarization of the magnetic ions in the mixed state is very small, this is reflected in the fact that the observed magnetization curves and the upper critical field curve are very similar to those observed in non-magnetic superconductors, with a peak value in the upper critical field curve of around 10 KG.[10] The upper critical field measured relative to the easy axis on the other hand, is markedly different from the hard axis measurements, with a peak value of around 2 KG at around $T \approx 5.5°K$.[10] Furthermore the magnetization curves measured with respect to the easy axis show that the transition from the mixed state to the normal state becomes first order at around $T \approx 3.5°K$. Both effects may be attributed to the polarization of the rare earth spin induced by the applied field, since the easy axis susceptibility is much larger than the hard axis susceptibility. The detailed nature of these measurements together with the effect of the anisotropy of the spin system provide an excellent testing ground for various models and treatments of the mixed state in ferromagnetic superconductors.

The aim of the work presented in this section is to provide a detailed analysis of $ErRh_4B_4$ and to demonstrate to what extent the single crystal measurements may be accounted for within the formalism presented in the previous section. In this we assume that the superconducting properties of the system are to a good approximation isotropic and hence that the difference between magnetic properties of the hard and easy axes, may be attributed entirely to the observed anisotropy of the spin system.

A number of important results emerge from this analysis. First, the critical field curves obtained are in good agreement with both the hard and easy axis curves presented in ref. [10] and secondly the resultant magnetization curves exhibit a first order transition on going from the mixed state to the normal state at H_{c2} as observed[11]. These results are obtained using a choice of parameters consistent with a large number of other measurements on $ErRh_4B_4$. In addition to this, a comparison between the results obtained with and without the effect of the scattering of the electrons by the localized spin fluctuations, is presented. The result of this comparison shows quite clearly that the peculiar magnetic properties of $ErRh_4B_4$ are due almost entirely to the effect of the Zeeman splitting of the electrons arising from the effective field induced by the d-f interaction through the polarization of the localized spins.

Two other points are perhaps worth noting before presenting the details of the analysis. The first is that it is only since the single crystal measurements have become available that such a detailed treatment of ferromagnetic superconductors has been possible, since many of the properties alluded to above cannot be observed in polycrystalline samples due to the averaging over the hard and easy axis properties. Secondly an important aspect of the work presented here is that it allows one to treat, in a unified manner, the entire temperature domain above T_p, the co-existence temperature, including the region wherein the transition from the mixed state to the normal state, at H_{c2}, is first order.

In the mixed state the magnetic field penetrates the superconducting system in the form of vortices. As explained in the previous section an individual vortex corresponds to the presence of a topological line singularity in the phase of the order parameter f(x). In the case of a vortex array the phase f(x) is given by Eq. (4.25)

$$f(x) = \sum_i \frac{1}{2}\, \theta[\vec{x}-\vec{\xi}_i] \tag{4.163}$$

where $\theta[\vec{x}-\vec{\xi}_i]$ corresponds to the cylindrical angle measured with respect to the line singularity at ξ_i. The phase f(x) specified in Eq. (4.163) gives the vortex density given by Eq. (4.26)

$$\vec{n}(x) = \vec{e}_3 \sum_i \delta(\vec{x}-\vec{\xi}_i) \ . \tag{4.164}$$

The problem posed in the analysis of the magnetic properties of the mixed state may be presented as follows, for a given applied external field H what is the equilibrium density of vortices that penetrate the system. In order to answer this question we compute the free energy given by Eq. (4.86), and which may be written as

$$F_s(n) = \frac{1}{V}\int d^3\vec{x}\,\Big[\frac{1}{8\pi}\,\vec{n}(x)\phi\cdot\langle\vec{H}(x)\rangle + \frac{1}{2}\,\vec{H}_M(x)\cdot\langle\vec{M}(x)\rangle$$
$$-\frac{N}{\beta}\,\ell n\, Z_J\{g_J\mu_B J\beta|\vec{H}_M(x)|\} - \frac{H_c^2}{8\pi} + E_{core}(x)\Big] \quad , \tag{4.165}$$

in the case of the vortex array specified by Eq. (4.164). For purposes of the present analysis we assume that the vectors $\{\xi_i\}$ form a triangular lattice in the x-y plane.

In order to treat the fields generated by the vortex lattice we follow the procedure outlined in ref. [28] and we separate the fields $\vec{B}$, $\vec{M}$ and $\vec{H}$ into their spatially averaged values and their spatial deviations,

$$\langle\vec{B}\rangle = n\phi\vec{e}_3 + \delta\vec{B} \quad , \tag{4.166}$$

$$\langle\vec{M}\rangle = M_o\vec{e}_3 + \delta\vec{M} \tag{4.167}$$

and

$$\langle\vec{H}\rangle = H_o\vec{e}_3 + \delta\vec{H} \quad , \tag{4.168}$$

where n denotes the vortex density and is given by

$$n = \lim_{V\to\infty} \frac{1}{V}\int_V n(x)\, d^3\vec{x} \quad . \tag{4.169}$$

Now from the expression for the magnetization given by Eq. (4.101) we obtain to lowest order in the spatial deviation

$$\delta\vec{M} = \chi(-i\nabla)\delta\vec{H} \tag{4.170}$$

$$= \frac{\chi(-i\nabla)}{1 + 4\pi\chi(-i\nabla)}\,\delta\vec{B} \tag{4.171}$$

where $\chi(\vec{k})$ is given by

$$\chi(\vec{k}) = \frac{C\alpha_J}{T - C\alpha_J\gamma} \quad . \tag{4.172}$$

In Eq. (4.172) the constant C denotes the Curie constant and α_J is given by Eq. (4.111) as

$$\alpha_J = \frac{3J}{J+1} B'_J \left\{\frac{g_J\mu_B J}{k_B T} |H_{MF}|\right\} \tag{4.173a}$$

where B_J is the Brillouin function and H_{MF} is given by

$$|H_{MF}| = H_o + \gamma(0) M_o \quad . \tag{4.173b}$$

The function $\gamma(\vec{k})$ is given by Eq. (4.114)

$$\gamma(\vec{k}) = \gamma_o(k) + I^2\chi_\sigma + 4\pi \tag{4.174}$$

where we have neglected the contribution from the paramagnetic interaction. Parameterizing $\gamma(k)$ as in Eq. (4.124) as $\gamma(\vec{k}) = T_m/C - D/C\,|\vec{k}|^2$ we obtain

$$\chi(k) = \frac{C}{T - T_m + D|\vec{k}|^2} \quad . \tag{4.175}$$

Now inverting the Maxwell equation given by Eq. (4.27) and neglecting the σ contribution, we obtain, to lowest order in the spatial deviations, the following expression for $\langle B(x)\rangle$ in terms of the vortex density $n(x)$

$$\langle B(\vec{x})\rangle = \frac{[1 + 4\pi\chi(-i\nabla)]\,C(-i\nabla)}{-\lambda_L^2\nabla^2 + [1 + 4\pi\chi(-i\nabla)]C(-i\nabla)}\; n(x)\,\phi \quad . \tag{4.176}$$

If we now introduce the effective single vortex fields

$$b_s(\vec{x}) = \frac{\phi}{(2\pi)^2} \int d^2\vec{k}\; e^{i\vec{k}\cdot\vec{x}} \; \frac{[1 + 4\pi\chi(\vec{k})]\,C(\vec{k})}{\lambda_L^2 k^2 + [1 + 4\pi\chi(\vec{k})]C(\vec{k})} \tag{4.177a}$$

and

$$h_s(\vec{x}) = \frac{\phi}{(2\pi)^2} \int d^2k \; e^{i\vec{k}\cdot\vec{x}} \; \frac{C(\vec{k})}{\lambda_L^2 k^2 + [1 + 4\pi\chi(\vec{k})]C(\vec{k})} \qquad (4.177b)$$

then the induction field $<B(x)>$ generated by the vortex lattice, given in Eq. (4.176), may be written as

$$<B(\vec{x})> = \sum_i b_s(\vec{x}-\vec{\xi}_j) \; , \qquad (4.178)$$

and using the relation

$$H_o = n\phi - 4\pi M_o \; , \qquad (4.179)$$

we obtain

$$<H(\vec{x})> = <B(x)> - 4\pi<M(x)>$$

$$= \frac{4\pi\chi(0)}{1+4\pi\chi(0)} u\phi - 4\pi M_o + \sum_i h_s(\vec{x}-\vec{\xi}_j) \quad . \qquad (4.180)$$

From Eq. (4.180) we obtain the result that

$$\frac{1}{V}\int d^3\vec{x} \; \frac{1}{8\pi} \vec{n}(x)\cdot<\vec{H}(x)> = \frac{n\phi}{8\pi}\{n\phi - 4\pi\tilde{M}_o + h(0)\} \; , \qquad (4.181)$$

where h(0) is given by

$$h(0) = n\phi \sum_{\vec{K}=0} \frac{\lambda_L^{-2}(t;n)C(\vec{K})}{|\vec{K}|^2 + [1 + 4\pi\chi(\vec{K})]\lambda_L^{-2}(t;n)C(\vec{K})} \qquad (4.182)$$

where the set $\{\vec{K}\}$ denotes the reciprocal lattice vectors of the vortex lattice.

The other contribution to the free energy that arises as a result of the vortex lattice, is the core energy denoted as $E_{core}(x)$. This term may be roughly thought of as arising from the potential due to the spatial variations in the magnitude of the order parameter $|\Delta(x)|$

induced by the vortex lattice. Since $|\Delta(x)|$ must vanish at the vortex centre, the effect of the spatial variation in $|\Delta(x)|$ is to increase the electron energy in the vortex core. Hence this term is referred to as the core energy. When the vortices form a lattice, we can define the core energy per vortex as

$$E(n) = \int_\Omega d^2x \; E_{core}(x) \; . \tag{4.183}$$

Expressing the core energy $E_{core}(x)$ in terms of the magnetic induction field $\langle B(\vec{x})\rangle$ and writing the field in the i^{th} lattice cell Ω_i as

$$\langle B(\vec{x})\rangle = b_s(\vec{x}) + b^{int}(\vec{x}) \; , \tag{4.184}$$

where we have chosen our coordinates such that $\vec{\xi}_i = 0$ and we have defined $b^{int}(\vec{x})$ as

$$b^{int}(\vec{x}) = \sum_{j\neq i} b_s(\vec{x}-\vec{\xi}_j) \; . \tag{4.185}$$

Now since $b_s(x)$ is well localized in the neighbourhood of the vortex and damps exponentially at large distances, one may expand $E_{core}(x)$ as

$$E_{core}[\vec{x};\langle B\rangle] = E_{core}[\vec{x};b_s] + \int d^3y \; E'_{core}[\vec{y}:b_s:\vec{x}]\, b^{int}(\vec{x}) + \ldots \; , \tag{4.186}$$

with

$$E'_{core}[\vec{y};b_s;\vec{x}] \equiv \frac{\delta E_{core}(\vec{x};\langle B\rangle)}{\delta b_s(\vec{y})} \; . \tag{4.187}$$

Now from the definition of the E'_{core} term together with the highly localized nature of the vortex induction field b_s, we may approximate

$$\int d^3x \int d^3y \; E'_{core}(x;b_s;y)\, b^{int}(\vec{y}) \simeq E_2\, b^{int}(0) \; . \tag{4.188}$$

Thus from Eqs. (4.187) and (4.188), E(n) may be parametrized in terms of two parameters E_1 and E_2

$$E(n) = E_1 - E_2 b^{int}(n) \ , \tag{4.189}$$

where we have defined

$$E_1 = \int d^3\vec{x}\ E_{core}(x;b_s) \tag{4.190}$$

and

$$\begin{aligned} b^{int}(n) &= \sum_{j\neq i} b_s(\vec{\xi}_j) \\ &= n\phi\left\{1 + \sum_{\vec{K}\neq 0} \frac{[1+4\pi\chi(\vec{K})]\lambda_L^{-2}(t;n)C(\vec{K})}{|\vec{K}|^2 + [1+4\pi\chi(\vec{K})]\lambda_L^{-2}(t;n)C(\vec{K})}\right\} \\ &\quad - \phi\int \frac{d^2k}{(2\pi)^2}\ \frac{[1+4\pi\chi(\vec{k})]\lambda_L^{-2}(t;n)C(\vec{k})}{|\vec{k}|^2 + [1+4\pi\chi(\vec{k})]\lambda_L^{-2}(t;n)C(\vec{k})} \end{aligned} \tag{4.191}$$

The contribution to the free energy from the core energy is thus given as

$$\frac{1}{V}\int_V d^3x\ E_{core}(\vec{x}) = n\{E_1 - E_2\, b^{int}(n)\}\ . \tag{4.192}$$

The calculation of the coefficients E_1 and E_2 in any precise fashion is extremely difficult, however the coefficient E_1 has been estimated using the virial theorem[7] and is given by

$$E_1 = \frac{\hbar c}{32e^2}\ \frac{1}{\lambda_L^2(t;n)}\ . \tag{4.193}$$

Thus Eq. (4.192) may be written as

$$\frac{1}{V}\int_V d^3\vec{x}\ E_{core}(x) = \frac{n\phi^2}{8\pi\lambda_L^2(t;n)}\left\{\frac{1}{4\pi} - \varepsilon_2 b^{int}(n)\right\}\ . \tag{4.194}$$

The parameter ε_2 therefore characterizes the multiple vortex effects and is determined by the requirement that there exists a second order transition point to the normal state.

The remaining terms, the condensation energy of the superconducting electrons and the free energy of the magnetic ions may be obtained from the expressions given in the preceding section. Thus we arrive at the following expression for the free energy $F_s(n)$ for a given vortex density n as

$$F_s(n) = \frac{n\phi}{8\pi}\left[n\phi + h(0) + \frac{\phi}{\lambda_L^2(n;t)}\{\frac{1}{4\pi} - \varepsilon_2 b^{int}(n)\}\right] + F_m[\tilde{\gamma};n] - \frac{H_c^2(t;n)}{8\pi}, \quad (4.195)$$

where

$$F_m(\tilde{\gamma};n) = \frac{1}{2}\tilde{\gamma}(\vec{k}=0)\, M_o^2 - \frac{N}{\beta}\ell n\, Z_J\{g_J\mu_B J\beta[n\phi + \tilde{\gamma}(0)M_o]\} \quad (4.196)$$

and $\tilde{\gamma}(0)$ is obtained from Eq. (4.118)

$$\tilde{\gamma}(0) = \gamma(0) - 4\pi \quad (4.197)$$

where, as before, we have neglected the paramagnetic interaction term $\sigma.B$.

Before going on to discuss the determination of the magnetic properties, it is worthwhile to consider how the various quantities appearing in the expression for the free energy given by Eq. (4.195) are affected by d-f interaction. First of all, the London penetration depth and the condensation energy, appearing in the third and fifth terms of Eq. (4.195) respectively, now depend on the polarization of the RE magnetic ions induced by the magnetic fields generated by the vortex lattice. Secondly, the superconducting currents generated by vortices will be modified by the change in the coherence length given by Eq. (4.100). Such effects were not included in the analysis of the mixed state presented in ref. [28], where it was argued that the effect of the d-f interaction was small and could be incorporated as a <u>temperature independent</u> renormalization of the various parameters.

With the free energy calculated as a function of the vortex density, the applied field H may be obtained as a function of the vortex density from the Gibbs free energy $G_s(n)$,

$$G_s(n) = F_s(n) - \frac{n\phi}{4\pi} H \,, \tag{4.198}$$

by the thermodynamic requirement that $G_s(n)$ be minimized with respect to the vortex density n. Thus we have that

$$\left.\frac{\partial G_s(n)}{\partial n}\right|_t = 0 \,, \tag{4.199}$$

which leads to

$$H(n) = \frac{4\pi}{\phi} \left.\frac{\partial F_s(n)}{\partial n}\right|_t \,. \tag{4.200}$$

The second order transition to normal state occurs when $n = n_c^o$ such that

$$G_s(n_c^o) = G_N(H_{c2}^o) \tag{4.201}$$

$$n_c^o \phi = H_{c2}^o + 4 M_{H_{c2}^o} \,, \tag{4.202}$$

where H_{c2}^o is defined by

$$H_{c2}^o = H(n_c^o) \,, \tag{4.203}$$

while $G_N(H)$ is the free energy of the normal state given by

$$G_N = -\frac{H^2}{8\pi} + F_m(\gamma;H) \tag{4.204}$$

with

$$F_m(\gamma;H) = \frac{1}{2}\{\gamma_o + I\chi_\sigma + 4\pi\}M_o^2 - \frac{N}{\beta}\ell n\, Z_J\{g_J\mu_B J\beta[H + (\gamma_o + I\chi_\sigma + 4\pi)M_o]\} \,, \tag{4.205}$$

and M_o is obtained from

$$M_o = g_J\mu_B JNB_J\{g_J\mu_B J\beta[H + (\gamma_o + I\chi_\sigma + 4\pi)M_o]\} \ . \tag{4.206}$$

Equations (4.201) and (4.202) serve to determine both the critical flux density n_c^o together with the parameter ε_2.

If it is the case, as one normally finds in non-magnetic type II superconductors, that

$$G_s(n) < G_N(H(n)) \tag{4.207}$$

for

$$n < n_c^o \ , \tag{4.208}$$

then the transition from the mixed state to the normal state will be second order and H_{c2}^o given by Eq. (4.203) will correspond to the physically observed upper critical field which we denote by H_{c2}.

It can happen, as we will see later in specific instances, that

$$G_s(n) = G_N(H(n)) \tag{4.209}$$

for certain n satisfying

$$n < n_c^o \ . \tag{4.210}$$

In this situation the observed critical flux density n_c is determined from Eq. (4.209) rather than Eqs.(4.201) and (4.202). Then we have that

$$n_c < n_c^o \ , \tag{4.211}$$

while the observed upper critical field H_{c2} is given by

$$\begin{aligned} H_{c2} &= H(n_c) \\ &> H_{c2}^o \end{aligned} \tag{4.212}$$

and the transition is first order being accompanied by a jump in the magnetization similar to that shown in figure 13. These rather peculiar effects we will discuss in greater detail later when we report on the results of various numerical calculations. It should be emphasized that the above change in the order of transition does not require any modification of the present formalism. What is assumed is that there is a point at which the second order transition occurs. This determines the parameter ε_2, then the theo[illegible]aturally predicts the first order transition if it occurs.

The value of the applied field from which transition from the pure Meissner state to the mixed state occurs may also be determined from Eq. (4.200) as

$$H_{c1}^{o} = H(n=0) . \tag{4.213}$$

It [illegible]cur that the free energy in the mixed state may actually in[illegible]s the vortex density increases. In such a situation the magnet[illegible]ion curve will be similar to that shown in figure 14 and the transition will be of first order and we will have that the observed lower critical field H_{c1} will be such that

$$H_{c1} < H_{c1}^{o} . \tag{4.214}$$

Calculations in the case of both non-magnetic and magnetic superconductors indicate that the difference between H_{c1} and H_{c1}^{o} is small and may be neglected for all practical purposes.

In order to apply the formalism summarized in the previous sections to the analysis of $ErRh_4B_4$ we need to know the various parameters characterizing the magnetic system, the superconducting system and the degree of coupling between the two systems. The Curie constant C and the saturation magnetization may be obtained from the observed lattice constant together with the values of J and g_J which may be assumed to have the same value as the free Er ion. The values given in table 1 are in reasonable agreement with those estimated from the inverse susceptibility measurements[131]. The Curie temperatures for the hard axis, $T_m^{(c)}$, and the easy axis, $T_m^{(a)}$, may be obtained from an extrapolation of the inverse susceptibility measurements measured with respect to the hard and easy axes respectively[131]. The condensation energy $H_{co}^2/8\pi$ may be estimated from the value obtained for $LuRh_4B_4$ $\{H_{co}(LuRh_4B_4) = 1.85$ KOe$\}$ from specific heat measurements[130] using the relation that

$$\frac{T_c(Lu)}{T_c(Er)} = \frac{H_{co}(Lu)}{H_{co}(Er)} . \tag{4.215}$$

This yields a value for Er of around 1.4 KG. The parameter κ_B has been estimated experimentally to be around 4.[132] The value of the field normalization ϕ/λ_{Lo}^2 may then be obtained from the relation $H_{co}^2 = \frac{3}{2}\frac{\kappa_B^2}{\pi^4}\left(\frac{\phi}{\lambda_{Lo}^2}\right)^2$. With the above values, we have estimated $\lambda_{Lo} \approx 825$ Å. The value of $g_oN(0)$ is chosen to be around 0.3. The ratio I^2/g_o may be estimated from the increase in the transition temperature as non-magnetic impurities are added to $ErRh_4B_4$. In the measurement on $Y_xEr_{(1-x)}Rh_4B_4$[119] it is observed that for low concentrations of Y (i.e. $x \ll 1$) the impurity concentration dependence of the magnetic transition temperature is given by

$$T_m^x \approx T_m(1 - x) . \tag{4.216}$$

This can be used together with Eq. (4.49) and Eqs. (4.121) and (4.129) to obtain the x dependence of the superconducting transition temperature T_c^x,

$$\frac{I^2}{g_0} = \frac{4\pi g_0 N(0)}{c^{(a)}} \; \frac{(1 - t_m^{(a)}(1 + t_m^{(a)}(d_f^{(a)}(1+\alpha) - 1))}{Z\, t_m^{(a)}} \; \frac{\frac{d}{dx}\log T_c(x)}{1 + \frac{d}{dx}\log T_c(x)}\Bigg|_{x=0} , \quad (4.217)$$

where Z is given by

$$Z = 2 + \frac{1 - t_m^{(a)}}{1 - t_m^{(c)}} \left\{\frac{t_m^{(a)}}{t_m^{(c)}}\right\} \frac{d_f^{(a)}(1+\alpha) + \varepsilon^{(a)}(t=1)}{d_f^{(c)}(1+\alpha) + \varepsilon^{(c)}(t=1)} \quad (4.218)$$

where the various dimensionless parameters appearing in Eq. (4.218) are given by

$$c^{(i)} = \frac{4\pi C}{T_m^{(i)}} , \qquad i = (a \text{ or } c)$$

$$d_f^{(i)} = 4 \frac{Dk_f^2}{T_m^{(i)}} , \qquad d^{(i)} = \frac{D\lambda_L^{-2}}{T_m^{(i)}} ,$$

$$D_i(\varepsilon) = (\varepsilon + d^{(i)}(1+\alpha))^2 - 4d_i(1+\alpha)c_i \quad (4.219)$$

and

$$\varepsilon_i(t) = \left\{\frac{t}{t_m^{(i)}} - 1\right\} , \quad (4.220)$$

where $t_m^{(a)}$ ($t_m^{(c)}$) denotes the reduced Curie temperature corresponding to the easy (hard) axis.

The value of $d/dx \log T_c(x)$ may be estimated from experiment[119] as

$$\frac{d}{dx} \log T_c(x)\Big|_{x=0} \simeq 0.14 . \quad (4.221)$$

Thus Eqs. (4.217) and (4.218) may be used to estimate the value of I^2/g_0 once $d_f^{(a)}$ and α are specified.

The remaining parameter $d^{(a)}$ may be estimated from the co-existence temperature T_p, since T_p is given by[15]

$$T_p \simeq T_m - 2\left\{\frac{4\pi c^{(a)}}{D\lambda_L^{-2}}\right\}^{1/2} = T_m\left[1 - 2\sqrt{\frac{c^{(a)}}{d^{(a)}}}\right] . \qquad (4.222)$$

The value of T_p shown in table 1 is estimated from the neutron scattering data on single crystal $ErRh_4B_4$.[23,133] The parameters α and d_f cannot as yet be obtained from any experimental values and are therefore adjusted to provide a reasonable overall fit to the data. If we choose $\alpha = 5$ and $d_f \simeq 20$ then condensation energy $H_c^2(T;h=0)$ may be computed, as a function temperature. The results shown in figure 5 are in reasonable agreement with recent estimates from the single crystal magnetization curves[122]. The resultant value of $\bar{I}$ ($\equiv I g_J J \mu_B N/\Delta_o$) is 3.555. This gives $\mathcal{J}(\equiv I \frac{g_J - 1}{g_J \mu_B N}) \simeq 1.5 \times 10^{-3}$ eV somewhat lower than other estimates[134]. The experimental parameters are summarized in table 1.

Using the above parameters we can now compute the upper and lower critical fields, by the methods summarized in this section and compare them with the single crystal data for $ErRh_4B_4$. We present the results of two separate analyses. In the first analysis, we simply apply the parameters presented in table 2, and proceed in the manner outlined to compute the critical fields. In the second analysis, we neglect the effect of the scaling and modify the parameters κ_B and $\bar{I}$ to obtain good fit to the experimentally observed upper and lower critical fields.

The reason for the two separate analyses is twofold. First of all, there is good reason to suppose that introducing the spin fluctuations by means of the effective coupling constant described in section 4.2 probably overestimates their effect, particularly at lower temperature. It is interesting therefore to compare this analysis with one in which the effect of the fluctuations is underestimated. Such a situation is obviously realized if they are neglected completely. The second reason is that a comparison of the two numerical analyses helps to illustrate the role played by the spin fluctuations.

The numerical results for the upper and lower critical fields H_{c2}, H^{o}_{c2} and H_{c1} ($\simeq H^{o}_{c1}$) including the effects of the spin fluctuations are shown in figure 15 for the easy axis direction, together with the single crystal measurements on $ErRh_4B_4$.[10] The parameters used are those shown in table 2. The upper solid line shows H_{c2} ($= H^{o}_{c2}$ when the transition to the normal state is second order). The dotted line shows the computed H^{o}_{c2} curve when the transition from the mixed state to the normal state is first order. It should be noted that the agreement with the experiment is rather good. Not only are the calculated values in good agreement with the experimental values but also the temperature at which the transition at H_{c2} changes from second to first order is in good agreement with the experimental value of $t \simeq 0.4$. Using the same parameter the hard axis upper critical field H_{c2} curve is shown in figure 16 together with the single crystal measurements. The lower critical field curve is similar to that obtained for the easy axis. The decrease in H_{c2} for low temperatures arises from the decrease in the condensation energy arising from the localized-spin fluctuations. The agreement with experiment is reasonably good.

The results of the numerical analyses of the upper and lower critical fields H_{c2}, H^{o}_{c2} and H_{c1} ($\simeq H^{o}_{c1}$) neglecting the effect of the spin fluctuations are shown in figure 17 for the easy axis direction, together with the corresponding single crystal measurements[10]. The parameters used are those shown in table 3. Again the upper solid line denotes H_{c2} and dotted line H^o_{c2}. The upper critical field in the case of the hard axis is shown in figure 18 together with the corresponding single crystal measurements. Again the agreement is quite acceptable.

A number of important conclusions may be drawn from these results. First of all, it would appear that both the measured upper and lower critical field curves along both the hard and easy axes may quantitatively be described using existing analytical methods suitably modified to include the d-f interaction using a set of parameters consistent with many other measurements. Secondly, it has become apparent in the course of our computations that it is difficult solely on the basis of the easy axis upper and lower critical field curves to distinguish between the effects of the electron polarization and the scattering by the spin fluctuations. Indeed qualitatively similar curves can be obtained with slightly modified parameters with or without the effect of the fluctuations or the polarization. If however one considers the hard axis critical field curves with the same sets of parameters, marked differences appear depending on which effects are included. This is seen to some extent by comparing the curves shown in figures 15 and 16 with those given in figures 17 and 18. This indicates the crucial role of the single crystal measurements in the understanding and interpretation of magnetic properties of these materials.

In addition to the upper and lower critical fields the expression for the applied field H(n), given in Eq. (4.200), together with our expression for the Gibbs free energy in Eq. (4.198), allows us to compute the bulk magnetization as a function of the applied external field H since

$$4\pi M = n\phi - H(n) . \tag{4.223}$$

The results of several magnetization curves computed for various values of the reduced temperature t are presented using the parameters given in table 2, including the effect of the spin fluctuations in figure 19. Two features are worth noting with regard to these curves. First of all, the magnetization for $t = 0.4$ clearly demonstrates a convex nature around H_{c2}, similar to that observed in the experimental magnetization curves[11]. Furthermore, as the temperature is lowered the convex nature of the magnetization becomes so pronounced that the curve exhibits a supercooling portion around H_{c2}^{o} and hence a first order transition at H_{c2}. This is clearly seen in the curves calculated for $t = 0.3$ and 0.2. Secondly, the magnetization curves also show the appearance at low temperature of a first order transition at H_{c1} as the temperature is lowered. This becomes quite pronounced below $t \simeq 0.15$. The appearance of the first order transition at H_{c1} may be attributed to two reasons; the modification of the vortex-vortex interaction induced by the dipole interaction[27,28,116,135] and the temperature and field dependent change in the superconducting current and the condensation energy arising from the scattering by the localized spin fluctuations.

These results indicate that the sequence of phase transitions as the temperature is lowered is given by

$$\text{type } II_{2,2} \longrightarrow \text{type } II_{1,2} \longrightarrow \text{type } II_{1,1} \longrightarrow \text{type } I \ ,$$

where we have defined the type $II_{i,j}$ $(i,j = 1,2)$ in the following way $i = 1$ $(j = 1)$ means a first order transition at H_{c1} (H_{c2}) and $i = 2$ $(j = 2)$ implies a second order transition at H_{c1} (H_{c2}).

Regarding the jump in the magnetization at H_{c1}, which will be referred to as ΔM_I, and illustrated in figure 21, it should be noted that for $t \gtrsim 0.15$ the calculated jump is relatively small. Given the difficulties inherent in the measurement of the magnetization curve around H_{c1} arising from the flux pinning and the fact that the slope of the magnetization curve around H_{c1} would be infinite anyway were it not for the pinning, it is quite likely that such a small jump would be extremely difficult to observe.

The results of several magnetization curves computed for various values of the reduced temperature using the parameters given in table 3 and neglecting the effect of the spin fluctuations are presented in figure 20. The behaviour in the vicinity of H_{c2} is seen to be qualitatively similar to that obtained in the previous analysis. However, the transition at H_{c1} was found to be second order indicating the sequence of the transitions as the temperature is lowered in this instance is given by

$$\text{type } II_{2,2} \longrightarrow \text{type } II_{2,1} \longrightarrow \text{type I} .$$

The jump in the magnetization at H_{c2} which will be denoted by ΔM_{II} may be obtained from the magnetization curves. The resultant curves together with some experimental points are shown in figure 22. The lower curve (labelled A) is that obtained using the parameters of table 2 including the spin fluctuations, the upper curve is that obtained using the parameters of table 3 neglecting the spin fluctuations. The points are somewhat lower than those observed experimentally.

Several features are worth noting. First of all, the appearance of the first order transition at H_{c2} appears to be a direct consequence of the polarization of the superconducting electrons induced by the d-f interaction. This result is consistent with other calculations[29,30], which show that the magnetization curve develops a convex curvature around H_{c2}, although no calculations, apart from those presented here, have considered the temperature domain, where the transition bcomes type $II_{i,1}$. The second point worth noting is the fact that, while the scaling effect induced by the localized spin fluctuations does not play a crucial role in determining the nature of the transition around H_{c2}, it does together with the dipole interaction have important consequences regarding the nature of the transition around H_{c1}. This is clearly shown by the fact that the jump in the magnetization appearing in figure 19 disappears when the scaling effect is neglected. In order, therefore, to draw any precise conclusion regarding the nature of the transition at H_{c1}, it is necessary to examine in more detail the pair breaking effect of the localized spin fluctuations and the long range structure of the vortex current.

To summarize in this section we have applied the formalism out lined in the preceding section to a detailed analysis of the mixed state in $ErRh_4B_4$. The analysis takes into account the Zeeman splitting of the electrons due to the polarization of the magnetic ions and the scattering of the electrons by the localized spin fluctuations. Both these effects are a result of the d-f interaction and both serve to suppress the superconductivity. In addition to the d-f interaction the interaction between the magnetic ions and the persistent current is contained within the Maxwell equation as well as the calculation of the magnetic susceptibilities. The effect of the anisotropic nature of the spin dynamics is also taken into account.

The nature of the formalism presented in Section 4.2 is such that these effects are included in an entirely self-consistent fashion.

The results of our analysis and the comparison with the experimental data allow us to draw a number of rather interesting conclusions. Most importantly, perhaps, we can state that many of the recently observed magnetic properties of $ErRh_4B_4$ may be adequately described within an existing theoretical framework developed by Matsumoto et al[28] provided the effect of d-f interaction is included. This includes the region where the transition to the normal state is first order and the observed magnetization curve is discontinuous. Since the analyses of both the hard and easy axis properties were performed using the same value of κ_B, the agreement between the results reported here and the experimental data, allows us to conclude that the observed differences between the hard and easy axes may be attributed to the observed anisotropy of the magnetic interaction between the rare earth ions. This seems to be supported by experimental measurements[132].

The results of our analysis also show that, while the scaling induced through the scattering of the electrons by the spin fluctuations can substantially affect the condensation energy and the detailed nature of transition around H_{c1}, its effect on the qualitative behaviour of the upper critical field curves and on the magnetization curve in the neighbourhood of H_{c2} is negligible. Indeed as is shown when the scaling effect is neglected, one may obtain good quantitative agreement regarding the latter two quantities by a rather minor modification of the parameters used. This is somewhat unfortunate since the measurement of the magnetization curve around H_{c1} and the temperature dependence of the condensation energy in $ErRh_4B_4$ is extremely difficult due to the amount of flux pinning present, making it very difficult to draw any definite conclusions regarding the effect of the spin fluctuations on the superconducting properties from the magnetization measurements. A corollary of this last observation is that the dominant effect arising from the d-f interaction observed in the existing magnetization measurements on $ErRh_4B_4$ arises from the polarization of the superconducting electrons by the Er moments.

It should be noted that the value of all but two of the parameters used in this analysis, α and d_f, may be determined experimentally.

To close this discussion we note that while the results of the analysis reported here suggest that the pair breaking effect of the spin fluctuation is not easily obtainable from the magnetization measurements of Crabtree et al[10,11], such effects will however have a strong effect on the temperature dependence of the condensation energy. This is clearly seen from the graph shown in figure 5 which deviates strongly from the BCS result to the effect of the spin fluctuations. Estimates of the condensation energy have been made from the hard and easy axis magnetization curves[122] and seem to be consistent with the results presented here.

Another measurement wherein the spin fluctuations play an important role is in the determination of the surface impedance. Recent measurements have been made of the surface impedance of polycrystalline $ErRh_4B_4$,[136] and an analysis using the parameters and assumption presented in this chapter is given in Appendix D together with a comparison with the data. The agreement is seen to be surprisingly good.

CHAPTER 5

CONCLUSIONS

The concept of spontaneously broken symmetry underlies many of the recent theoretical developments in modern condensed matter physics. It provides a unified conceptual framework for a number of wide and diverse areas of many body theory. Magnetism and superconductivity, both of which have been considered at length in this thesis, provide two examples. What one very quickly comes to realize in the study of physical systems which manifest the phenomena of spontaneously broken symmetry is that if one wishes to describe such systems by means of a well-defined and systematic scheme of approximation, then such a scheme must be consistent with the various symmetry requirements which underly the broken symmetry state.

In this regard the field theoretical formalism is well suited to the often subtle and complex facets of condensed states. The dual language of the Heisenberg fields and the physical fields, the Green's function technique together with the Feynman diagram realization of perturbation theory and devices such as the spectral representation, all provide powerful if not essential tools in analysis of spontaneously broken symmetry. Thus while much of the work presented in this thesis may be considered to be of a rather formal nature, the motivation is to try and account for certain empirical aspects of condensed states in many body systems.

Perhaps the most novel application of the field theoretical techniques in the work presented in this thesis was the use of the TFD formalism to construct a low temperature expansion for various experimentally accessible quantities in itinerant electron ferromagnets presented in Section 2.2. Here we were able, not only to obtain explicit expressions for the corrections arising from the thermal excitation of the elementary quanta, but also demonstrate how the requirements of th[illegible] rotational invariance, as realized in the W-T identities, allow us to determine in an explicit and model independent fashion, detailed information regarding the low temperature properties of these systems. In this way we were able to show how the empirically well established Bloch $T^{3/2}$ law for the magnetization together with the $T^{5/2}$ dependence of the quasi-particle spectrum arising from the magnon excitations were to be regarded as strict requirements of the spin rotational invariance.

These rather general considerations were complemented by the approximate calculation of the magnetization, presented in Appendix B, where the approximation was determined in such a way as to be consistent with the rigorous requirements of the W-T identities. This means therefore that despite the approximate nature of the calculation, it does nevertheless manifest the correct leading thermal correction (i.e. $T^{3/2}$) arising from the thermally excited magnons. This suggests that the approximation scheme outlined in Appendix B provides a useful starting point for a more realistic treatment of the itinerant electron model of ferromagnetism.

While the considerations of Section 2.2 concerned themselves with the particular case of spontaneously broken spin symmetry in itinerant electron systems, the method is of a sufficiently general character so as to be able to compute not only the leading magnon corrections to a large number of observable quantities, but also may be applied to consider analogous situations in other types of condensed states. The reason for this lies in the fact that all the essential features of the analysis presented in Section 2.2, such as the appearance of the Goldstone mode and the manner in which it couples to various operator quantities, have their analogue in other ordered states since such features are a general property of spontaneously broken symmetry. One would expect therefore the low temperature expansion, together with the W-T identities, to be applicable in areas such as triplet superfluidity, triplet superconductivity and phonon dynamics in crystals, since all are ordered states characterized by the appearance of an order parameter and all of which manifest an observable gapless collective excitation (the Goldstone mode). This provides us with an obvious extension of this work.

While the important role played by the W-T relations in the analysis of the ferromagnetic state is perhaps not surprising, their application to the analysis of the paramagnetic domain of ferromagnetic (and nearly ferromagnetic) itinerant spin systems presented in Section 2.3 is rather surprising. In the paramagnetic domain one would suppose that the requirements of spin rotational invariance and the corresponding W-T identities would be satisfied in a very trivial sense and hence be of little computational value. This however is not in fact the case. In Section 2.3, you will recall, we were able to exploit the spin rotational invariance in a non-trivial fashion by considering the response of the system to a small symmetry breaking term. This, we found, was due to the fact that the response of the system is severely controlled by the requirements of the spin rotational invariance and the corresponding W-T identities. Indeed it was shown how an exact expression for the low momentum limit of the electron paramagnon vertex could be obtained in terms of the induced magnetization together with the splitting of the electron self-energy. This allowed us to obtain an exact expression for the static susceptibility. This result is of more than formal interest and may be regarded in one of two ways. In the first instance it may be taken as a consistency requirement for the low momentum limit in any approximate calculation of the electron paramagnon vertex Γ, in order to ensure that the static long wavelength limit of the transverse susceptibility is consistent with the response of the induced magnetization M to the "applied field" h. Thus

$$\lim_{q\to 0} \chi(q) = \lim_{h\to 0} \frac{M}{h}, \tag{5.1}$$

as required by the spin rotational invariance. In the second instance it may be regarded as a simple means whereby the vertex Γ and hence the static susceptibility, may be calculated in terms of the electron self-energy. It was this latter aspect contained within the W-T relations with which we concerned ourselves in the remainder of Section 2.3. What we found was that we were able to obtain, in the case of the local contact interaction model, an exact expression for the corrections to RPA susceptibility arising from the spin fluctuations entirely in terms of the paramagnon contributions to the electron self-energy. Within the context of this result an explicit expression for the leading order correction to the static susceptibility arising from the spin fluctuations was obtained and it was shown how the results of previous work, by other authors, could be recovered and hence to what extent the requirement of the spin rotational invariance were satisfied. In particular we were able to give a rather systematic explanation of the so-called SCR method of Moriya and Kawabata, in terms of the lowest order paramagnon corrections to the electron self-energy[9].

As we emphasized in the discussion in Section 2.1, if the itinerant electron model is to account for the finite temperature properties of ferromagnetic metals, then it is essential that corrections arising from the spin fluctuations be included. At the present time the SCR technique provides one of the few methods whereby such effects may be included and it has had considerable success in accounting for a wide range of the observed properties in weak itinerant electron systems[137]. The discussion of the SCR method within the context of the formalism presented in Section 2.3 is important in that it indicates to what extent the SCR procedure is consistent with the requirements of spin rotational invariance, within the paramagnetic region. More than this however, the result of Section 2.3 shows quite clearly the basic assumptions and approximations underlying the SCR procedure. It should be possible therefore to construct other renormalization schemes for the self-consistent treatment of the spin fluctuations which allow us to go beyond the SCR procedure. One important extension of the work presented in Section 2.3, together with the considerations of Section 2.2, would be the development of a renormalization prescription which allowed us to include the effects of the spin fluctuations in both the ferromagnetic and paramagnetic domains in an entirely consistent fashion, both in the case of an applied field (induced symmetry breaking) and in the case of zero field (spontaneous symmetry breaking when $T < T_c$). Such a unified treatment would have application in many aspects of itinerant electron ferromagnetism.

The phenomena of superconductivity in metals also finds its explanation within the framework of spontaneously broken symmetry. In the case of superconductivity it is the phase symmetry of the electrons which is spontaneously broken. While there exist many close analogies between the superconducting state and the ferromagnetic state, in itinerant electron systems, there exist many important differences between the two. In the first place the phase symmetry is an abelian symmetry, whereas the spin symmetry represents a non-abelian symmetry. This means, for example, that the ferromagnetic state offers a far richer variety of singular topological structures than does the superconducting state where all topological singularities may be regarded as superpositions of the basic line or vortex singularity[7], discussed in Chapter 4. The second main difference, from a theoretical point of view, between the superconducting state and the ferromagnetic state in itinerant electron systems is the peculiar role played by the gauge degree of freedom in the superconducting state. The most important manifestation of this is the fact that the Goldstone fields are not observable as gapless particle like excitations; this may be understood in terms of the Anderson-Kibble-Higgs mechanism[138,139,140,141]. It is this rather subtle relationship between the broken phase symmetry and the requirements of gauge invariance which give rise to many of the properties peculiar to the superconducting state[7]. Indeed it may be argued that despite the somewhat simple abelian nature of the phase symmetry, the superconducting state represents the most puzzling of all the ordered states in condensed matter physics, the possible exception being perhaps the superfluid state.

The recent discovery, therefore, of the magnetic superconductors, such as the Chevrel and the $ReRh_4B_4$ compounds, which exhibit both a ferromagnetic as well as a superconducting nature, provide us with what must be among one of the most exotic of physical systems. It is therefore hardly surprising that such materials exhibit a wide range of peculiar properties; the co-existence phase together with the modulated spin ordering, the re-entrant phenomena and the first order transition to the normal state at H_{c2}, are examples of properties peculiar to these materials.

Given the rather complex nature of these compounds it is perhaps rather surprising that many of their properties may be understood in a qualitative sense at least, solely through the electromagnetic interaction between the persistent current and the magnetic moment of the rare earth ions[142]. This approach is based on the assumption that the effect of the d-f interaction may be incorporated through a temperature independent renormalization of the physical parameters. This rather simple approximation is inadequate however when one wishes to make a more detailed quantitative comparison between theory and experiment. This is particularly true in the light of the recent magnetization measurements on single crystal $ErRh_4B_4$.[10,11] There exists therefore, a clear need for a unified treatment of ferromagnetic superconductors which includes, in a unified and consistent fashion, the d-f interaction as well as the electromagnetic interaction. Thus while the presentation of such a formalism in Section 4.2 may be considered to be of a rather formal nature, the motivation for such a detailed treatment of the mutual interactions between the rare earth moments and the superconducting electrons is nevertheless, largely empirical in origin.

Despite the apparent complexity of the derivation presented in Section 4.2 the resultant formalism is relatively straightforward. The expression for the free energy given in Eq. (4.91), for example, is formally equivalent to that obtained in the earlier work[28], although the more detailed treatment of the effects of the d-f interaction means that the individual terms appearing in the free energy are of a somewhat complex nature. The calculation of the various quantities appearing in the expression for the free energy is not quite so complicated as one might expect and is contained entirely in the calculation of the spin splitting parameter μ, which may be thought of as the spatial average of the mean field experienced by the electrons due to the polarization of the rare earth ions, together with the scale factor s(t;h), which arises from the temperature and field dependent renormalization of the BCS coupling constant arising from the scattering of the superconducting electrons by the fluctuations in the localized spins. The definition and evaluation of these quantities is contained in Section 4.2.

The definition of the spin splitting term μ together with the scale factor s allows us to express the effect of the d-f interaction on the various superconducting quantities such as the superconducting gap, the coherence length, the field dependent condensation energy and the London penetration depth, through the scaling of a set of two parameter functions. A summary of the results was presented in Eqs. (4.146), (4.147) and (4.148) together with the definitions contained in Eqs. (4.149) to (4.162).

The formalism developed in Section 4.2 was applied to the analysis of the Meissner state of $ErRh_4B_4$ in Section 4.2 and to the mixed state in $ErRh_4B_4$. In the analysis of the Meissner state it was shown how the condensation energy and the superconducting gap are strongly affected by the scattering of the electrons by the localized spin fluctuations. In the case of the London penetration depth the effect was not so pronounced until the temperature was very close to T_p ($\simeq T_{c2}$).

The results are shown in figures 4, 5 and 6.

The results of the condensation energy are in good agreement with the unpublished estimates obtained from the magnetization curves of single crystal $ErRh_4B_4$.[122] While the London penetration depth is not a quantity which is directly observed from experiment an analysis of the effective penetration depth λ may be defined in terms of certain experimentally accessible quantities such as the change in the resonant frequency of a cavity. An analysis of the effective penetration depth λ for the case of $ErRh_4B_4$ together with some recent experimental measurements on polycrystalline samples is presented in Appendix D. At high temperatures ($T \lesssim T_c$) the effective penetration depth and the London penetration depth may be shown to be related by means of a simple scale factor $[1 + 4\chi(T)]^{1/2}$. The values obtained in this region are in reasonable agreement with the results obtained in Chapter 4. At lower temperatures however there is no straightforward relationship between the effective penetration depth and the London penetration depth due to the critical spin fluctuations associated with the appearance of the surface magnetization sate at T_s.

The application of the formalism presented in Section 4.2 to the analysis of the magnetic properties of the mixed state is relatively straightforward. From the expression of the free energy given by Eq. (4.91) one computes the Gibbs free energy for a given vortex density n and a given external field H. The minimization of the Gibbs free energy with respect to the vortex density, for a given external field H, yields the equilibrium flux density n for a given applied field, which we denote by H(n). The details of this procedure were presented in Section 4.3.

Now from a knowledge of the applied field H(n) and the equilibrium value of the Gibbs free energy we can obtain a number of important results. For example the lower critical field H_{c1} is given by $H(n_{c1})$, where n_{c1} is determined from the condition

$$G_s(n_{c1};H(n_{c1})) = G_s(0;H(n_{c1})) ,$$

where $G_s(n;H)$ denotes the Gibbs free energy calculated in the superconducting state for flux density n and applied field H. Two situations can arise; $n_{c1} = 0$ in which case the transition from the Meissner state to the mixed state is second order and $n_{c1} \neq 0$ in which case the transition is first order. Usually the difference between $H(n_{c1})$ and $H(n=0)$ is negligible.

The analysis of the lower critical field was performed for both the hard and easy axes in $ErRh_4B_4$, both with and without the effect of the spin fluctuations. The results obtained were found to be in reasonable agreement with the observed values. Little qualitative difference was found between the hard and easy axes or between the results with and the results without the effect of the spin fluctuations. The only result worthy of note was the fact that the analysis including the spin fluctuations exhibited a small first order transition at H_{c1} at low temperatures whereas the analysis without the pair breaking effect of the fluctuations did not. This may be attributed to the suppression of the spin fluctuations as the vortex density increases and the consequent decrease in the pair breaking effect due to the fluctuations. Thus we see that the effect of the spin fluctuations enhances the effect of the electromagnetic interaction to induce a first order transition at H_{c1} at lower temperatures[27,28,116,135].

As the flux density increases the corresponding increase in the induced polarization of the rare earth magnetic moments, means that the differences between the hard and easy axes become more apparent. This is clearly seen when one compares the results of the upper critical field shown in figures 15 and 17 for the easy axis with those of the hard axis shown in figures 16 and 18. In the case of the easy axis, the upper critical curve has a peak value of around 2.2 at $t\,(=T/T_c) = 0.7$ K while the hard axis curves are qualitatively similar to those observed in the non-magnetic case, with a peak value just above T_p of around 8-10 KG, although it should be noted that the pair breaking effect of the spin fluctuations does indicate a slight reduction in H_{c2} before T_p. While the rather marked difference between the upper critical field is accounted for some extent by the induced magnetization ($H_{c2} = n_{c2} - 4\pi M$) and the effect of the electromagnetic interaction, the sharp reduction in the upper critical field below $t \simeq 0.7$, is due mainly to the reduction in the critical flux density n_{c2} resulting from the pair breaking effect of the Zeeman splitting of the electron spins arising from the d-f interaction.

While the results for the upper and lower critical field, presented in Section 4.3, are in reasonably good agreement with the experimental results for single crystal $ErRh_4B_4$, it could be argued that the effects of the d-f interaction are essentially quantitative. One could still claim, therefore, that the observed properties of $ErRh_4B_4$ may be understood qualitatively,at least, solely on the basis of the electromagnetic interaction.

Such a viewpoint becomes difficult to sustain when we turn our attention to the effect of the d-f interaction on the easy axis magnetization curves and the nature of the transition to the normal state at H_{c2}. In figures 19 and 20 the calculated easy axis magnetization curves exhibit a distinctly convex nature around H_{c2}. Indeed we find that as the temperature is lowered the convex nature of the magnetization curve becomes so pronounced that the magnetization curve exhibits a supercooling portion at low temperatures. This implies that the magnetization curve exhibits a jump at H_{c2} and hence the transition to the normal state at H_{c2} is first order. This is in accordance with the experimental results on single crystal $ErRh_4B_4$.[11]

A number of comments are perhaps appropriate in regard to the above results. The first is that it is important to appreciate that the application of the formalism presented in Section 4.2 to the analysis of the mixed state allows one to treat the entire temperature domain above T_p, including the region in which the transition at H_{c2} is first order, in an entirely consistent manner. The first order transition at H_{c2} and the consequent jump in the magnetization were seen to emerge from the calculations outlined in Section 4.3 in a very natural way and were not in any sense "put in by hand". The second comment is that the results of this analysis allow us to conclude that despite the relatively weak nature of the d-f interaction,its effect on the magnetization measured with respect to the easy axis in $ErRh_4B_4$ is quite dramatic and gives rise to the observed first order transition to the normal state at H_{c2}.

The success of the formulation presented in Section 4.2 in describing many of the observed quantities in the recent measurements on $ErRh_4B_4$, suggests that it does contain the essential aspects of magnetic superconductors such as the $RERh_4B_4$ compounds. It is worthwhile to consider therefore extensions of this formulation to other materials, such as the antiferromagnetic superconductors and other geometries such as thin films. While most of the data presently available in these situations is on polycrystalline samples there is a good chance that single crystal samples will become available in the near future. It would be interesting, therefore, to see to what extent the analysis presented in Chapter 4 would be applicable.

In the magnetic superconducting compounds, such as $ErRh_4B_4$ and the other ternary compounds, the physical description is that of a lattice of rare earth ions immersed in a sea of conduction electrons. The atomic-like character of the core electrons associated with the rare earth ions thus allows us to treat the system as an array of localized magnetic moments interacting weakly, in the case of the ternary superconductors at least, with the conduction electrons through the various exchange interactions and the electromagnetic interaction. Recent investigations have uncovered a number of other metallic alloys whose physical properties appear to involve an interplay between the magnetism and superconductors, but for which such a tidy separation, into conduction electron and localized moment, is no longer appropriate.

One example of such a material is the binary alloy Y_4Co_3[143,144] (or Y_9Co_7); this shows a transition to a magnetically ordered state at around 6-8°K and a transition to the superconducting state at around 2-3°K. Thus we see that the order of the transition is reversed from that observed in the rare earth ternary compounds $ErRh_4B_4$ and $HoMo_6S_8$. Another difference arises from the fact that the magnetic properties of the Y_4Co_3 seem to suggest that it is a weak itinerant ferromagnet[145]. If this is in fact the case then it is the conduction electrons which produce both the superconducting order as well as the magnetic order. In addition to this it would appear that the effect of the spin fluctuations is important and the measured magnetization is qualitatively similar to that predicted by the SCR theory[145]. It would seem therefore that the work on itinerant electron systems presented in Chapter 3 could be profitably combined with the work on magnetic superconductors to investigate such materials.

Yet another puzzling class of compounds are the so-called heavy fermions systems such as the ternary compound $CeCu_2Ci_2$[146] and the binary compound UBe_{13}[147], both of which exhibit a number of interesting and unusual features at low temperature. Both for example are characterized by an anomalously large specific heat, indicating the presence of itinerant electrons with an effective mass about three orders of magnitude greater than that of a free electron. Furthermore both materials become superconducting as the temperature is lowered at 0.65°K in the case of the $CeCu_2Si_2$ and 0.85°K in the case of the UBe_{13}. The experimental evidence accumulated so far indicates that the large specific heat and the appearance of the superconductivity is due to the presence of an unfilled f shell which lies just below the fermi energy. This may also account for the anomalous nature of the resistivity and the inverse magnetic susceptibility observed at higher temperatures. As yet no suitable theory exists which can account for these peculiar and exotic materials.

And with these enigmatic compounds in our minds and the promise that the subtle interplay of magnetism and superconductivity is by no means a closed book, we draw this discussion to a close.

Table 1. Various experimental data used in the analysis of the mixed state in single crystal $ErRh_4B_4$. See Section 4.3.

$T_{c1} = 8.7°K$	$J = 15/2$
$T_{c2} = 0.7°K$	$g_J = 6/5$
$T_m^{(a)} = 1.0°K$	$C = 0.184°K$
$T_m^{(c)} = -20.0°K$	$4\pi g_J \mu_B JN = 10.11$ KOe
$T_p = 0.8°K$	$\frac{1}{T_c}\frac{dT_c(x)}{dx} = 10.11$
$H_{co} = 1.4$ KG	

Table 2. Dimensionless parameters used in the analysis of the mixed state presented in Section 4.3, including the effect of the spin fluctuations.

$t^{(a)} = T_m^{(a)}/T_c = 0.115$	$g_o N(0) = 0.3$
$t_m^{(c)} = T_m^{(c)}/T_c = -2.300$	$d = (\frac{D}{T_m \lambda_{Lo}^2}) = 0.452 \times 10^{-2}$
$t_p = T_p/T_c = 0.092$	$J = 7.5$
$c^{(a)} = 4\pi C/T_m^{(a)} = 2.312$	$\kappa_B = 4$
$d_f = 4Dk_f^2/T_m^{(a)} = 20$	$\alpha = 5$
$\bar{I} = \frac{I g_J \mu_B J N}{\Delta_o} = 3.55$	

Table 3. Dimensionless parameters used in the analysis of the mixed state presented in Section 4.3, not including the effect of the spin fluctuations s = 1.

$t_m^{(a)} = T_m^{(a)}/T_c = 0.115$	$g_oN(0) = 0.3$
$t_m^{(c)} = T_m^{(c)}/T_c = -2.300$	$d = \left(\frac{D}{T_m^{\lambda} L_o^2}\right) = 0.452 \times 10^{-2}$
$t_p = T_p/T_c = 0.092$	$J = 7.5$
$c^{(a)} = 4\pi C/T_m^{(a)} = 2.312$	$\kappa_B = 3.5$
$\bar{I} = \frac{I g_J \mu_B JN}{\Delta_o} = 4.285$	

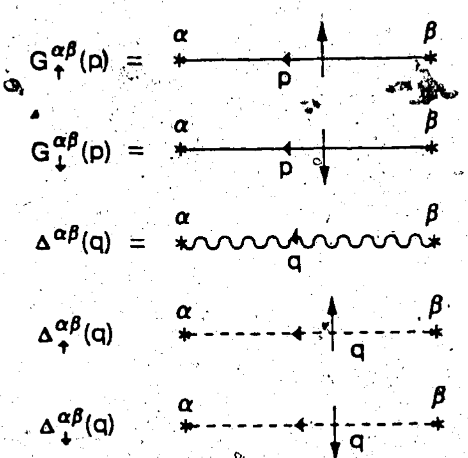
Table 4. Dimensionless parameters used in the calculation of the effective coupling constant shown in figure 3 together with corresponding scale factor. The quantities d_f and are chosen so as to emphasize the effect of the fluctuations.

$t_m^{(a)} = T_m^{(a)}/T_c = 0.115$	$d_f = 4Dk_f/T_m^{(a)} = 1.0$
$t_m^{(c)} = T_m^{(c)}/T_c = -2.300$	$\alpha = 2.0$
$t_p = T_p/T_c = 0.092$	$I^2/g_o = 1.26$
$c^{(a)} = 4\pi C/T_m^{(a)} = 2.312$	$d = (\frac{D}{T_m \lambda_{Lo}^2}) = 0.45 \times 10^{-2}$

Table 5. Calculated values of the condensation energy $H_c^2(t;h)/H_{co}^2$ for various values of $h(=H/\phi\lambda_L^2)$ and $t(=T/T_c)$. The parameters used are those given in table 2.

h	t = 0.2	t = 0.4	t = 0.6
0.00	0.523616	0.466289	0.269145
0.01	0.523638	0.466290	0.269145
0.02	0.523702	0.466295	0.269147
0.03	0.523805	0.466303	0.269149
0.04	0.523940	0.466313	0.269152
0.05	0.524097	0.466327	0.269155
0.06	0.524261	0.466342	0.269160
0.07	0.524410	0.466359	0.269165
0.08	0.524512	0.466377	0.269170
0.09	0.524519	0.466395	0.269176
0.10	0.524365	0.466414	0.469182

Fig. 1. Lowest order electron self-energy corrections arising from the traverse and longitudinal spin fluctuations. See Eqs (3.170a) and (3.170b). (Source Ref. 67)


G↑αβ(p) =
G↓αβ(p) =
Δαβ(q) =
Δ↑αβ(q)
Δ↓αβ(q)
α
β
p
q

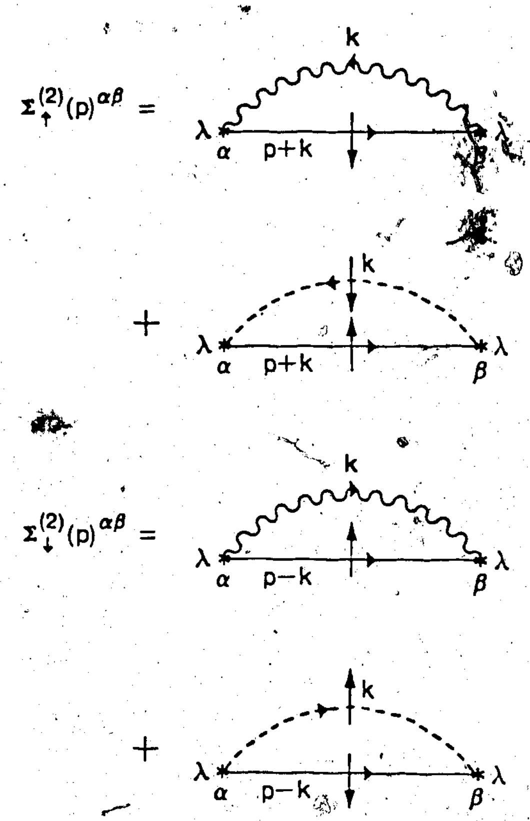

Σ↑(2)(p)αβ =
Σ↓(2)(p)αβ =
+
k
λ
α
β
p+k
p−k

Fig. 2. Contour for the complex integral contained in the expression for $\Phi_i(x;y)$. See Eq. (4.156). (Source Ref. 153)

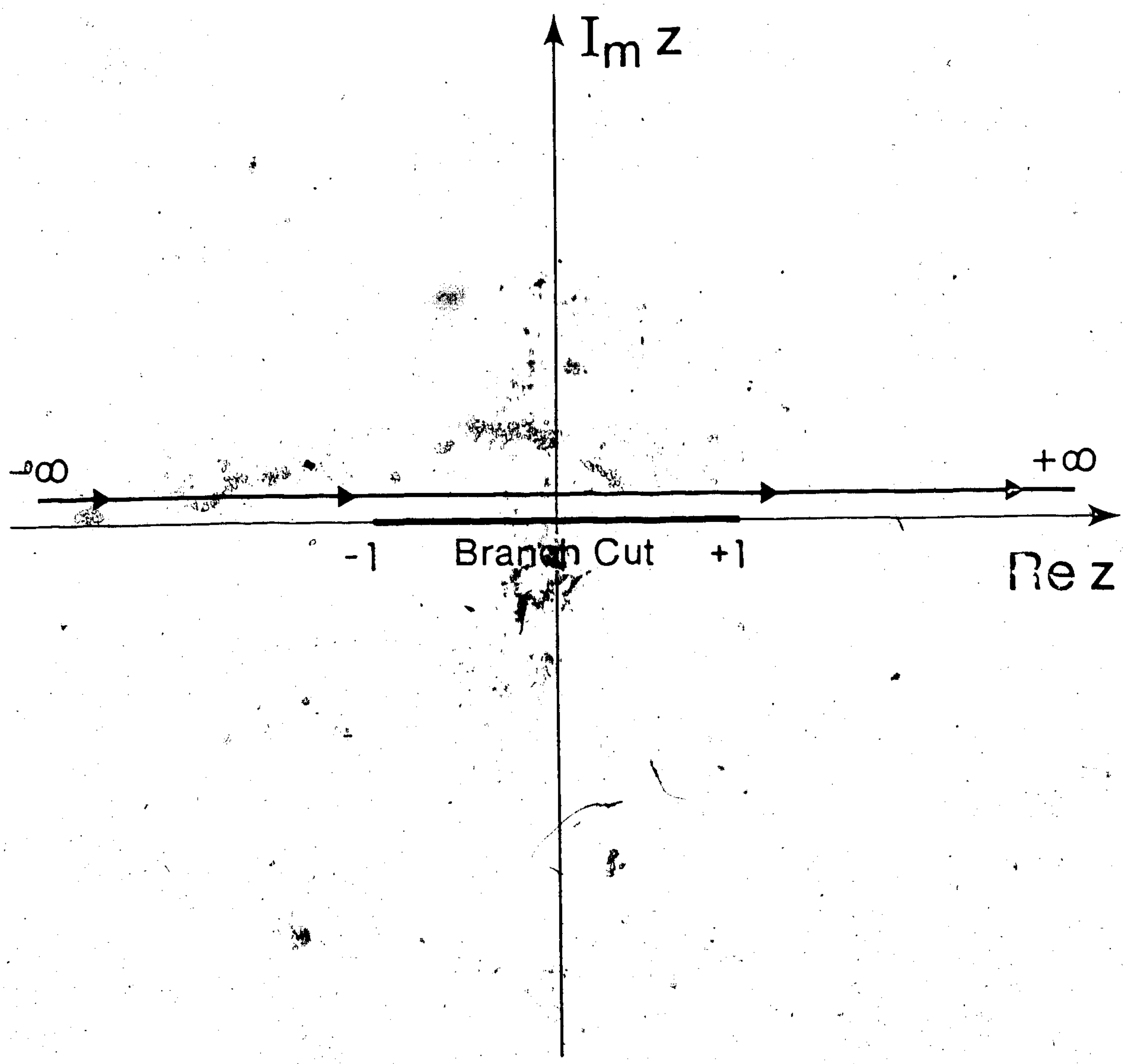
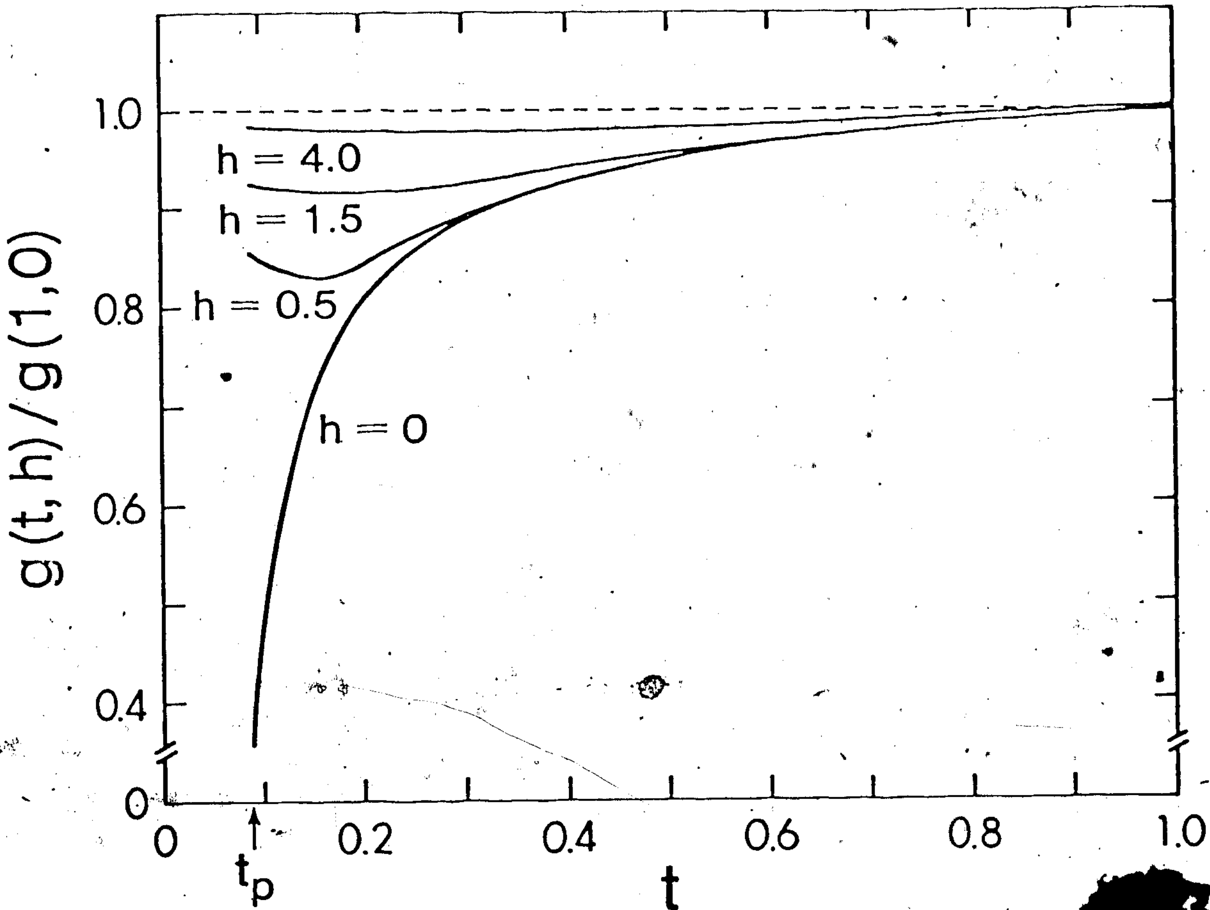

Im z
-∞
+∞
-1
Branch Cut
+1
Re z

Fig. 3. The temperature dependent coupling constant $g(t;h)/g(1;0)$ and the corresponding scale factor $s(t;h)$, calculated using the parameters shown in table 4.


1.0
0.8
0.6
0.4
0
g(t, h)/g(1,0)
h = 4.0
h = 1.5
h = 0.5
h = 0
0
0.2
0.4
0.6
0.8
1.0
t_p
t

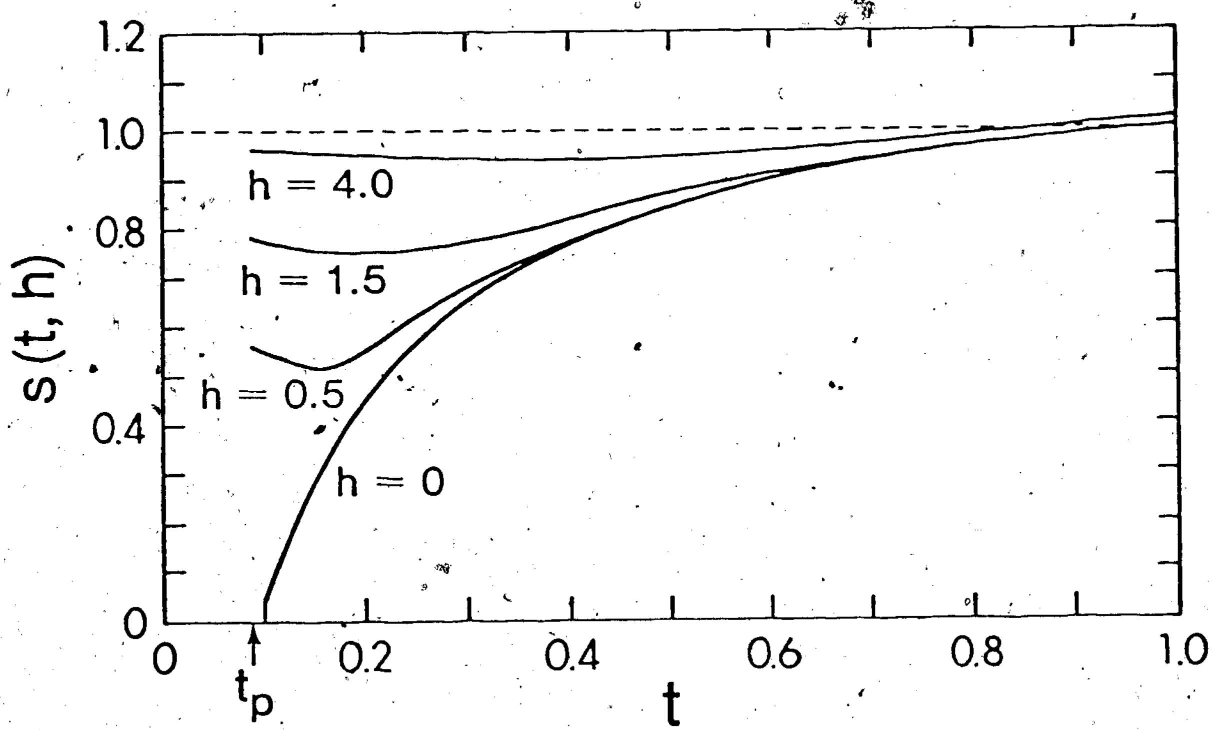
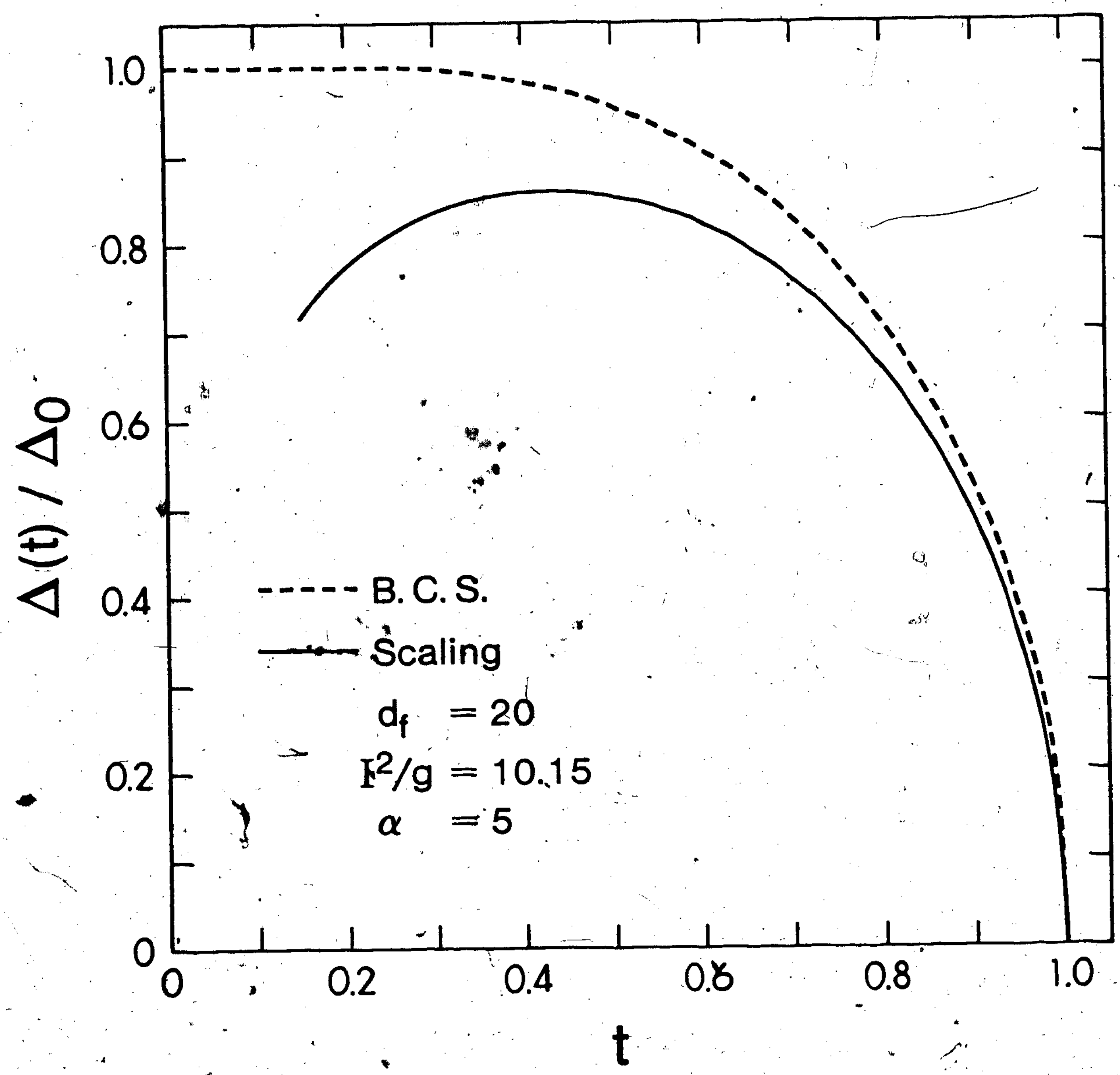

1.2
1.0
0.8
0.4
0
s(t, h)
h = 4.0
h = 1.5
h = 0.5
h = 0
0
0.2
0.4
0.6
0.8
1.0
t_p
t

Fig. 4. Temperature dependence of the superconducting gap including the effect of the spin fluctuations (solid curve) and the BCS result for comparison (dotted curve). The parameters used are those given in table 2. (Source Ref. 153)



Δ(t) / Δ0
1.0
0.8
0.6
0.4
0.2
0
0
0.2
0.4
0.6
0.8
1.0
t
B. C. S.
Scaling
d_f = 20
F²/g = 10.15
α = 5

Fig. 5. Temperature dependence of the condensation energy including the effect of the spin fluctuations (solid curve) and the BCS result (dotted curve) for comparison. The parameters used are those given in table 2. (Source Ref. 153)

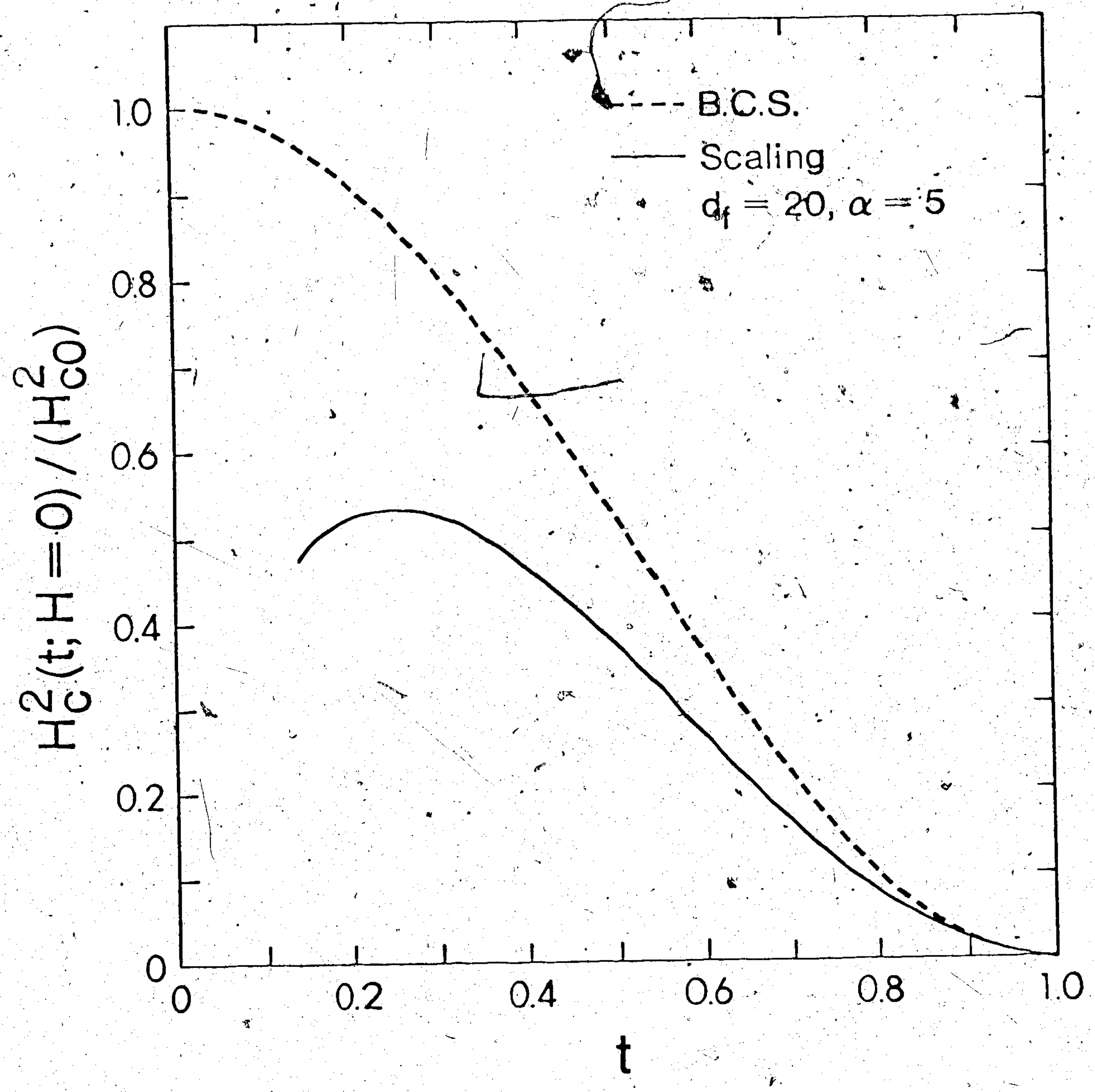

B.C.S.
Scaling
$d_f = 20, \alpha = 5$
1.0
0.8
0.6
0.4
0.2
0
$H_c^2(t; H=0)/(H_{c0}^2)$
0
0.2
0.4
0.6
0.8
1.0
t

Fig. 6. Temperature dependence of the London penetration depth including the effect of the spin fluctuations (solid curve) and the BCS result (dotted curve) for comparison. The parameters used are those given in table 2. (Source Ref. 153)

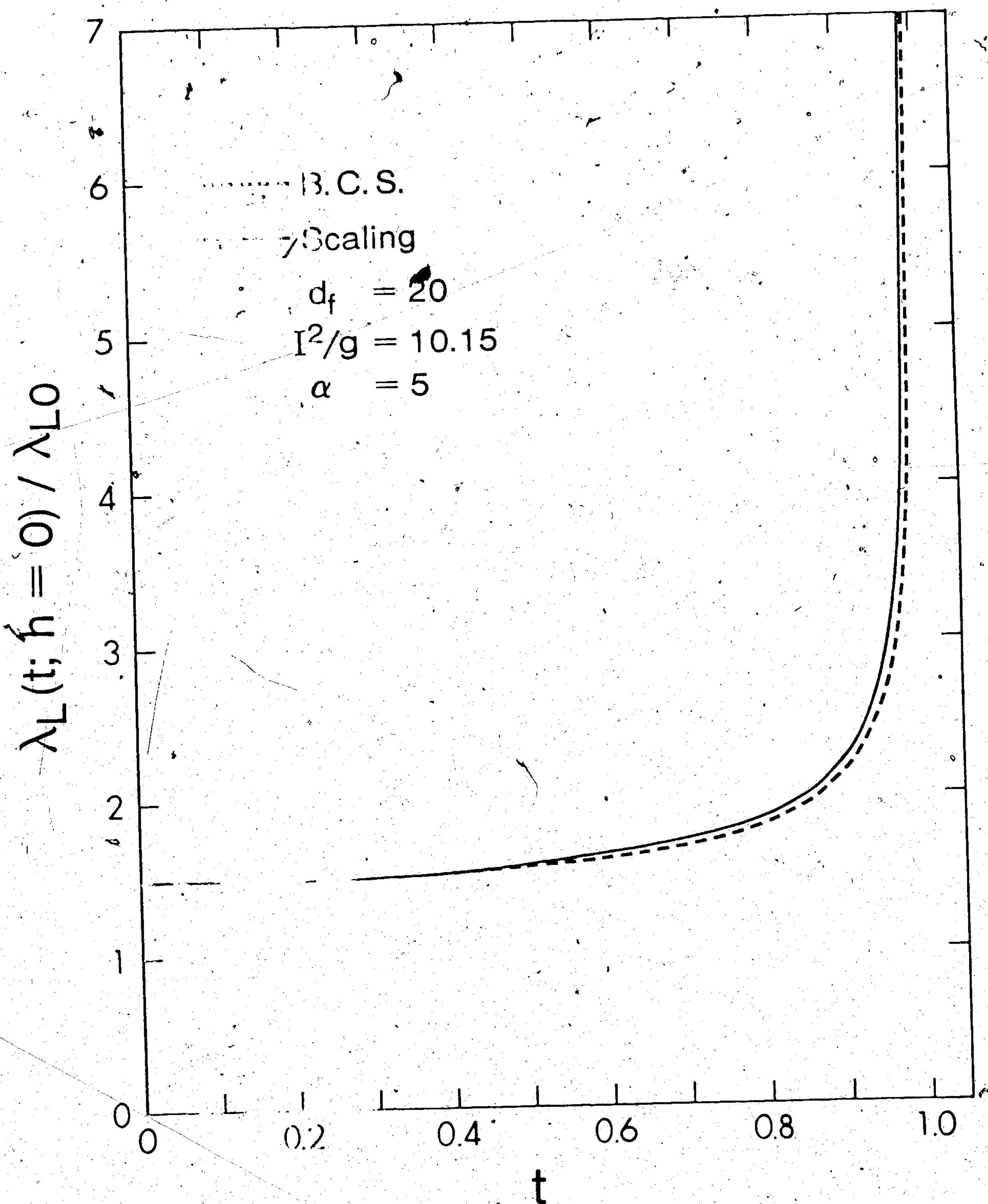
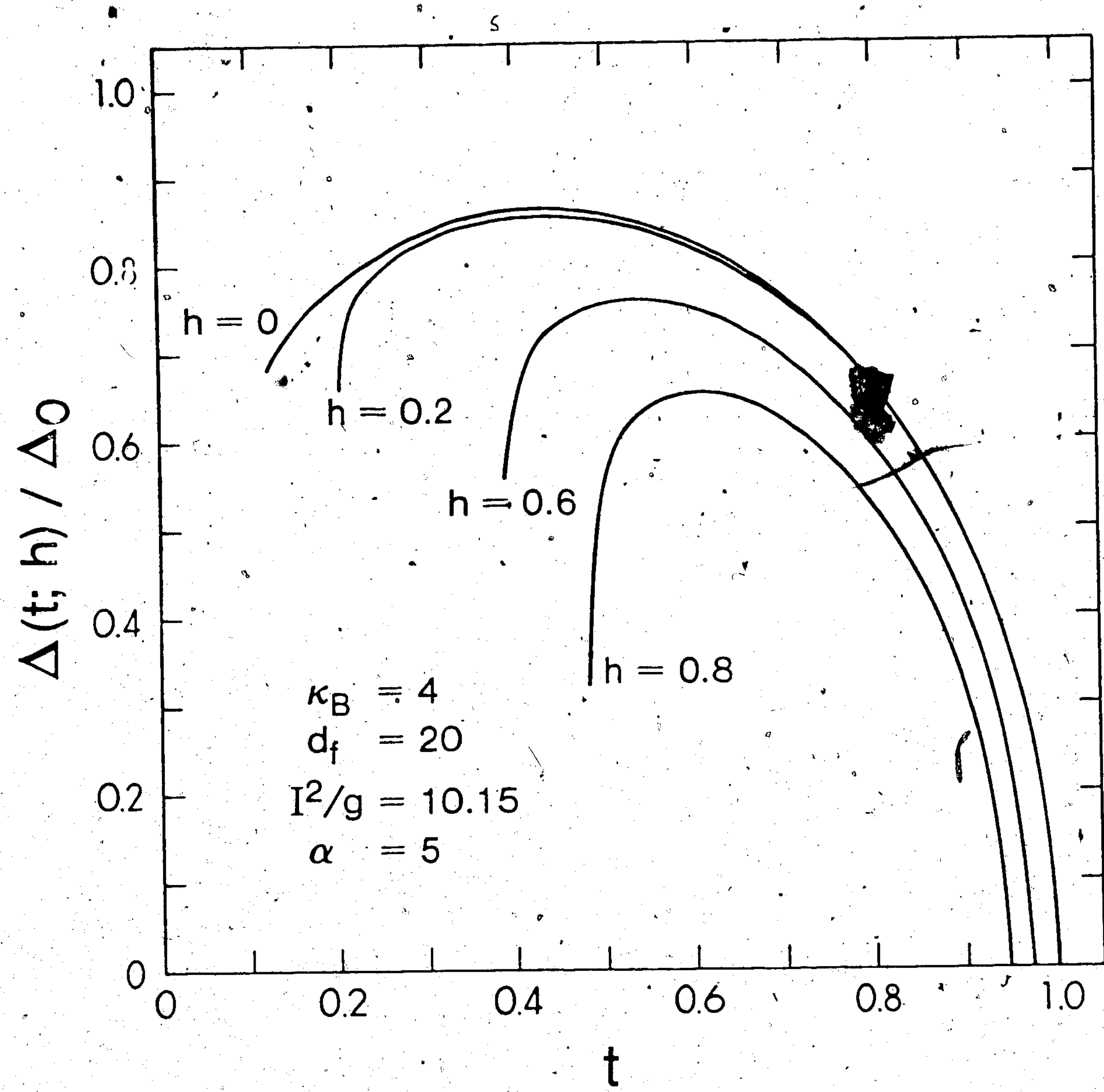
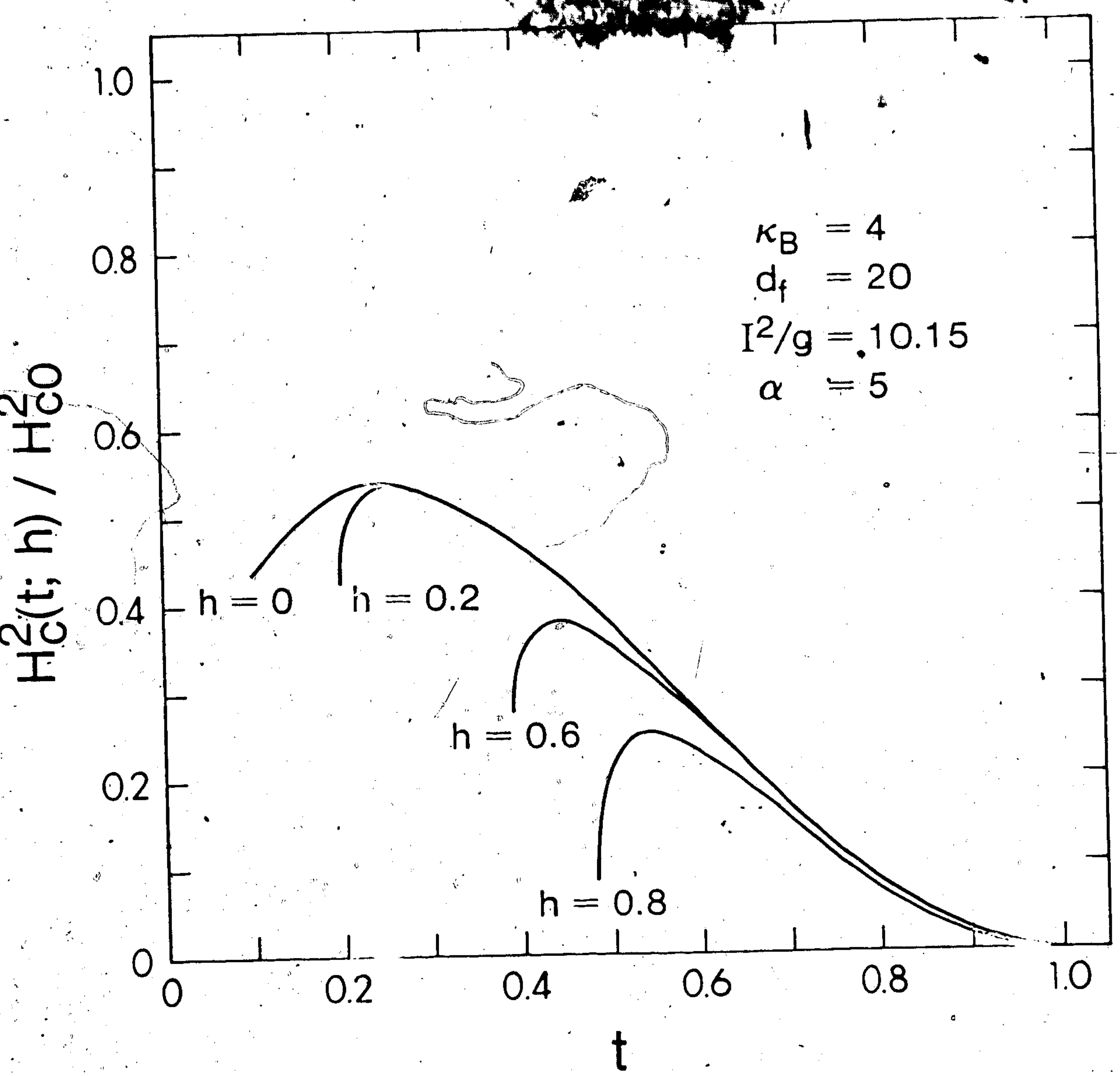

B.C.S.
Scaling
d_f = 20
I^2/g = 10.15
α = 5
$\lambda_L(t; h=0) / \lambda_{L0}$
t
0
1
2
3
4
5
6
7
0.2
0.4
0.6
0.8
1.0

Fig. 7. Temperature dependence of the gap for various values of the reduced internal field h ($\equiv H/\phi\lambda_{Lo}^{-2}$). The parameters used are those given in table 2. (Source Ref. 153)



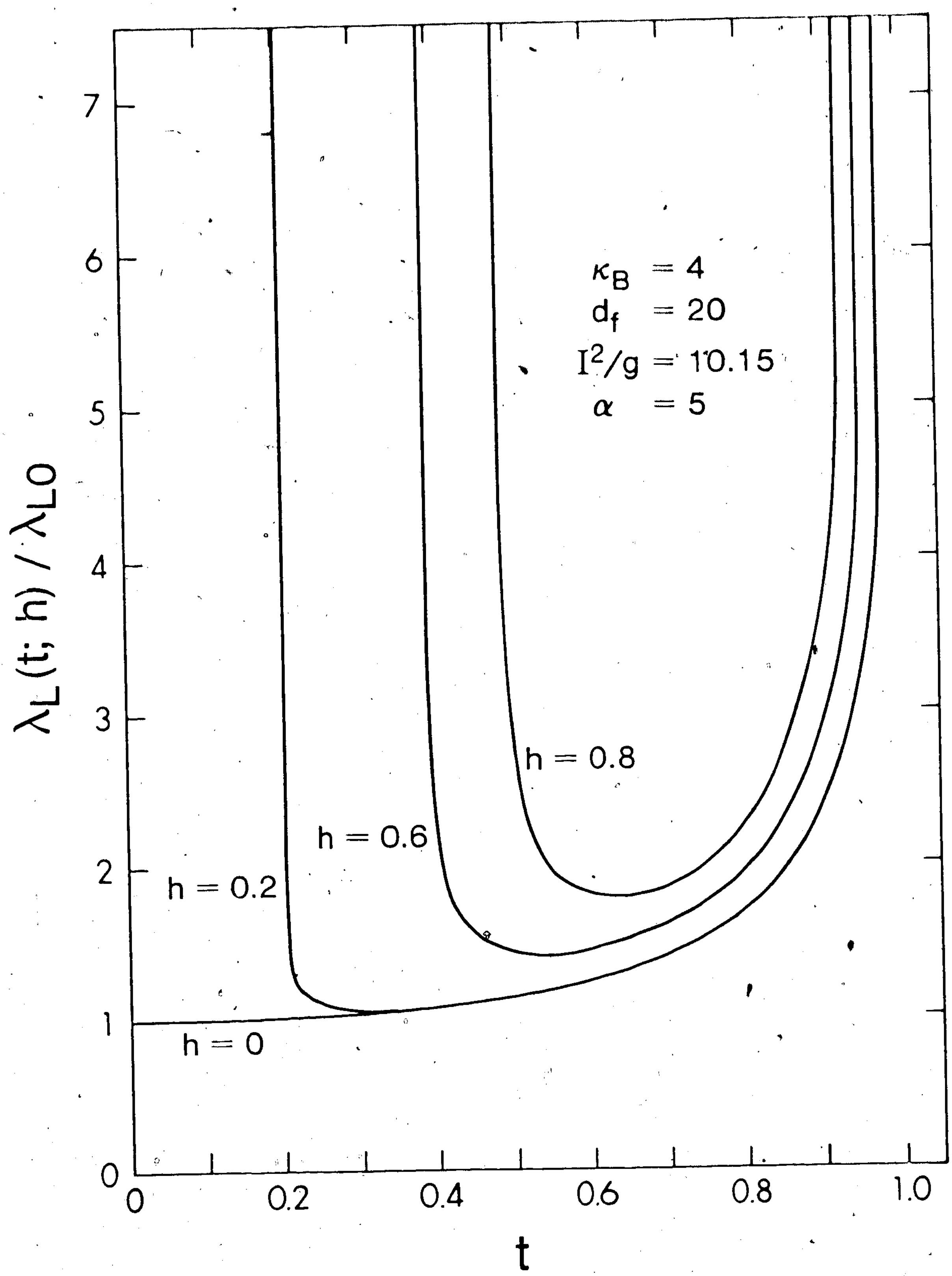
1.0
0.8
0.6
0.4
0.2
0
0
0.2
0.4
0.6
0.8
1.0
Δ(t; h) / Δ0
t
h = 0
h = 0.2
h = 0.6
h = 0.8
κB = 4
df = 20
I²/g = 10.15
α = 5

Fig. 8. Temperature dependence of the field dependent condensation energy for various values of the reduced internal field $h \equiv (H/\phi\lambda_{Lo}^{-2})$. The parameters used are those given in table 2.



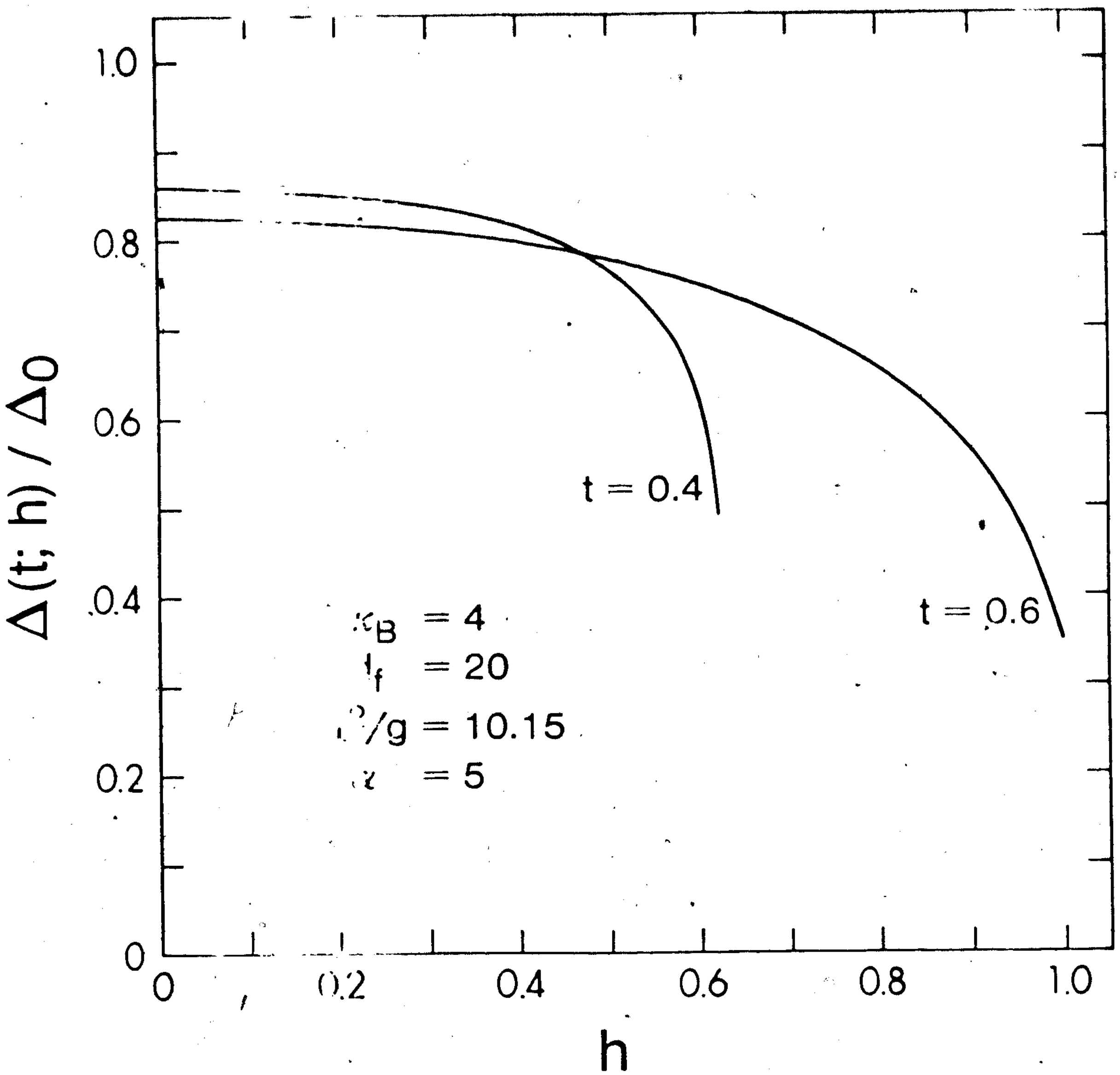
1.0
0.8
0.6
0.4
0.2
0
$H_c^2(t; h) / H_{c0}^2$
$\kappa_B = 4$
$d_f = 20$
$I^2/g = 10.15$
$\alpha = 5$
h = 0
h = 0.2
h = 0.6
h = 0.8
0
0.2
0.4
0.6
0.8
1.0
t

Fig. 9. Temperature dependence of the London penetration [illegible] for various values of the reduced internal field $h = (H\phi\lambda_{Lo}^{-2})$. The parameters used are those given in table 2. (Source Ref. 153)



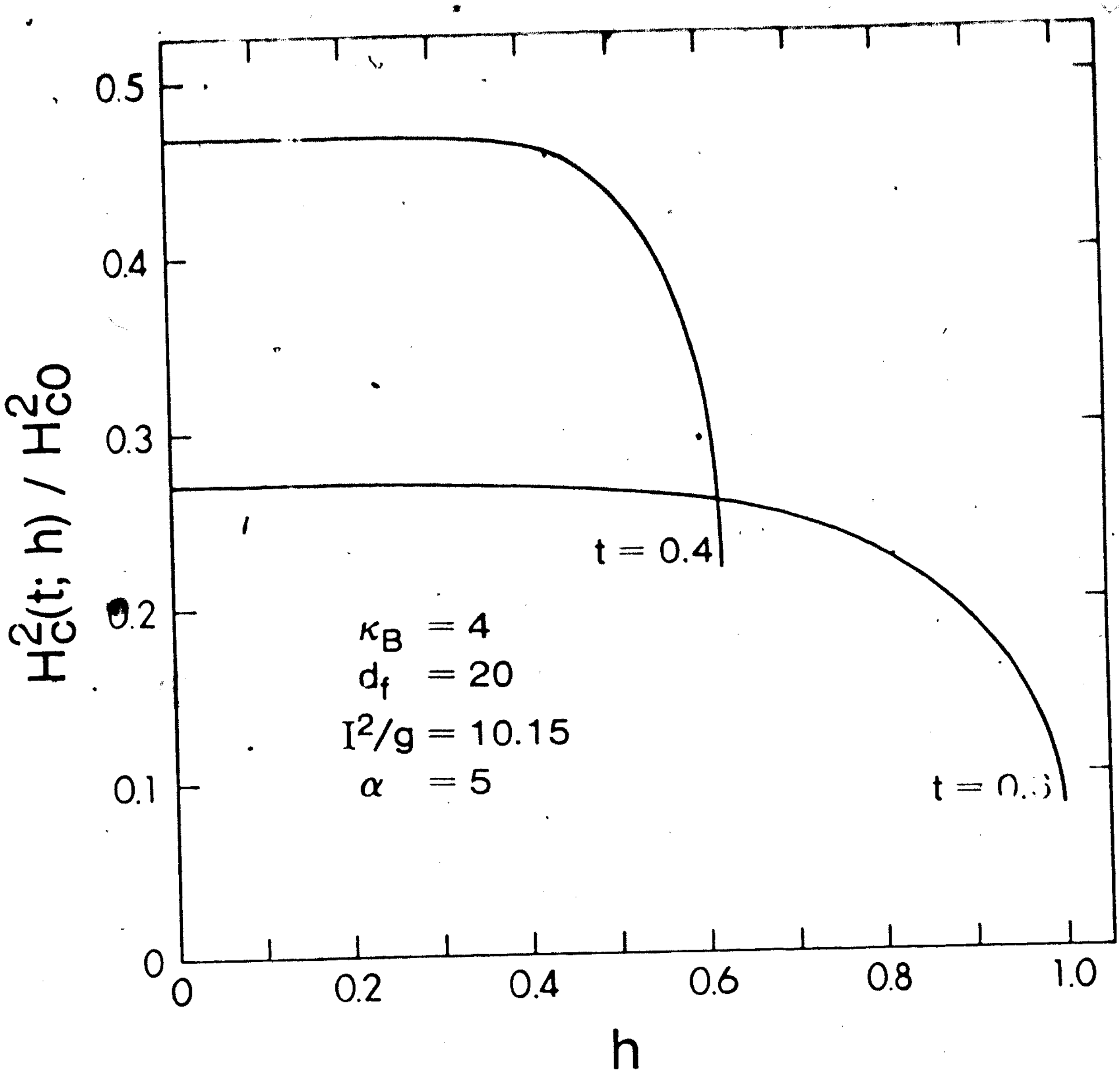
$\kappa_B = 4$
$d_f = 20$
$I^2/g = 10.15$
$\alpha = 5$
h = 0.8
h = 0.6
h = 0.2
h = 0
$\lambda_L(t; h) / \lambda_{LO}$
t
0
1
2
3
4
5
6
7
0.2
0.4
0.6
0.8
1.0

Fig. 10. Field dependence of the superconducting gap for various values of the reduced temperature. The parameters used are those given in table 2. (Source Ref. 153)



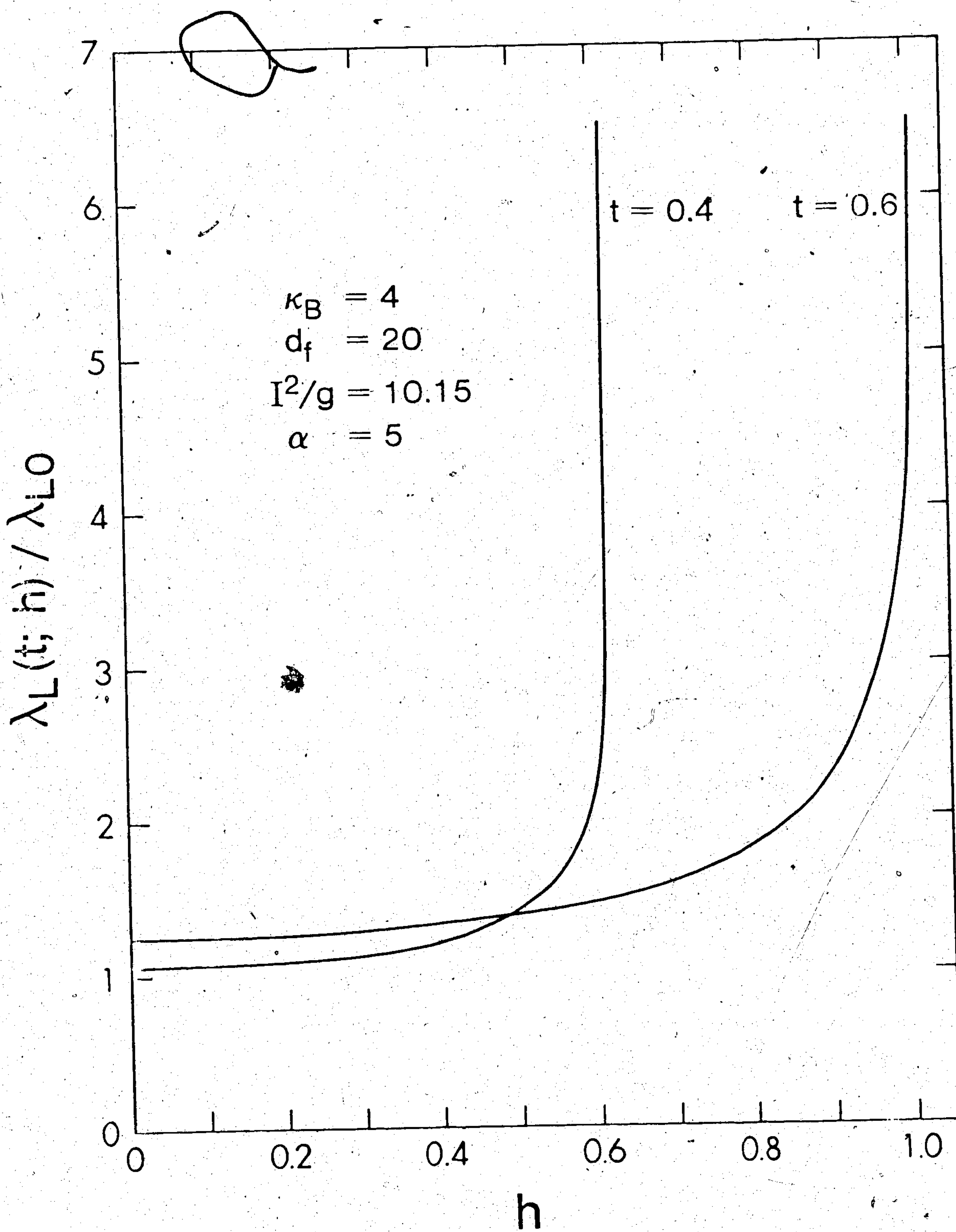
Δ(t; h) / Δ0
h
0
0.2
0.4
0.6
0.8
1.0
t = 0.4
t = 0.6
= 4
= 20
/g = 10.15
= 5

Fig. 11. Field dependence of the London penetration depth for various values of the reduced temperature. The parameters used are those given in table 2. (Source Ref. 153)



0.5
0.4
0.3
0.2
0.1
0
$H_c^2(t; h) / H_{c0}^2$
t = 0.4
t = 0.6
$\kappa_B = 4$
$d_f = 20$
$I^2/g = 10.15$
$\alpha = 5$
0
0.2
0.4
0.6
0.8
1.0
h

Fig. 12. Field dependence of the London penetration depth for various values of the reduced temperature. The parameters used are those given in table 2. (Source Ref. 153)



7
6
5
4
3
2
1
0
0
0.2
0.4
0.6
0.8
1.0
h
$\lambda_L(t; h) / \lambda_{LO}$
t = 0.4
t = 0.6
$\kappa_B = 4$
$d_f = 20$
$I^2/g = 10.15$
$\alpha = 5$

Fig. 13. Schematic illustration of the magnetization curve in the neighbourhood of H_{c2} for a type $II_{i,1}$ superconductor. (Source Ref. 154)

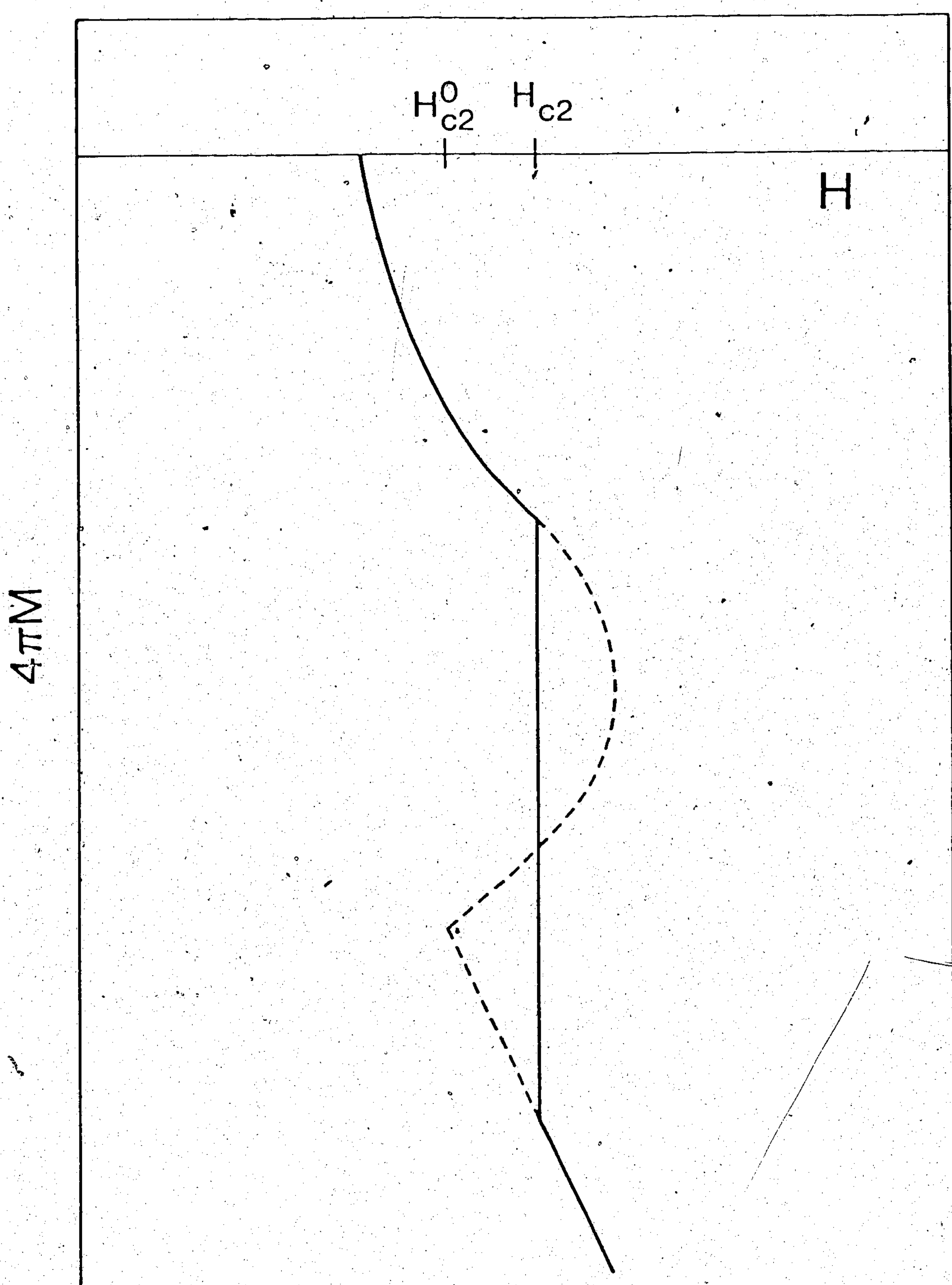
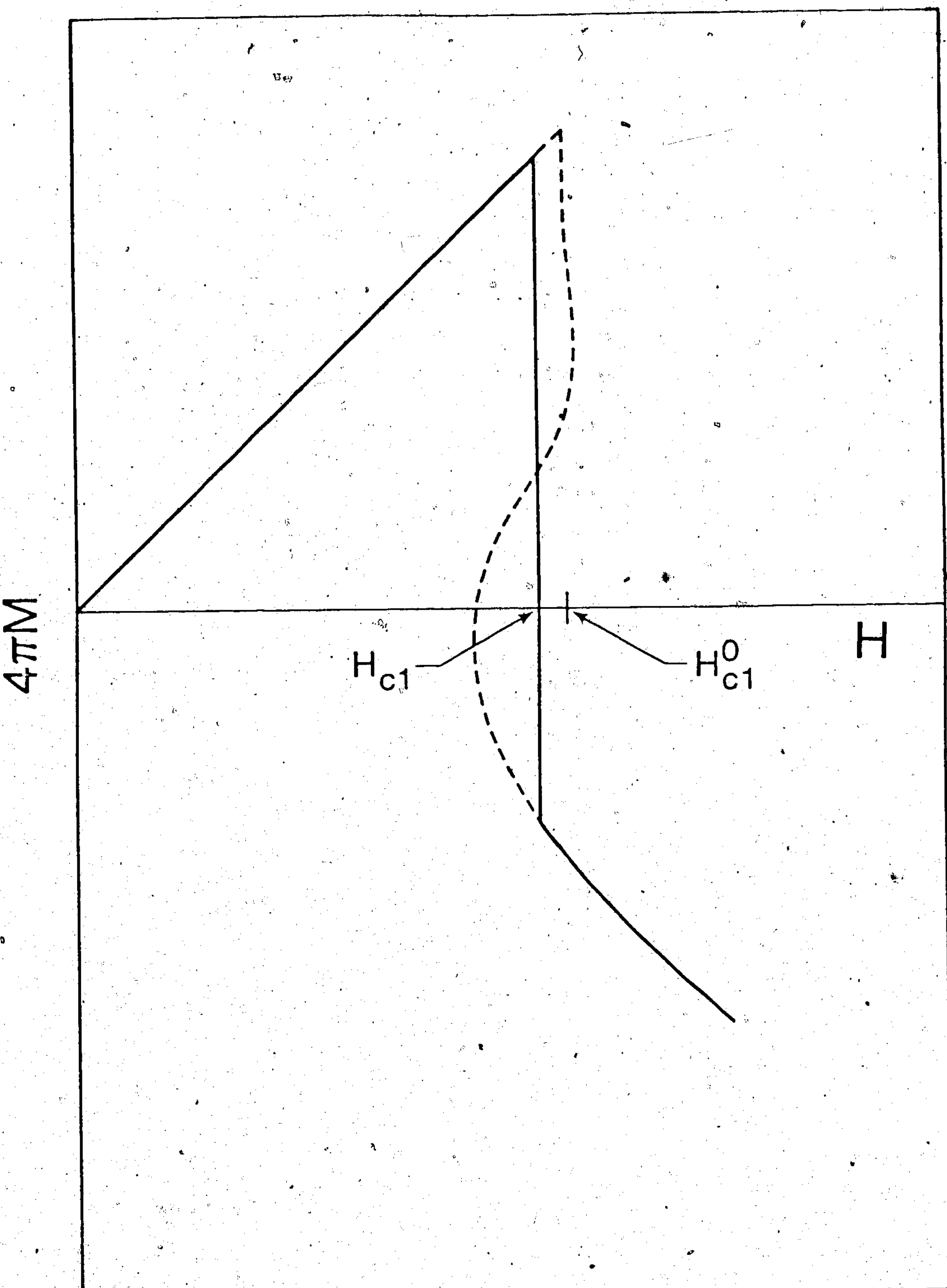

H^0_{c2}
H_{c2}
H
$4\pi M$

Fig. 14. Schematic illustration of the magnetization curve in the neighbourhood of H_{c1} for a type $II_{1,i}$ superconductor. (Source Ref. 154)



4πM
H
Hc1
H0c1

Fig. 15. The easy axis upper and lower critical fields H_{c2} and H_{c1} calculated using the parameters given in table 2 <u>including</u> the effect of the spin fluctuations. The dotted portion represents H^{o}_{c2}. Also shown are the experimental measurements after Crabtree et al.[10] (Source Ref. 154)

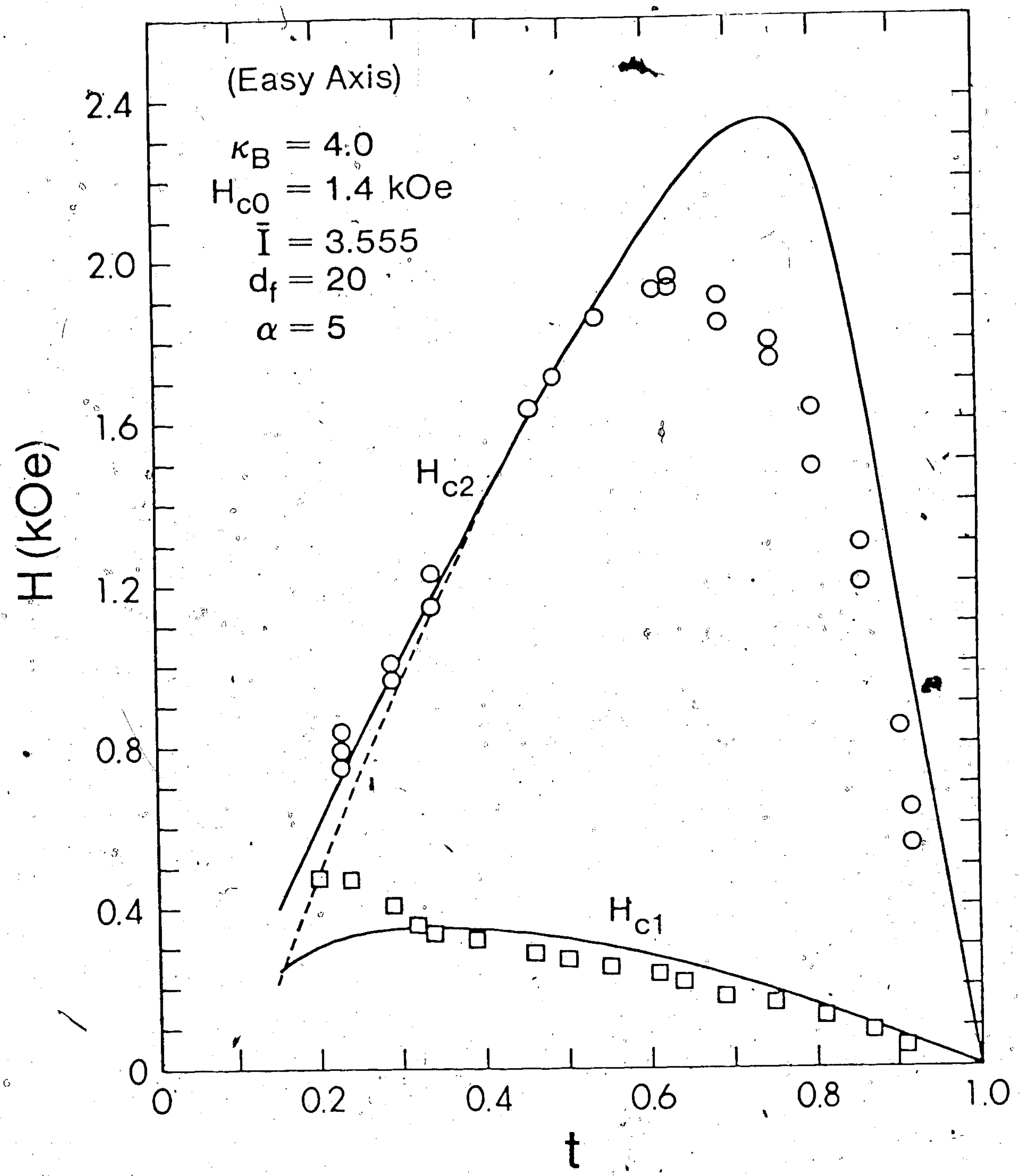

(Easy Axis)
κ_B = 4.0
H_{c0} = 1.4 kOe
$\bar{I}$ = 3.555
d_f = 20
α = 5
H_{c2}
H_{c1}
H (kOe)
t
2.4
2.0
1.6
1.2
0.8
0.4
0
0
0.2
0.4
0.6
0.8
1.0

Fig. 16. The hard axis upper critical field H_{c2} calculated using the parameters given in table 2 including the effect of the spin fluctuations. Also shown are the experimental measurements after Crabtree et al.[10] (Source Ref. 154)

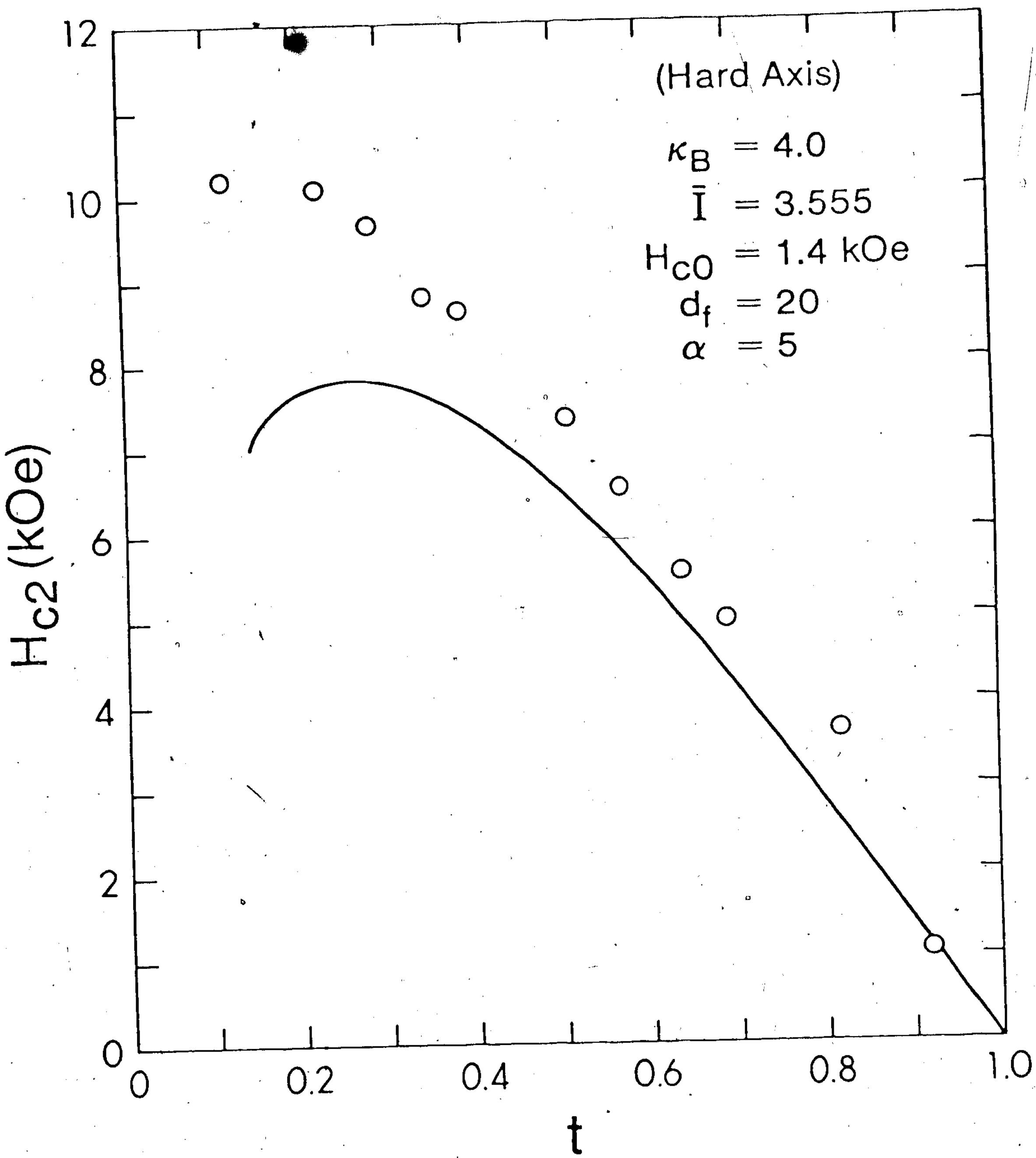

(Hard Axis)
$\kappa_B = 4.0$
$\bar{I} = 3.555$
$H_{c0} = 1.4$ kOe
$d_f = 20$
$\alpha = 5$
H_{c2} (kOe)
t
0
2
4
6
8
10
12
0.2
0.4
0.6
0.8
1.0

Fig. 17. The easy axis upper and lower critical fields H_{c2} and H_{c1} calculated using the parameters given in table 3 <u>neglecting</u> the effect of the spin fluctuations (i.e. s = 1). The dotted portion represents H^{o}_{c2}. Also shown are the experimental measurements after Crabtree et al.[10] (Source Ref. 154)

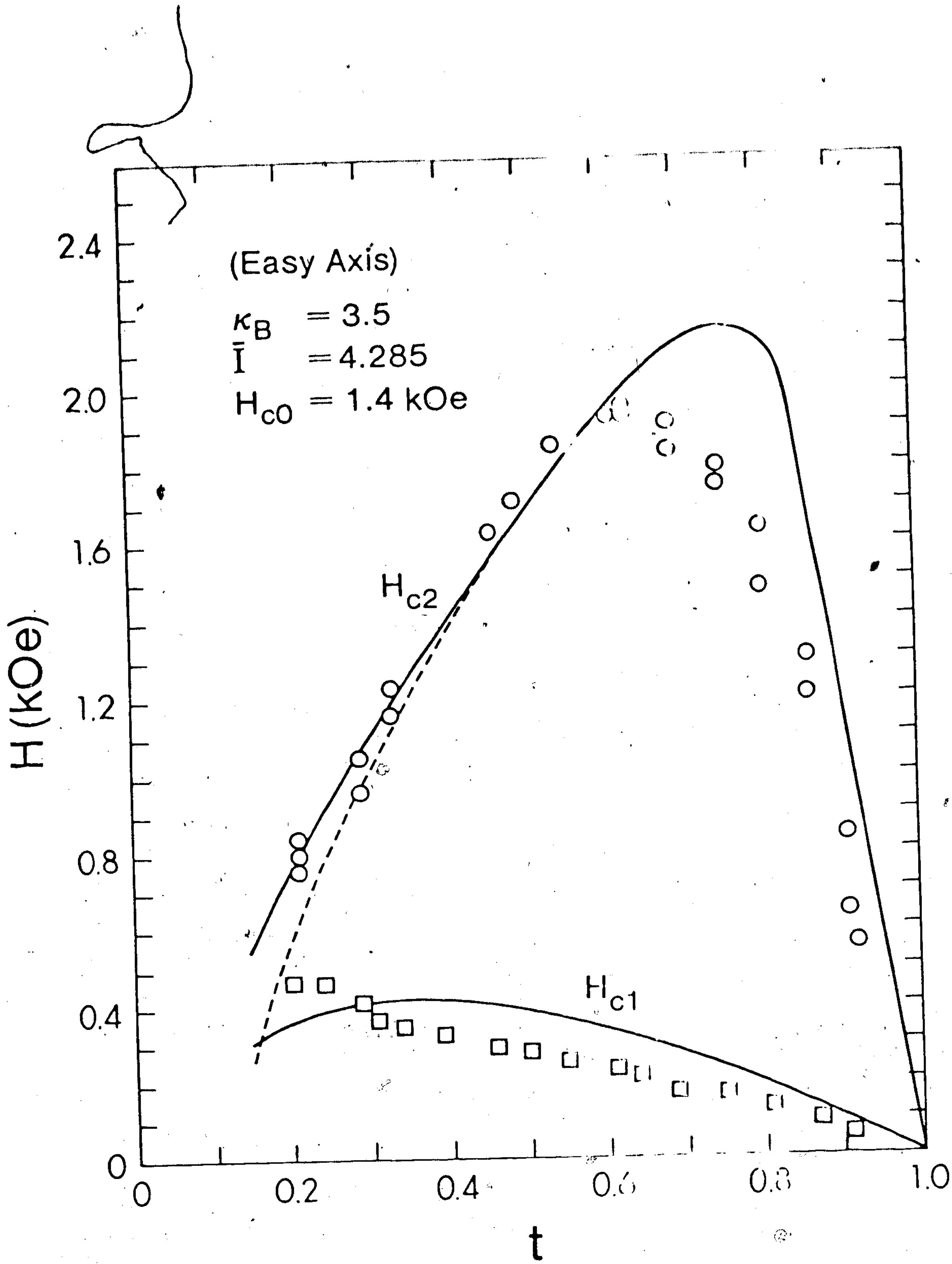

(Easy Axis)
κ_B = 3.5
$\bar{I}$ = 4.285
H_{c0} = 1.4 kOe
H_{c2}
H_{c1}
H (kOe)
t
2.4
2.0
1.6
1.2
0.8
0.4
0
0.2
0.4
0.6
0.8
1.0

Fig. 18. The hard axis upper critical field H_{c2} calculated using the parameters given in table 3 neglecting the effect of the spin fluctuation (i.e. $s = 1$). Also shown are the experimental results after Crabtree et al.[10] (Source Ref. 154)

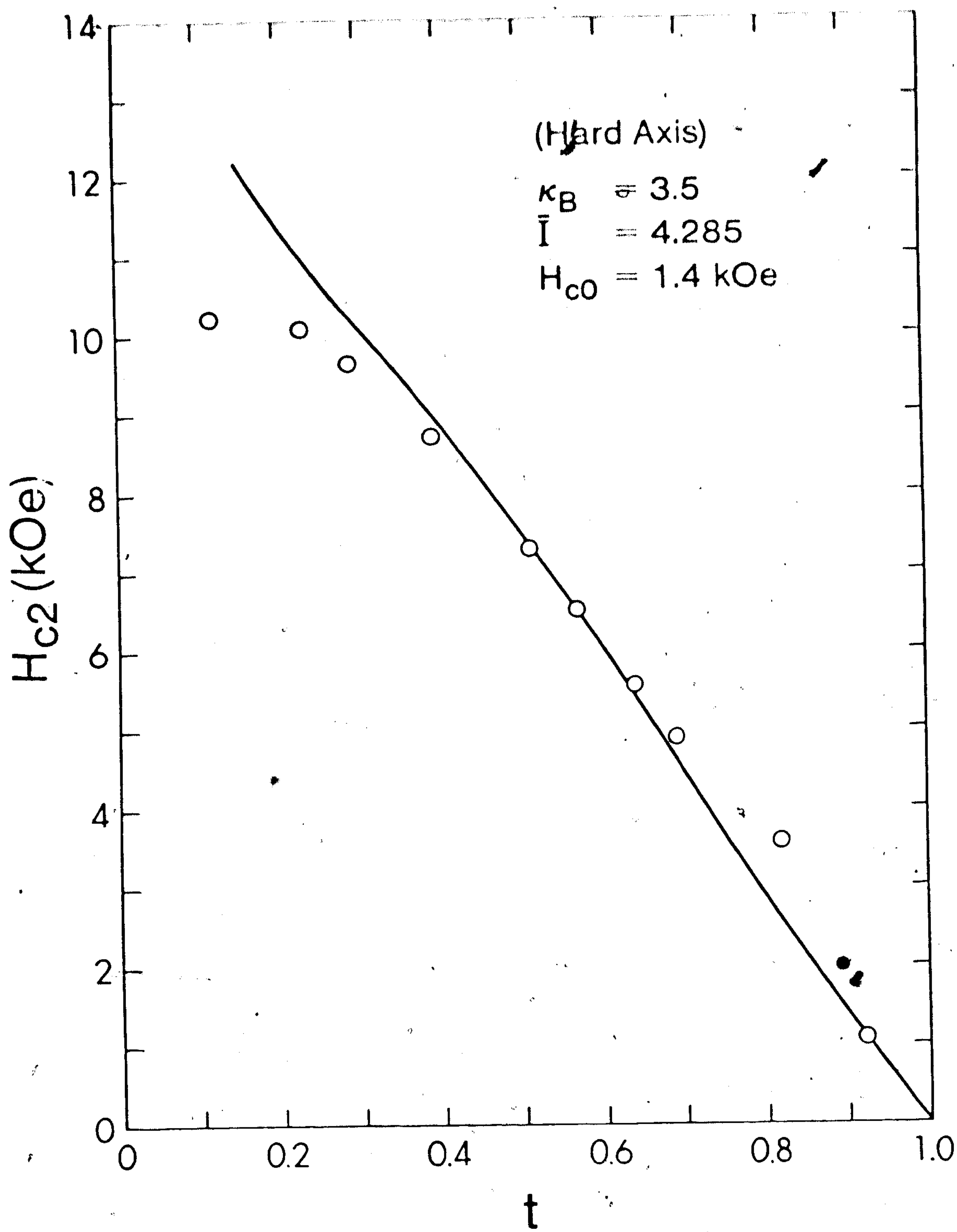

(Hard Axis)
κ_B = 3.5
$\bar{I}$ = 4.285
H_{c0} = 1.4 kOe
H_{c2} (kOe)
t
0
2
4
6
8
10
12
14
0.2
0.4
0.6
0.8
1.0

Fig. 19. Easy axis magnetization curves for various values of the reduced temperature calculated using the parameters given in table 2 including the effect of the spin fluctuations. (Source Ref. 154)

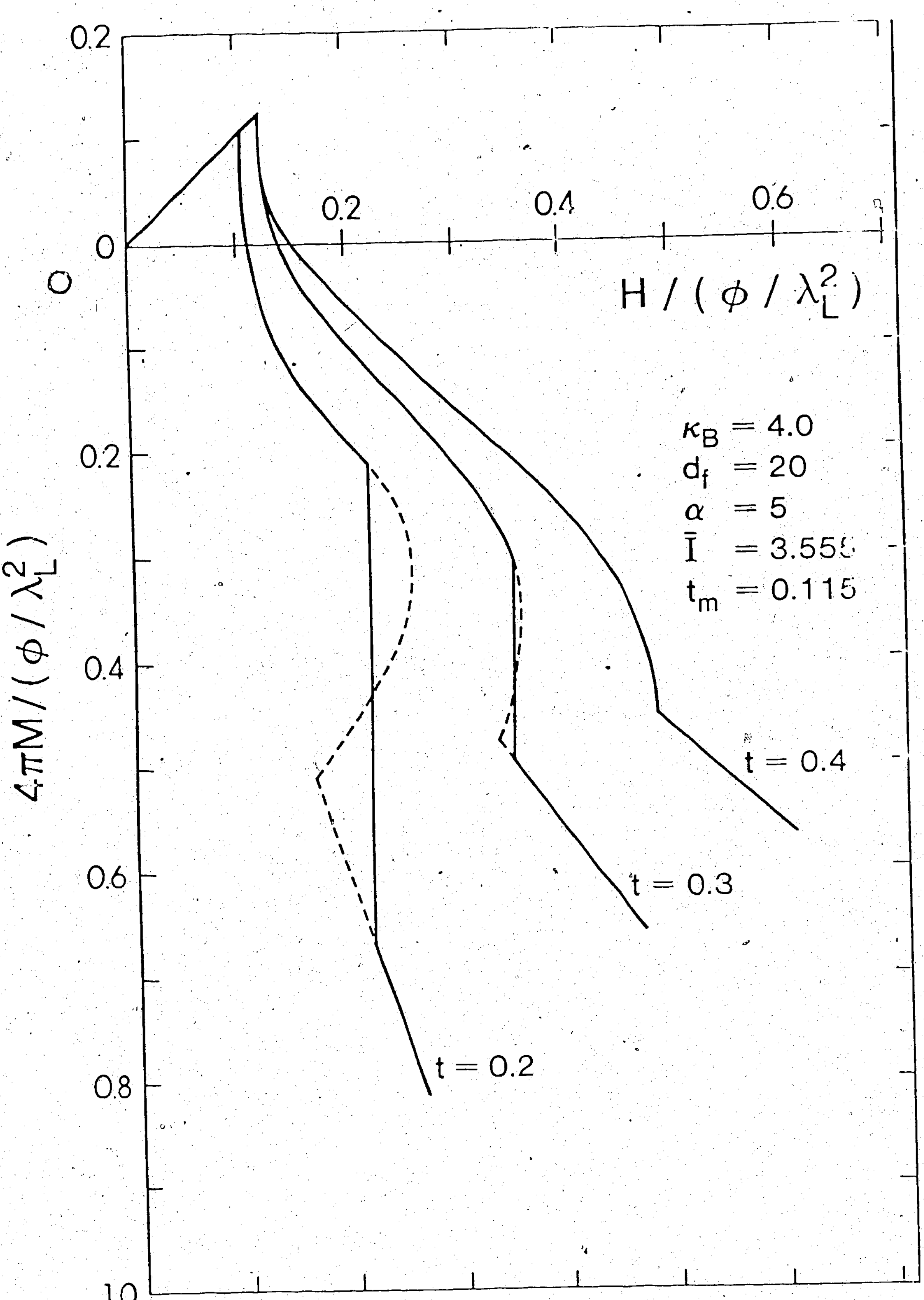

0.2
0
0.2
0.4
0.6
0.8
1.0
0.2
0.4
0.6
O
$H / (\phi / \lambda_L^2)$
$4\pi M / (\phi / \lambda_L^2)$
$\kappa_B = 4.0$
$d_f = 20$
$\alpha = 5$
$\bar{I} = 3.555$
$t_m = 0.115$
t = 0.4
t = 0.3
t = 0.2

Fig. 20. Easy axis magnetization curves for various values of the reduced temperature calculated using the parameters given in table 3 neglecting the effect of the spin fluctuations. (Source Ref. 154)

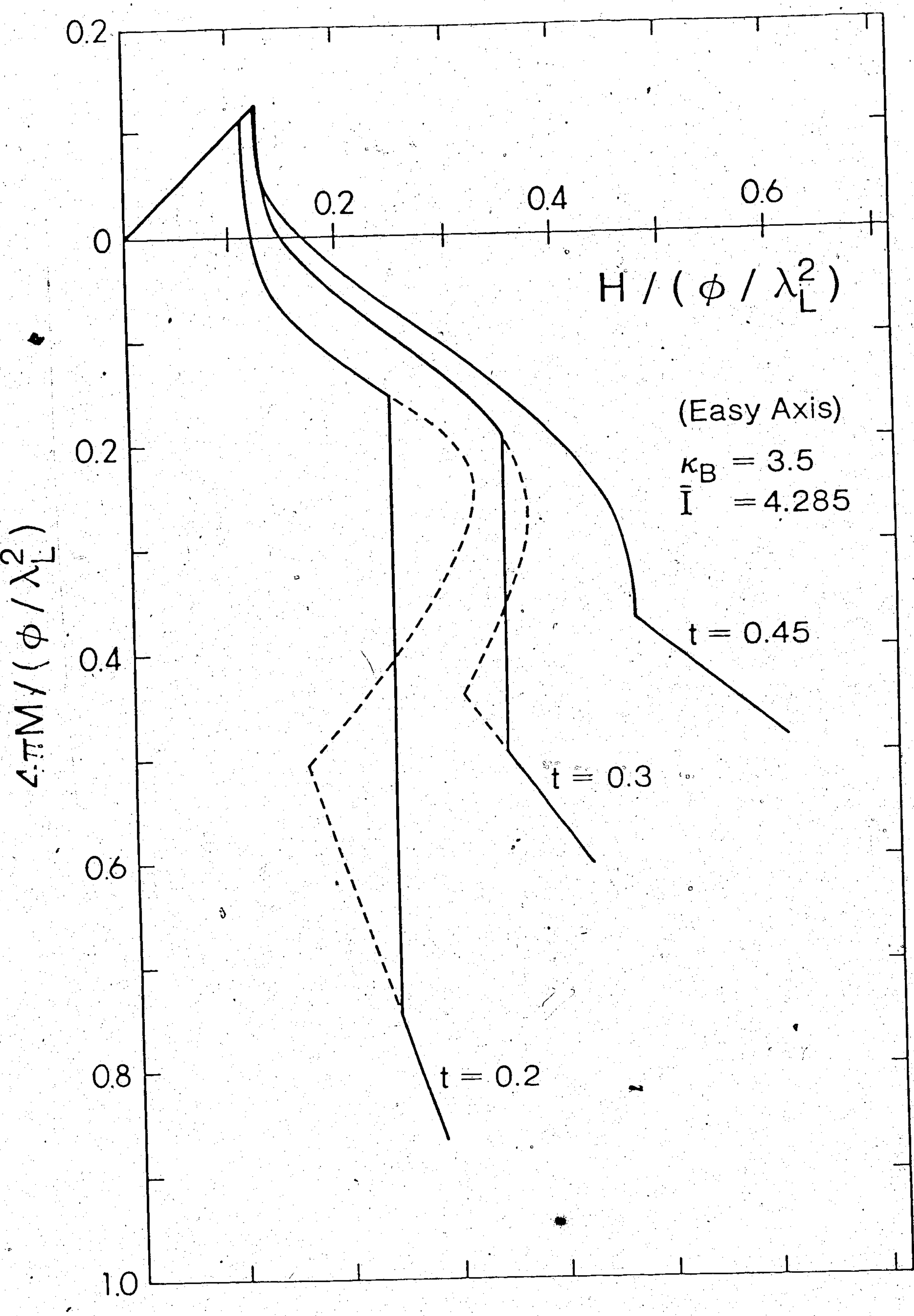

0.2
0
0.2
0.4
0.6
0.8
1.0
0.2
0.4
0.6
H / (φ / λ_L^2)
4πM / (φ / λ_L^2)
(Easy Axis)
κ_B = 3.5
Ī = 4.285
t = 0.45
t = 0.3
t = 0.2

Fig. 21. The jump in the magnetization at H_{c1}, ΔM_I, calculated from the curves similar to those shown in figure 19. (Source Ref. 154)

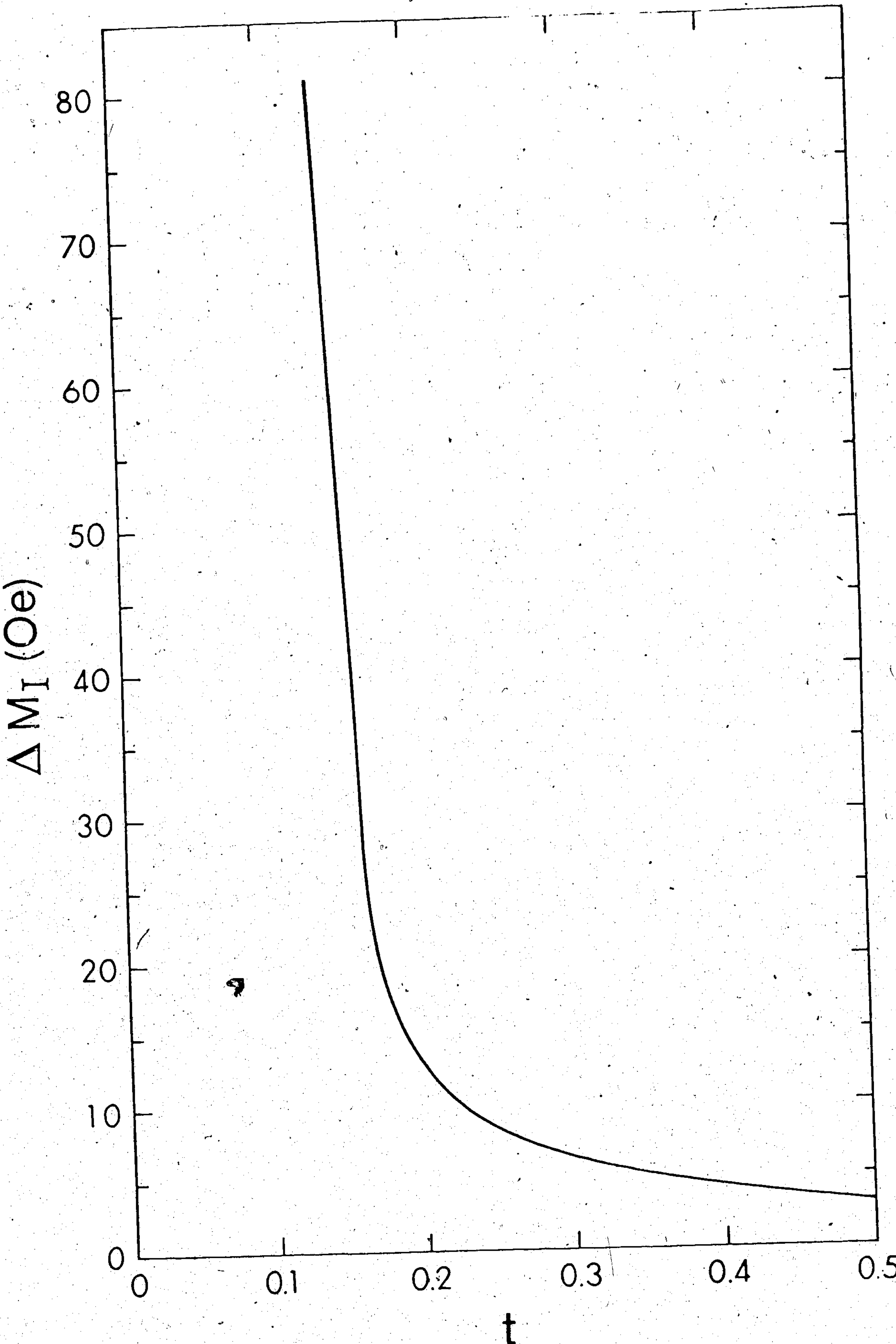
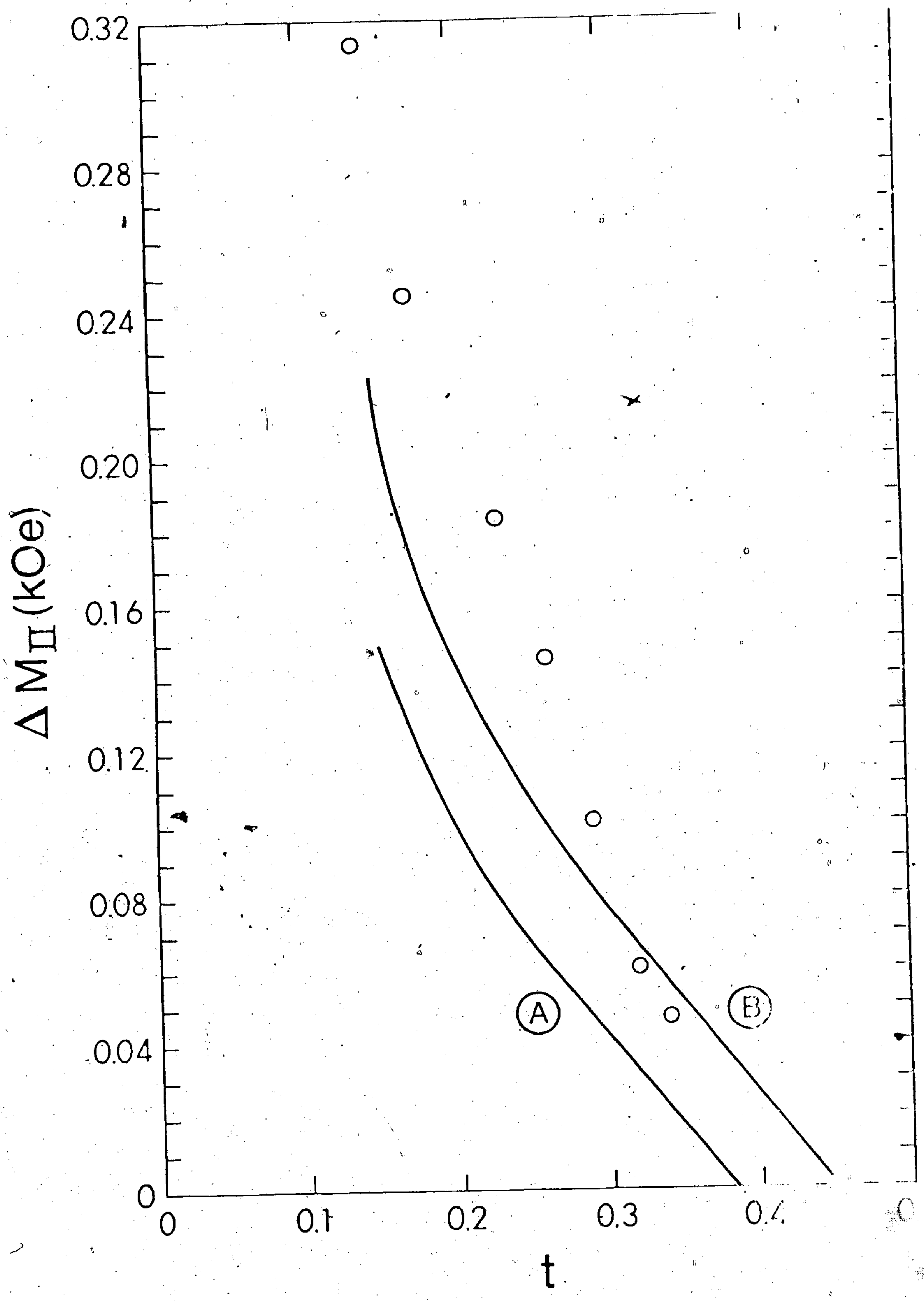
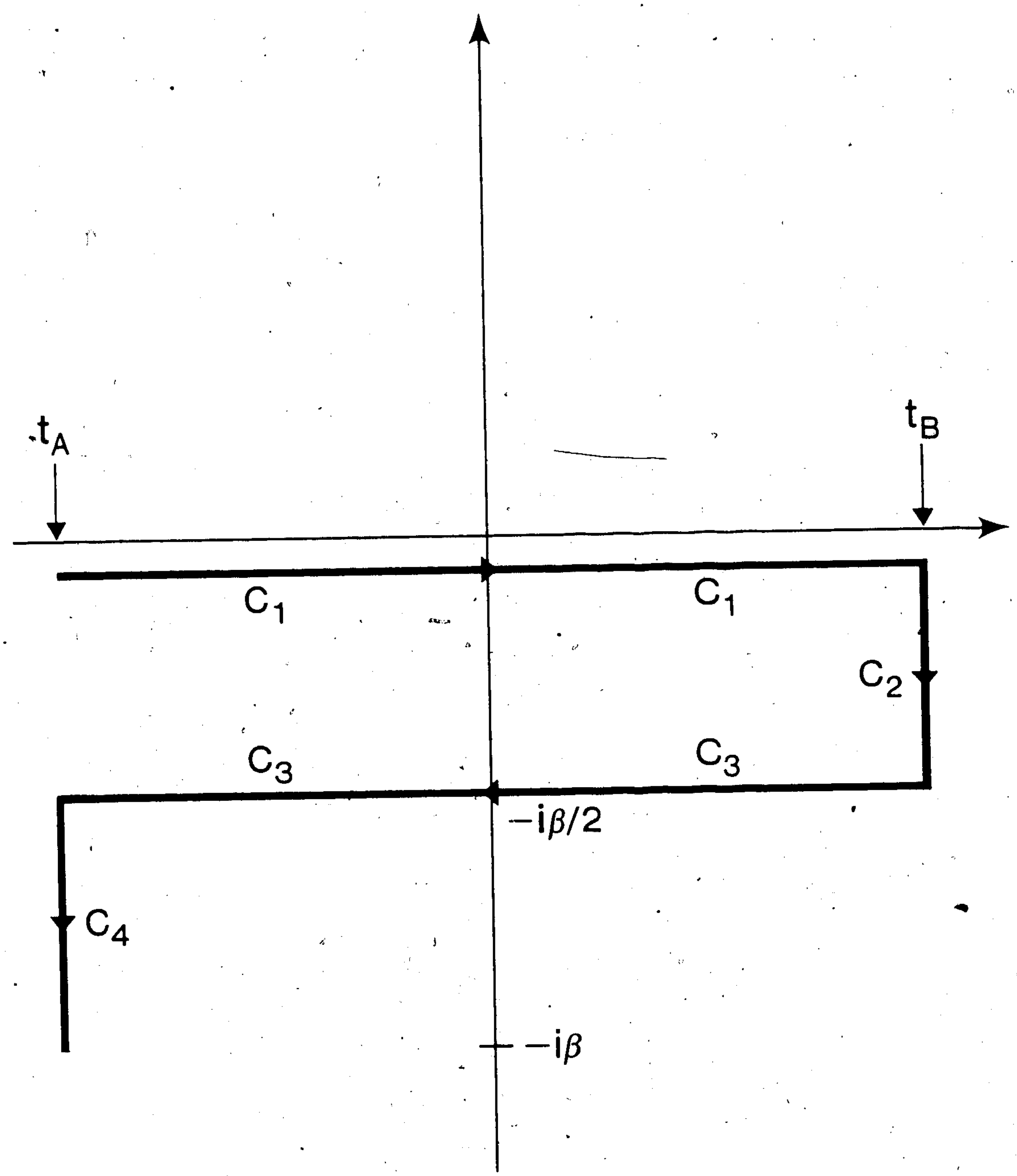

80
70
60
50
40
30
20
10
0
ΔM_I (Oe)
0
0.1
0.2
0.3
0.4
0.5
t

Fig. 22. The jump in the magnetization at H_{c2}, ΔM_{II}. The lower curve (labelled A) is calculated from the parameters given in table 2 including the effect of the spin fluctuations. The upper curve (labelled B) is calculated from the parameters given in table 3 neglecting the effect of the spin fluctuations. (Source Ref. 154)



0.32
0.28
0.24
0.20
0.16
0.12
0.08
0.04
0
Δ M_{II} (kOe)
0
0.1
0.2
0.3
0.4
t
A
B

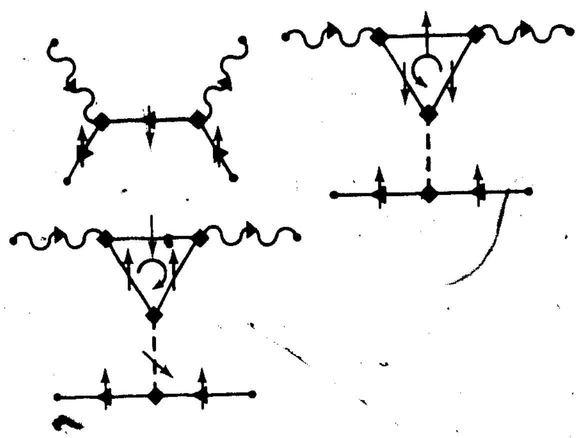
Fig. 23. The contour C employed in the path ordering method, described in Appendix, to generate the real time finite temperature Green's functions.



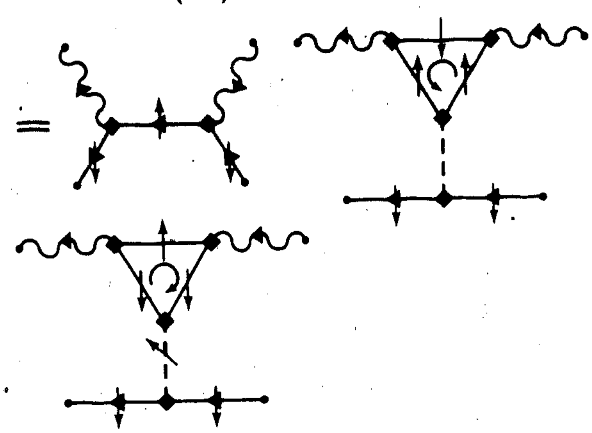
t_A
t_B
C_1
C_1
C_2
C_3
C_3
$-i\beta/2$
C_4
$-i\beta$

Fig. 24. Diagrammatic contributions to the vertices $\Gamma_{\uparrow M}$ and $\Gamma_{\downarrow M}$ used to obtain the expressions given in Eqs. (B.3a) and (B.3b).

$$G_\uparrow(p)\Delta(q)\,\frac{i}{(2\pi)^4}\,\Gamma_{\uparrow M}(p;q;q';p')\Delta(q')G_\uparrow(p')$$

$=$ 

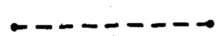
$$G_\downarrow(p)\Delta(q)\,\frac{i}{(2\pi)^4}\,\Gamma_{\downarrow M}(p;q;q';p')\Delta(q')G_\downarrow(p')$$

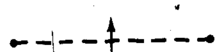
$=$ 

$G_\uparrow(p) =$ 

$G_\downarrow(p) =$ 

$\Delta(q) =$ 

$\frac{1}{1-\lambda^2 D_\uparrow D_\downarrow} =$ 

$\frac{D_\uparrow}{1-\lambda^2 D_\uparrow D_\downarrow} =$ 

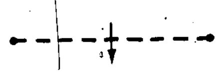
$\frac{D_\downarrow}{1-\lambda^2 D_\uparrow D_\downarrow} =$ 

Fig. 25. Geometry near the surface for calculation of surface impedance in Appendix D.

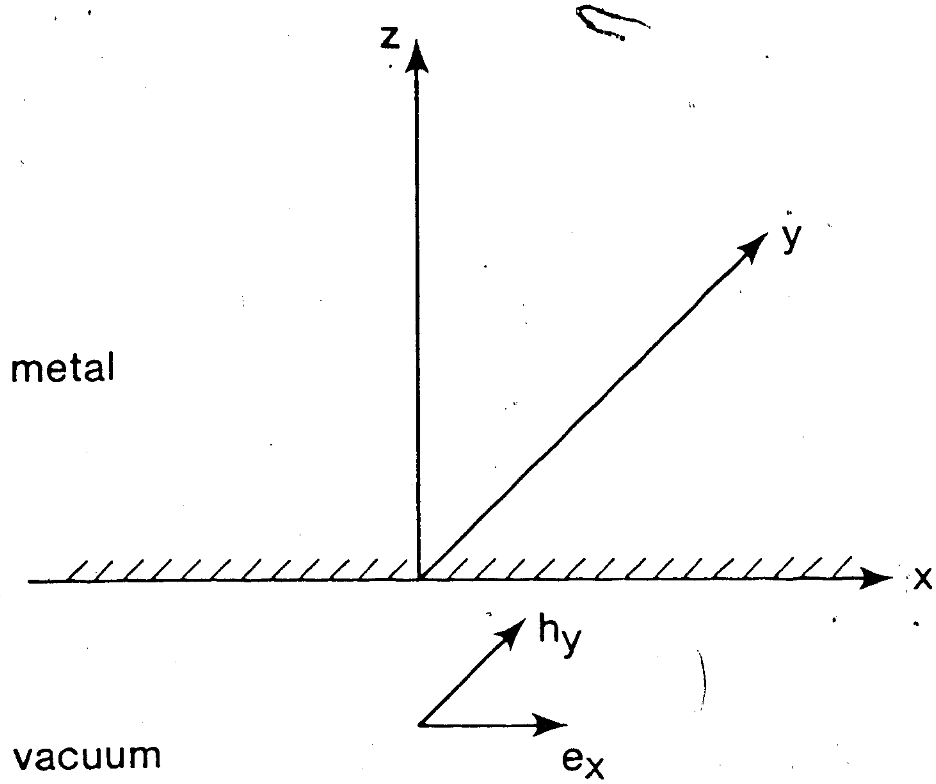
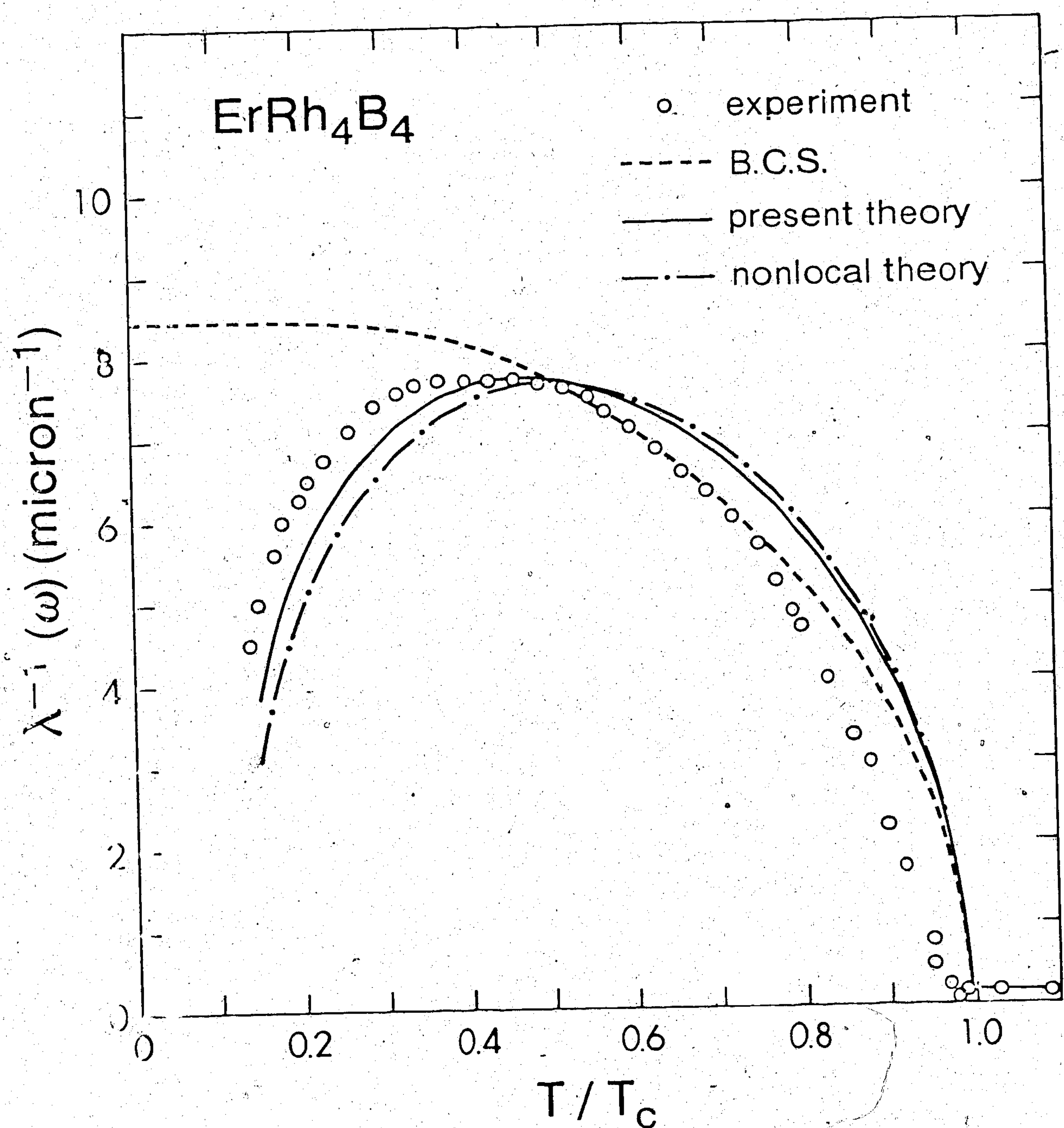
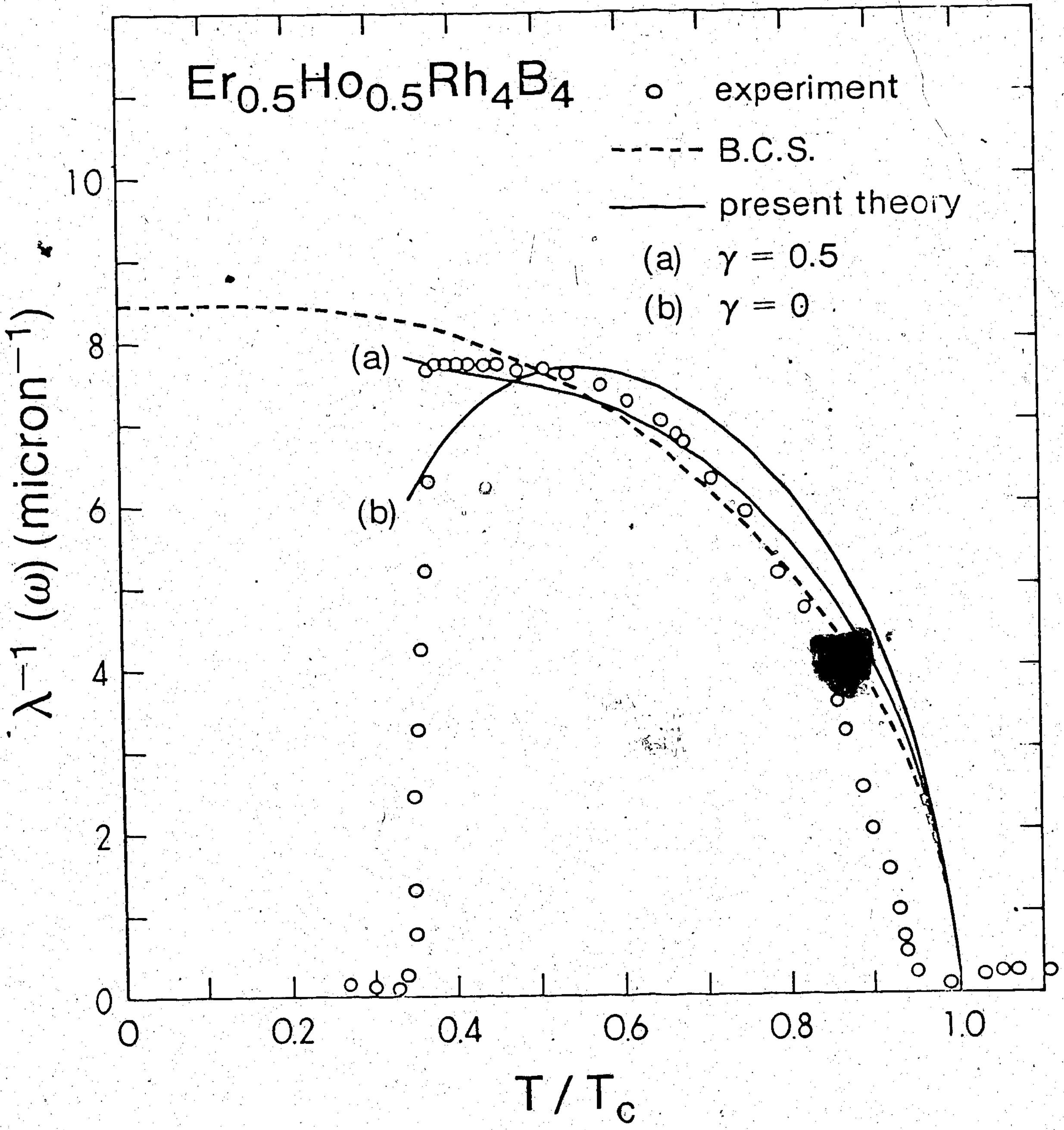

z
y
metal
x
h_y
vacuum
e_x

Fig. 26. Penetration depth $\lambda(\omega)$ for $ErRh_4B_4$. The circles are experimental values ($\omega = 9.3$ GHz, $T_c = 8.7°K$). The solid line is the theoretical curve ($T_m = 1.0°K$, $4\pi C/T_m = 2.3$, $\lambda_L(0) = 908$ Å, $d_o = 0.2529 \times 10^{-2}$, $\delta/\lambda_L = 86.4$, $\mu = \gamma = 0$). The dashed line is for the BCS theory ($\lambda_L(0) = 1184$ Å). The dot-dashed line is for the static non-local theory in refs. [150] and [149] ($\kappa_B = 4$, $d_o = 0.4254 \times 10^{-2}$, $\lambda_L(0) = 749$ Å. Other parameters are the same as for the solid line.)



ErRh4B4
experiment
B.C.S.
present theory
nonlocal theory
λ⁻¹ (ω) (micron⁻¹)
10
8
6
4
2
0
0
0.2
0.4
0.6
0.8
1.0
T / Tc

Fig. 27. Penetration depth $\lambda(\omega)$ for $Er_{0.5}Ho_{0.5}Rh_4B_4$. The circles are experimental values ($\omega = 9.3$ GHz, $T_c = 7.35$ °K). The solid line is the theoretical curves ($T_m = 3.2$ °K, $4\pi C/T_m = 2.3$, $d_0 = 1.0$, $\mu = 0$ and for (a), $\gamma = 0.5$, $\delta/\lambda_L(0) = 52.2$, $\lambda_L(0) = 868$ Å and for (b), $\gamma = 0$, $\delta/\lambda_L(0) = 59.1$, $\lambda_L(0) = 767$ Å). The dashed line is for the BCS theory ($\lambda_L(0) = 1186$ Å).



$Er_{0.5}Ho_{0.5}Rh_4B_4$
o experiment
B.C.S.
present theory
(a) $\gamma = 0.5$
(b) $\gamma = 0$
(a)
(b)
λ^{-1} (ω) (micron^{-1})
0
2
4
6
8
10
0
0.2
0.4
0.6
0.8
1.0
T / T_c

REFERENCES

[1] L. Laplae, H. Umezawa and F. Mancini, Phys. Rep. 10C, 151 (1974).

[2] Y. Takahashi and H. Umezawa, Collect. Phen. 2, 151 (1975).

[3] J.C. Ward, Phys. Rev. 78, 182 (1950).

[4] Y. Takahashi, Nuovo Cim. 6, 370 (1957).

[5] H. Matsumoto and H. Umezawa, Fortschr. der Phys. 24, 357 (1977).

[6] H. Matsumoto, M. Tachiki and H. Umezawa, Fortschr. der Phys. 25, 273 (1977).

[7] H. Umezawa, H. Matsumoto and M. Tachiki, "Thermo Field Dynamics and Condensed States", North Holland, Amsterdam (1982).

[8] M.T. Béal-Monod, S.K. Ma and D.R. Fredkin, Phys. Rev. Lett. 20, 929 (1968).

[9] T. Moriya and A. Kawabata, J. Phys. Soc. of Japan 34, 639 (1973).

[10] G.W. Crabtree, F. Berhoozi, S.A. Cambell and D.G. Hinks, Phys. Rev. Lett. 49, 1342 (1982).

[11] F. Berhoozi, G.W. Crabtree, S.A. Cambell and D.G. Hinks, Phys. Rev. B27, 6849 (1983).

[12] W.A. Fertig, D.C. Johnson, L.E. DeLong, R.E. McCallum, M.B. Maple and B.T. Matthias, Phys. Rev. Lett. 38, 987 (1977).

[13] M. Ishikawa and Ø. Fisher, Solid State Commun. 23, 37 (1977); Solid State Commun. 24, 747 (1977).

[14] M. Tachiki, A. Kotani, H. Matsumoto and H. Umezawa, Solid State Commun. 31, 927 (1979).

[15] H. Matsumoto, H. Umezawa and M. Tachiki, Solid State Commun. 31, 157 (1979).

[16] E.I. Blount and C.M. Varma, Phys. Rev. Lett. 42, 1079 (1979).

[17] H.S. Greenside, E.I. Blount and C.M. Varma, Phys. Rev. Lett. 46, 49 (1981).

[18] H. Suhl, in Felix Bloch Festschrift (1980).

[19] S.C. Schneider, M. Levy, R. Chen, M. Tachiki, D.C. Johnson and B.T. Matthias, Solid State Commun. 40, 61 (1981).

[20] N. Toyota, S.B. Woods and Y. Muto, Solid State Commun. 37, 547 (1981).

[21] D.E. Moncton, J. Appl. Phys. 50, 1880 (1979).

[22] D.E. Moncton, D.B. McWhan, P.H. Schmidt, G. Shirane, W. Thomlinson, M.B. Maple, H.M. McKay, L.D. Woolf, Z. Fisk and D.C. Johnston, Phys. Rev. Lett. 45, 2060 (1980).

[23] S.K. Sinha, G.W. Crabtree, D.G. Hinks and H. Mook, Phys. Rev. Lett. 48, 950 (1982).

[24] J.W. Lynn, G. Shirane, W. Thomlinson and R.N. Shelton, Phys. Rev. Lett. 48, 950 (1982).

[25] J.W. Lynn, G. Shirane, W. Thomlinson, R.N. Shelton and D.E. Moncton, Phys. Rev. B 24, 3817 (1981).

[26] I. Shapira, M.N. Shah and H. Umezawa, Physica, 84B, 213 (1976).

[27] M. Tachiki, H. Matsumoto and H. Umezawa, Phys. Rev. B 20, 1915 (1979).

[28] H. Matsumoto, R. Teshima, H. Umezawa and M. Tachiki, Phys. Rev. B 27, 158 (1983).

[29] O. Sakai, M. Suzuki, S. Maekawa, M. Tachiki, G.W. Crabtree and F. Berhoozi, J. Phys. Soc. of Japan 52, 134 (1983).

[30] T. Koyama, S. Maekawa and M. Tachiki, J. Phys. Soc. of Japan 52, 1750 (1983).

[31] T. Matsubara, Progr. Theor. Phys. 14, 351 (1955).

[32] L.P. Kadanoff and G. Baym, "Quantum Statistical Mechanics: Green's Function Methods in Equilibrium and Non-Equilibrium Problems", W.A. Benjamin, Reading, Mass. (1964).

[33] P.C. Martin and J. Schwinger, Phys. Rev. 115, 1342 (1959).

[34] G. Baym and N.D. Mermin, J. Math. Phys. 2, 232 (1961).

[35] R. Mills, Unpublished Preprint (1962).

[36] R. Mills, "Propagators for Many Particle Systems", Gordon and Breach, N.Y. (1969).

[37] L.V. Keldysh, Sov. Phys. JETP 20, 1018 (1965).

[38] R.A. Craig, J. Math. Phys. 9, 605 (1968).

[39] A.S. Wightman, Phys. Rev. 101, 860 (1956).

[40] H. Matsumoto, Fortschr. der Phys. 25, 1 (1977).

[41] H. Schmutz, Z. Phys. B 30, 97 (1978).

[42] H. Matsumoto, Y. Nakano, H. Umezawa and F. Mancini, Prog. Theor. Phys. 70, 599 (1983).

[43] H. Matsumoto, Y. Nakano and H. Umezawa, to be published, J. Math. Phys. (1984).

[44] A.J. Niemi and G.W. Semenoff, Ann. of Phys. 152, 105 (1984).

[45] G.W. Semenoff and H. Umezawa, Nucl. Phys. B 220, 196 (1983).

[46] L. Dolan and R. Jackiw, Phys. Rev. D 9, 3320 (1974).

[47] I. Ojima, Ann. of Phys. 137, 1 (1981).

[48] R. Haag, N.W. Hugenbortz and M. Winnhik, Comm. Math. Phys. 5, 215 (1967).

[49] H. Matsumoto, I. Ojima and H. Umezawa, Ann. of Phys. 152, 348 (1984).

[50] H. Matsumoto, Y. Nakano and H. Umezawa, Phys. Rev. D 28, 1931 (1983).

[51] D. Lurie, "Particles and Fields", Interscience Publishers (1968).

[52] J.D. Bjorken and S.D. Drell, "Relativistic Quantum Mechanics", McGraw-Hill (1965).

[53] A.L. Fetter and J.D. Walecka, "Quantum Theory of Many particle Systems", McGraw-Hill (1971).

[54] M. Gell-Mann and M. Levy, Nuovo Cim. 16, 705 (1960).

[55] M.W. Goldberger and S.B. Trieman, Phys. Rev. 110, 1178 (1958).

[56] D.R. Yennie, S.C. Frautschi and H. Suura, Ann. of Phys. 13, 379 (1961).

[57] H. Matsumoto, N.J. Papastimatio and H. Umezawa, Nucl. Phys. B 68, 236 (1974); Nucl. Phys. B 82, 45 (1974).

[58] F.J. Wegner, Z. Phys. B 25, 327 (1975); Z. Phys. B 35, 207 (1979).

[59] P.B. Littlewood and C.M. Varma, Phys. Rev. B 26, 4883 (1982).

[60] M. Wadati, Phys. Rep. 50, 87 (1979).

[61] E. Tablot and A. Griffen, Ann. of Phys. 151, 71 (1983).

[62] T. Toyda, Ann. of Phys. 141, 154 (1982); Ann. of Phys. 147, 244 (1983).

[63] J.A. Hertz and D.M. Edwards, J. Phys. F 3, 2174 (1973).

[64] D.M. Edwards and J.A. Hertz, J. Phys. F 3, 2191 (1973).

[65] H. Matsumoto, H. Umezawa, S. Seki and M. Tachiki, Phys. Rev. B 17, 2276 (1978).

[66] J.P. Whitehead, H. Matsumoto and H. Umezawa, Phys. Rev. B 29, 423 (1984).

[67] J.P. Whitehead, H. Matsumoto and H. Umezawa, Phys. Rev. B 25, 4737 (1982).

[68] Y. Takahashi, Phys. Rev. D 15, 1589 (1977).

[69] Y. Takahashi and T. Gotō, Prog. Theor. Phys. 57, 1732 (1977).

[70] See for example, R.M. White, "Quantum Theory of Magnetism", 2nd Edition, Section 4.1.1, Springer Verlag (1983).

[71] W. Pauli, Z. Phys. 41, 81 (1927).

[72] J.C. Slater, Phys. Rev. 49, 537 (1936).

[73] E.C. Stoner, Proc. Roy. Soc. (London) A 165, 372 (1938).

[74] P. Hohenberg and W. Kohn, Phys. Rev. B 136, 864 (1964).

[75] W. Kohn and L.J. Sham, Phys. Rev. A 140, 1133 (1965).

[76] V.L. Moruzzi, J.F. Janack and A.R. Williams, "Calculated Electronic Properties of Metals", Pergamon Press, N.Y. (1978).

[77] O.K. Andersen, J. Madsen, U.K. Poulsen, O. Jepsen and J. Kollar, Physica 86-88B, 249 (1977).

[78] J. Calloway and C.S. Wang, Physica 91B, 337 (1977).

[79] J. Hubbard, Proc. Roy. Soc. (London) A 276, 238 (1963).

[80] For the definition of the Wannier functions see for example, C. Kittel, "Qauntum Theory of Solids", Wiley, N.Y. (1963).

[81] See for example the review by S. Doniach, Adv. in Phys. 18, 819 (1969).

[82] F. Bloch, Z. Phys. 61, 206 (1930); Z. Phys. 74, 295 (1932).

[83] O. Gunnarson, J. Appl. Phys. 49, 1399 (1978).

[84] B.T. Matthias and R.M. Bozorth, Phys. Rev. 100, 604 (1958).

[85] B.T. Matthias, A.M. Clogston, H.J. Williams, E. Coreniwitz and R.C. Sherwood, Phys. Rev. Lett. 7, 7 (1961).

[86] G.S. Knapp, F.Y. Fradin and H.V. Culbert, J. Appl. Phys. 42, 1341 (1971).

[87] W.E. Gardener, T.F. Smith, B.F. Howlett, C.W. Chu and A. Sweedler, Phys. Rev. 166, 577 (1968).

[88] D.M. Edwards and E.P. Wohlfarth, Proc. Roy. Soc. (London) A 303, 127 (1968).

[89] R.D. Lowde, Proc. Roy. Soc. (London) A 235, 305 (1956).

[90] V.J. Minkiewicz, M.F. Collins, R. Nathans and G. Shirane, Phys. Rev. 182, 624 (1969).

[91] H.A. Mook, R.M. Nicklow, E.D. Thompson and M.K. Wilkinson, J. Appl. Phys. 40, 1450 (1969).

[92] T. Holstien and H. Primakoff, Phys. Rev. 58, 1098 (1940).

[93] F.J. Dyson, Phys. Rev. 102, 1217 (1956).

[94] A.J. Niemi and G.W. Semenkoff (to be published) (1983).

[95] J.F. Cornwell, Proc. Roy. Soc. (London) A 284, 423 (1965).

[96] I. Izuyama and R. Kubo, J. Appl. Phys. 35, 1074 (1964).

[97] J. Mathon and E.P. Wohlfarth, Proc. Roy. Soc. (London) A 302, 409 (1968).

[98] S.U. Tyablikov,"Methods in the Quantum Theory of Magnetism", Plenum, N.Y. (1967).

[99] W.F. Brinkman and S.F. Engelsberg, Phys. Rev. 169, 417 (1968).

[100] K.K. Murata and S. Doniach, Phys. Rev. Lett. 29, 285 (1972).

[101] G. Gumbs and A. Griffen, Phys. Rev. B 13, 5054 (1976).

[102] A. Kawabata, J. Phys. F 4, 1477 (1974).

[103] The term paramagnon appears widely in the literature and is used in analogy with the term magnon to denote certain low lying excitations in the dynamical spin susceptibility. While these do not have the particle-like behaviour of their ferromagnetic counterparts the magnons, consisting instead of a continuum of excitations they nevertheless play an important role in determining the temperature dependence of various quantities such as the static susceptibility, particularly in the domain $T \geq T_c$.

[104] Here we refer to $\Delta_\uparrow$ and $\Delta_\downarrow$ as paramagnon propagators. Strictly speaking, however, $\Delta_\uparrow$ and $\Delta_\downarrow$ can be decomposed into the spin fluctuation contribution (the paramagnon part) and a term corresponding to the density fluctuations. Calculations[101] however show that, in the region of interest, the contribution of the density fluctuations is negligible.

[105] T. Moriya and A. Kawabata, J. Phys. Soc. of Japan 35, 669 (1973).

[106] V.L. Ginzberg, Sov. Phys. JETP 4, 153 (1957).

[107] H. Suhl and B.T. Matthias, Phys. Rev. Lett. 2, 5 (1959); Phys. Rev. 114, 977 (1959).

[108] A.A. Abrikosov and L.P. Gorkov, Sov. Phys. JETP 12, 1243 (1961).

[109] K. Maki, "Superconductivity", R.D. Parks (ed.), Marcel Dekker, N.Y., 1038 (1969).

[110] M. Tachiki, A. Kotani, S. Takahashi, T. Koyama, H. Matsumoto and H. Umezawa, Solid State Commun. 37, 113 (1981).

[111] A. Kotani, M. Tachiki, H. Matsumoto and H. Umezawa, Phys. Rev. B 23, 5960 (1981).

[112] M. Tachiki, A. Kotani, H. Matsumoto and H. Umezawa, Solid State Commun. 32, 599 (1979).

[113] This possibility was also pointed out by B.T. Matthias and H. Suhl, Phys. Rev. Lett. 4, 51 (1960).

[114] M. Tachiki, H. Matsumoto, T. Koyama and H. Umezawa, Solid State Commun. 34, 19 (1980).

[115] M. Tachiki, S. Takahashi, H. Matsumoto and H. Umezawa, Solid State Commun. 32, 393 (1980).

[116] H. Matsumoto, M. Tachiki and H. Umezawa, Phys. Rev. B 25, 6633 (1982).

[117] H.R. Ott, W.A. Fertig, D.C. Johnson, M.B. Maple and B.T. Matthias, J. Low Temp. Phys. 33, 159 (1978).

[118] H. Adrian, K. Müller and Ischenko-Salemann, Phys. Rev. B 22, 4424 (1980).

[119] K. Okuda, Y. Nakakura and K. Kodowaki, Solid State Commun. 32, 185 (1979).

[120] C.P. Umbach, L.E. Toth, E.D. Dahlberg and A.M. Goldman, Physica 108B, 803 (1981).

[121] U. Poppe, Physica 108B, 805 (1981).

[122] G.W. Crabtree, F. Berhoozi and D.G. Hinks, (unpublished), private communication (1983).

[123] H. Matsumoto, H. Umezawa and J.P. Whitehead, "Interplay Between d-f Interaction and the Dipole Interaction in Magnetic Superconductors", presented at the Argonne Workshop on Magnetic Superconductors, Argonne National Labs, 1983 (unpublished).

[124] N. Nakanishi, Prog. Theor. Phys. 49, 640 (1973).

[125] B. Lautrap, Mat. Fys. Medd. Dan. Vid. Salsk. 35, 1 (1967).

[126] V. Jaccarino and M. Peter, Phys. Rev. Lett. 9, 290 (1962).

[127] S. Maekawa and M. Tachiki, Phys. Rev. B 18, 4688 (1978).

[128] H. Matsumoto, G. Semenoff, R. Teshima, M. Tachiki and H. Umezawa, University of Alberta, Preprint (1979) unpublished.

[129] G. Sarma, J. Phys. and Chem. of Solids 24, 1029 (1963).

[130] L.D. Woolf, D.C. Johnston, H.B. McKay, R.W. McCallum and M.B. Maple, J. Low Tem. Phys. 35, 651 (1979).

[131] G.W. Crabtree, Private Communication (1982).

[132] F. Berhoozi, Private Communication (1983).

[133] S.K. Sinha, G.W. Crabtree, D.G. Hinks and H. Mook, Physica 109 and 110B, 1693 (1983).

[134] M.B. Maple, "Ternary Superconductors", Page 131, Ed. Shenoy, Dunlap and Fradin, Elsevier, North Holland (1981).

[135] M. Tachiki, Physica 109-110B&C, 1699 (1982); J. Magn. and Magn. Mat. 31-34, pt. 2, 484 (1983).

[136] C.Y. Huang, G. Kozlowski, F. Mancini, M.B. Maple, H. Matsumoto, C.E. Olsen, H. Umezawa and J.P. Whitehead, "Penetration Depth in Some Re-entrant Superconductors", presented at APS Meeting, Detroit, March 1983; "Penetration Depth Anomalies in Ferromagnetic Superconductors", submitted to Phys. Rev. Lett. for publication.

[137] For a review of the applications and results of the SCR method see T. Moriya, J. Magn. and Magn. Mat. 14, 1 (1979).

[138] P.W. Anderson, Phys. Rev. 110, 827, 1900 (1958).

[139] K. Yosida, Prog. Theor. Phys. 21, 731 (1959).

[140] P. Higgs, Phys. Rev. 45, 1156 (1960).

[141] T.W.B. Kibble, Phys. Rev. 155, 1554 (1957).

[142] For a review of the electromagnetic interaction and its various applications in ferromagnetic superconductors see, H. Matsumoto and H. Umezawa, Interplay between Magnetism and Superconductivity, Cryogenics, January (1983).

[143] A. Koldziejczyck, B.V.B. Sarkissian and B.R. Coles, J. Phys. F 10, L333 (1980).

[144] W. Cheng, G. Cruezet, P. Garoche, I.A. Cambell and E. Gratz, J. Phys. F 12, 475 (1982).

[145] Y. Yamaguchi, Y. Nishihara and S. Ogawa, J. Magn. and Magn. Mat. 21, 191 (1980).

[146] F. Steglich, J. Aarts, C.D. Bredl, W. Lieke, D. Meschede, W. Franz and H. Schafer, Phys. Rev. Lett. 43, 1892 (1979).

[147] H.R. Ott, H. Rudigier, Z. Fish and J.L. Smith, Phys. Rev. Lett. 50, 1595 (1983).

[148] P.M. Morse and H. Feshbach, "Methods of Mathematical Physics", Vol. II, McGraw-Hill (1953).

[149] T. Koyama, A. Kotani, S. Takahashi, M. Tachiki, H. Matsumoto and H. Umezawa, J. Phys. Soc. of Japan 51, 3469 (1982).

[150] F. Mancini and M. Fusco Girard, Phys. Lett. 95A, 447 (1983).

[151] H.A. Mook, W.C. Koehler, M.B. Maple, Z. Fisk, D.C. Johnston and L.D. Woolf, Phys. Rev. B 25, 372 (1982).

[152] S. Maekawa, J.L. Smith and C.Y. Huang, Phys. Rev. B 22, 164 (1980).

[153] H. Matsumoto, H. Umezawa and J.P. Whitehead, Phys. Rev. B 30, 1294 (1984).

[154] J.P. Whitehead, H. Matsumoto, R. Teshima and H. Umezawa, Phys. Rev. B 30, 1314 (1984).

APPENDIX A
The Path Ordering Method

In this section we wish to briefly discuss the finite temperature Green's function method using the path ordering technique presented by Mills[35,36] and its relation to the TFD formalism following Matsumoto et al[42,43]. The reason for including this short digression is that while the path ordering method really only provides us with a formulation for the perturbation theory in terms of Feynman diagrams for the real time finite temperature Green's functions as opposed to the complete finite temperature field theoretic formulation provided us by thermo-field dynamics, it does serve to highlight the relation between the more familiar Matsubara method and TFD. It also provides as I shall demonstrate a somewhat different raison d'etre for the tilde degrees of freedom than that provided in the discussion of section 2.1.

We begin by considering the two point G_{AB} defined by

$$G_{AB}(x-y) = \mathrm{Tr}\{e^{-\beta H}A(x)B(y)\}/\mathrm{Tr}\{e^{-\beta H}\} \tag{A.1}$$

inserting a complete set of energy eigenstates we note that

$$G_{AB}(x-y) = \sum_{nm} e^{iE_n(x_0-y_0+i\beta)} \langle n|A(\vec{x};x_0=0)|m\rangle$$
$$e^{-E_m(x_0-y_0)} \langle m|B(\vec{y};y_0=0)|n\rangle/\mathrm{Tr}\{e^{-\beta H}\} \tag{A.2}$$

From this we see that the Greens function G_{AB} may be analytically continued to imaginary times provided

$$-\beta < \mathrm{Im}(x_0-y_0) < 0 \tag{A.3}$$

in which case the summation will converge exponentially, since the eigenvalues $\{E_n\}$ are positive definite. This allows us to define a somewhat more general quantity than that given by Eq. (A.1). If we define a contour C running from t_0 to $t_0 - i\beta$, then we can define with respect to this contour C, the function

$$G^{c}_{AB}(\vec{x}-\vec{x}';z,z') = Tr\{e^{-\beta H}T_c[A(\vec{x};z)B(\vec{x}';z')]\}/Tr\{e^{-\beta H}\}. \qquad (A.4)$$

where T_c denotes that the operators appearing in the product are ordered according to their position along the contour C. From condition Eq. (A.3) we see that G^{c}_{AB} is well defined provided the contour C has a monotically decreasing imaginary part. Obviously the definition of the path ordering product defined for the two point function can be generalised to consider other multi-point functions, we will however restrict the discussion to the two point function of Eq. (A.4).

As with the evaluation of the time ordered operators products in thermofield dynamics the computation of Eq. (A.4) may be best achieved by means of the interaction representation. Separating the Hamiltonian into a free part H_0 and an interacting part the H_I

$$H = H_0 + H_I \qquad (A.5)$$

we may define the operators in the interaction representation with complex times as

$$\psi_I(\vec{x};z) = e^{iH_0 z}\psi(\vec{x};0)e^{-iH_0 z}. \qquad (A.6)$$

These are related to the Heisenberg field through the evolution operator as

$$\psi(x;z) = U(0;z)\psi_I(\vec{x};z)U(z;0) \qquad (A.7)$$

where $U(z;z')$ is given by

$$U(z;z') = e^{iH_o z} e^{-iH(z-z')} e^{-iHz'} \tag{A.8}$$

This may be computed perturbatively for points z and z' on the contour C as

$$U(z;z') = \sum_n \frac{(-i)^n}{n!} \oint_{z'}^{z} dz_1 \ldots \oint_{z'}^{z} dz_n \, T_c [H_I'(z_1) \ldots H_I(Z_n)]$$

$$= T_c[\exp - i \oint_{z_o}^{z} H_I'(z) dz] \tag{A.9}$$

where $H_I'(z)$ simply denotes $H_I[\psi_I(z);\psi_I(z')]$ and $\oint$ means the integral is along the path C in the complex plane. Defining the single particle Greens function in the path ordering formalism as

$$G^c(\vec{x}-\vec{x}';z',z') = Tr\{e^{-\beta H} T_c[\psi(\vec{x};z)\psi^{\dagger}(\vec{x};z')]\}/Tr\{e^{-\beta H}\} \tag{A.10}$$

$$= Tr\{e^{-\beta H_o} e^{(\beta+it_o)H_o} e^{-(\beta+it_o)} \psi(\vec{x};z)\psi^{\dagger}(\vec{x}';z') e^{i\tau H} e^{-i\tau H_o}\}$$

$$/Tr\{e^{-\beta H}\} \tag{A.11}$$

for $Im(z-z') < 0$. Eq. (A.7) together with Eq. (A.8) allows us to write Eq. (A.11) as

$$G^c(\vec{x}-\vec{x}';z',z') = Tr\{e^{-\beta H_o} U(t_o-i\beta;z)\psi_I(\vec{x};z)U(z;z')$$

$$\psi(\vec{x}';z')U(z';t_o)\}/Tr\{e^{\beta H}\} \tag{A.12}$$

$$= \langle T_c[S_c \psi_I(\vec{x};z)\psi_I^{\dagger}(\vec{x}';z')]\rangle_o \; [Tr\{e^{-\beta H_o}\} Tr\{e^{-\beta H}\}^{-1}] \tag{A.13}$$

where

$$S_c = T_c[\exp - i \oint_{t_o-i\beta}^{t_o} H_I'(z) dz] \tag{A.14}$$

and

$$\langle O \rangle_o = \mathrm{Tr}\{e^{-\beta H_o} O\}/\mathrm{Tr}\{e^{-\beta H_o}\} \qquad \text{(A.15)}$$

The perturbative expression of Eq. (A.13) may be expressed in terms of the Feynman diagrams by means of the finite temperature Wick's theorem.

$$\langle T_c[\prod_{i=1}^{2p} A_i(z_i)]\rangle_o = (-1)^p \sum_{r=2}^{2p} (-\rho_F)^{r-1} \langle T_c[A_1(z_1)A_r(z_r)]\rangle_o$$

$$\langle T_c[\prod_{\substack{i\neq 1\\ i\neq r}} A_i(z \text{[illegible]} \qquad \text{(A16)}$$

where the operators $\{A_i(z_i)\}$ denote the fields $\psi_I(z)$ and their canonical conjugates $\psi_I^\dagger(z)$. By virtue of Eq. (A.16) and the expression for S_c given in Eq. (A.14) the path ordered Greens functions of Eq. (A.10) may be computed perturbatively in terms of a sum of products of the propagator $\langle T_c[\psi_I(z)\psi_I^\dagger(z')]\rangle_o$. The association of the various contributions to the individual terms in the perturbation series is then straightforward and Feynman rules similar to those obtained at zero temperature may be defined.

Now while it is the case that the Feynman rules for the path ordered Green's function Eq. (A.10) are identical to those generated by the zero temperature theory the resultant integrals involve the path ordered propagator $\langle T_c[\psi_I(z)\psi_I^\dagger(z')]\rangle_o$, the particular form of which depends on the choice of contour. If for example we choose z to be pure imaginary and define C as a contour running from 0 to $-i\beta$ then we generate the Matsubara Green's function and it is fairly straightforward to show that the perturbation scheme reduces to the familiar imaginary time method. A more useful contour for our purposes is that shown in Fig. (23), where the portions C_1 and C_3 have an infinitesimally decreasing imaginary part, since if we let z and z' belong to the portion of the contour C_1 then the path ordered products, which we have denoted by $T_c[\ldots]$, reduce to time ordered products, $T[\ldots]$. Furthermore one finds if the quantities t_A and t_B are taken to $-\infty$ and $+\infty$ respectively, then the contribution arising from these positions, to the path ordered Green's function of Eq. (A.10) will factor out and can be absorbed by the normalisation. We see then that the fields appearing in Eq. (A.13) are of two types, those lying on the portion of the contour C_1 $\psi_I(t)$ and $\psi_I^\dagger(t)$ and those lying on the portion of the contour C_3 $\psi_I(t-i\beta/2)$ and $\psi_I^\dagger(t-i\beta/2)$. The resulting Feynman rules may then be neatly summarised in terms of the four component propagator.

$$S_c^{ab}(x-x') \equiv \langle T_c\left[\begin{Bmatrix}\psi_I(\vec{x};t)\\ \psi_I(\vec{x}'t-i\beta/2)\end{Bmatrix}\{\psi^\dagger(\vec{x}';t)\psi^\dagger(\vec{x}'+-i\beta/2)\}\right]\rangle . \quad (A.17)$$

Calculation shows that this propagator is exactly that obtained in thermofield dynamics and that the Feynman rules obtained from the path ordering method of Mills employing the contour shown in Fig. (23) are equivalent to those obtained in the TFD formalism. Indeed the equivalence of the two theories may be made explicit through the identification.

$$\psi^{\alpha=1}(x;t) \longrightarrow \psi(x't); \quad \psi^{\alpha=1}(x't)^\dagger \longrightarrow \psi^\dagger(x;t) \quad (A.18)$$

and

$$\psi^{\alpha=2}(x;t) \longrightarrow \psi(x;t-i\beta/2); \quad \psi^{\alpha=2}(x't)^\dagger \longrightarrow \psi^\dagger(x;+i\beta/2) \quad (A.19)$$

It is a somewhat surprising fact that the fields ψ^1 and ψ^2 may be chosen so as to commute (anti-commute). This is by no means obvious from the path ordering method where $\psi^{(1)}$ and $\psi^{(2)}$ denote the same fields on separate parts of the contour.

In addition to clarifying the relationship between the Matsubara formalism and thermofield dynamics the work of Matsumoto et al, on which this discussion is based, also shows that while other choices of contour in the path ordering method may be used to construct other finite temperature quantum field theories of which TFD is a special case, the resultant Hamiltonian density except in the case of TFD is not Hermitian in the usual sense and requires the introduction of a metric operator. This somewhat unique property of the TFD formalism explains the rather straightforward structural equivalence of TFD with conventional zero temperature field theory and hence why so many devices of conventional field theory may be extended to finite temperature in a rather obvious way by means of TFD.

APPENDIX B

Thermal Excitation of Magnons at Low Temperature: An Example

In Section 3.2 we presented a rather formal argument regarding the W-T identities generated by the spin rotational invariance and their role in determining the effect of the thermally excited magnons. From this we were able to obtain certain exact results regarding the magnetisation and the quasi particle excitation spectra by means of a low temperature expansion in thermo-field dynamics. In this appendix we wish to present an explicit calculation, in the low temperature expansion of the temperature dependence of the magnetisation which arises from the thermal excitation of the magnons. The purpose of this is two fold, first of all it serves to demonstrate the computational value of the low temperature expansion, and secondly it provides the basis for what could be an extremely useful approximation scheme for the analysis of spin fluctuation effects in metals. The $T^{5/2}$ contribution is calculated explicitly.

Following the outline in Section (3.2) the zero temperature quantities we require are the zero temperature electron propagator, which we calculate in the mean field (MF) approximation, and the electron-magnon vertex. From the results presented in Section (3.2) we know, that if we wish our expression to have the correct $T^{3/2}$ behaviour, then we require that the electron magnon vertex must be calculated in such a way that it satisfies Eq. (3.105) in the case of the spin up electrons and Eq. (3.106) in the case of the spin down. This in effect determines our approximation in the calculation of the electron magnon vertex.

In order to keep the discussion relatively simple we consider the case of the local contact interaction model, expressed by the Lagrangian given in Eqs. (3.9a, 3.9b and 3.15b). Although we point out that the approach is by no means limited to such a simple Lagrangian. The zero temperature electron Green's functions, calculated in the MF approximation are given by

$$G^0_\uparrow(p) = \frac{\theta[\varepsilon(p) - \lambda M_0/2]}{p_0 - \varepsilon(p) + \lambda M_0/2 + i\delta} - \frac{\theta[-\varepsilon(p) + \lambda M_0/2]}{p_0 - \varepsilon(p) + \lambda M/2 - i\delta} \tag{B.1a}$$

and

$$G^0_\uparrow(p) = \frac{\theta[\varepsilon(p) + \lambda M_0/2]}{p_0 - \varepsilon(p) - \lambda M_0/2 + i\delta} - \frac{\theta[-\varepsilon(p) - \lambda M_0/2]}{p_0 - \varepsilon(p) - \lambda M_0/2 - i\delta} , \tag{B.1b}$$

where M_0 denotes the zero temperature magnetisation calculated self consistently from the expression

$$M_0 = - \frac{i}{(2\pi)^4} \int d^4p\{G^0_\uparrow(p) - G^0_\downarrow(p)\} . \tag{B.2}$$

The spin up electron magnon vertex, defined in Eq. (3.96), is given by

$$\begin{aligned} \frac{i}{(2\pi)^4} \Gamma_{\uparrow M}(p,q;q',p+q-q') &= \lambda^2 G^0_\downarrow(p+q) \\ &- \lambda^3[1 - \lambda^2 D_\uparrow(q-q')D_\downarrow(q-q')]^{-1} R_\downarrow(q;q') \\ &+ \lambda^4 D_\downarrow(q-q')[1 - \lambda^2 D_\uparrow(q-q')D_\downarrow(q-q')]^{-1} R_\uparrow(q;q') \end{aligned} \tag{B.3a}$$

and the spin down electron magnon vertex, defined in Eq. (3.98), is given by

$$\begin{aligned} \frac{i}{(2\pi)^4} \Gamma^*_{\downarrow M}(p;q;q';p+q-q') &= \lambda^2 G^0_\uparrow(p-q) \\ &- \lambda^3[1 - \lambda^2 D_\uparrow(q-q')D_\downarrow(q-q')]^{-1} R_\uparrow(q',q') \\ &+ \lambda^4 D_\uparrow(q-q')[1 - \lambda^2 D_\uparrow(q-q')D_\downarrow(q-q')] R_\downarrow(q;q') . \end{aligned} \tag{B.3b}$$

where

$$D_\uparrow(q) = \frac{i}{(2\pi)^4}\int d^4p\ G_\uparrow^o(p-q/2)G_\uparrow^o(p+q/2) \ , \tag{B.4a}$$

$$D_\downarrow(q) = \frac{i}{(2\pi)^4}\int d^4p\ G_\downarrow^o(p-q/2)G_\downarrow(p+q/2) \ ; \tag{B.4b}$$

$$R_\uparrow(q_1;q_2) = \frac{i}{(2\pi)^4}\int d^4p\ G_\uparrow^o(p-q_1)G_\downarrow^o(p)G_\uparrow^o(p-q_2) \ , \tag{B.4c}$$

and

$$R_\downarrow(q_1;q_2) = \frac{i}{(2\pi)^4}\int d^4p\ G_\downarrow^o(p+q_1)G_\uparrow^o(p)G_\downarrow^o(p+q_2) \ . \tag{B.4d}$$

The expressions for the electron magnon vertices given by Eqs. (B.3a and B.3b) are shown diagramatically in Fig. (24).

The electron magnon vertices, given above are determined in such a way that they satisfy the W-T relations given in Eqs. (3.105 and 3.106). This is relatively straightforward to show, in the case of $\Gamma_{\uparrow M}$ we have that

$$\begin{aligned}\frac{i}{(2\pi)^4}\Gamma_{\uparrow M}(p,0;0;p) &= \lambda^2 G_\downarrow^o(p) \\ &- \lambda^3[1-\lambda^2 D_\uparrow(0)D_\downarrow(0)]^{-1}\{R_\downarrow(p;0) - \lambda D_\downarrow(0)R_\uparrow(0;0)\}.\end{aligned} \tag{B.5}$$

The terms $R_\uparrow(0;0)$ and $R_\downarrow(0;0)$ are easily calculated.

$$\begin{aligned}R_\uparrow(0;0) &= \frac{i}{(2\pi)^4}\int d^4p\ G_\uparrow^o(p)G_\downarrow^o(p)G_\uparrow^o(p) \\ &= -\frac{1}{\lambda M_o}\frac{i}{(2\pi)^4}\int d^4p\ G_\uparrow^o(p)[G_\uparrow^o(p)-G_\downarrow^o(p)] \\ &= -\frac{1}{\lambda M_o}D_\uparrow(0) - \frac{1}{(\lambda M_o)^2}\frac{i}{(2\pi)^4}\int d^4p[G_\uparrow^o(p) - G_\downarrow^o(p)] \\ &= -\frac{1}{\lambda M_o}D_\uparrow(0) + \frac{1}{\lambda^2 M_o} \ ,\end{aligned} \tag{B.6}$$

where we have used the result that

$$G_\uparrow^o(p)G_\downarrow^o(p) = -\frac{1}{\lambda M_o}\{G_\uparrow^o(p) - G_\downarrow^o(p)\} \ , \tag{B.7}$$

which follows from the definition of $G^o_{\uparrow(\downarrow)}$ given in Eq. (B.1a) (Eq. (B.1b)). A similar result for $R_\downarrow(0;0)$ gives

$$R_\downarrow(0;0) = \frac{1}{\lambda M_o} D_\downarrow(0) - \frac{1}{\lambda^2 M_o} . \tag{B.8}$$

Substituting Eq. (B.8) and Eq. (B.6) into the result of Eq. (B.5) we obtain

$$\frac{i}{(2\pi)^4} \Gamma_{\uparrow M}(p;0;0;p) = \lambda^2 G^o_\downarrow(p) + \frac{\lambda}{M_o} . \tag{B.9a}$$

By an entirely analogous argument we obtain

$$\frac{i}{2\pi^4} \Gamma_{\downarrow M}(p;0;0;p) = \lambda^2 G^o_\uparrow(p) - \frac{\lambda}{M_o} \tag{B.9b}$$

Using the result given by Eq. (B.7) together with Eq. (B.9a) we obtain, after some perfectly straightforward algebra

$$G^o_\uparrow(p) \frac{i}{(2\pi)^4} \Gamma_{\uparrow M}(p;0;0,p) G^o_\uparrow(p) = -\frac{1}{M^2} \{G^o_\uparrow(p) - G^o_\downarrow(p)\}. \tag{B.10a}$$

while Eq. (B.7) together with Eq. (B.9b) yields the corresponding result for the spin down electron magnon vertex.

$$G^o_\downarrow(p) \frac{i}{(2\pi)^4} \Gamma_{\downarrow M}(p;0;0;p) G^o_\downarrow(p) = \frac{1}{M^2} \{G^o_\uparrow(p) - G^o_\downarrow(p)\} . \tag{B.10b}$$

Thus confirming that the choice of vertices given by Eqs. (B.3a and B.3b) do in fact satisfy the W-T identities given in Eqs. (3.105 and 3.106), thus assuming that the thermal corrections to the magnetisation will have the correct $T^{3/2}$ contribution. Thus we find that the requirements of spin rotational invariance as expressed through the W-T identities severly restricts the possible approximations which may be utilised in the calculation of the electron magnon vertex.

Now from Eqs. (3.90 and 3.91) together with Eqs. (3.97 and 3.99) we obtain the following expressions for the ($\alpha = 1$; $\beta = 1$) component of the finite temperature electron propagators, $G_{\uparrow}^{\alpha\beta}$ and $G_{\downarrow}^{\alpha\beta}$ as

$$G_{\uparrow}^{11}(p) = G_{\uparrow}^{0}(p) + G_{\uparrow}^{0}(p) \int \frac{d^3\vec{q}}{(2\pi)^3} \frac{i}{(2\pi)^4} \Gamma_{\uparrow M}(p,q;q;p) Z_B^0(\vec{q}) f_B(\omega_B^0(\vec{q}))\Big|_{q_0=\omega_B(\vec{q})}$$

$$G_{\uparrow}^{0}(p) + \ldots \tag{B.11a}$$

and

$$G_{\downarrow}^{11}(p) = G_{\downarrow}^{0}(p) + G_{\downarrow}^{0}(p) \int \frac{d^3q}{(2\pi)^3} \frac{i}{(2\pi)^4} \Gamma_{\downarrow M}(p;q;q,p) Z_B(\vec{q}) f_B(\omega_B(\vec{q}))\Big|_{q_0=\omega_B(\vec{q})}$$

$$G_{\downarrow}^{0}(p) + \ldots , \tag{B.11b}$$

where we have neglected the thermal excitation of the quasi electrons in order to simplify our analysis.

Now from Eq. (B.11a) and Eq. (B.3a) we have that

$$n_{\uparrow}(T) = -\frac{i}{(2\pi)^4} \oint^{+} d^4p\, G_{\uparrow}^{11}(p)$$

$$= n_{\uparrow}(T=0) - \lambda^2 \int \frac{d^3q}{(2\pi)^3} Z_B^0(\vec{q}) f_B(\omega_B^0(\vec{q}))$$

$$\left\{ \frac{R_{\uparrow}(q;q) - \lambda D_{\uparrow}(0) R_{\downarrow}(q;q)}{1 - \lambda^2 D_{\uparrow}(0) D_{\downarrow}(0)} \right\}_{q_0=\omega_B(\vec{q})} + \delta\mu(T) \frac{\partial n_{\uparrow}}{\partial \mu}(T=0)$$

$$+ \ldots \tag{B.12a}$$

and from Eq. (B.11b) and Eq. (B.3b) we have that

$$n_{\downarrow}(T) = -\frac{i}{(2\pi)^4} \oint^{+} d^4p\, G_{\downarrow}^{11}(p)$$

$$= n_{\downarrow}(T=0) - \lambda^2 \int \frac{d^3q}{(2\pi)^3} Z_B^0(q) f_B(\omega_B^0(q))$$

$$\left\{ \frac{R_{\downarrow}(q;q) - D_{\downarrow}(0)R_{\uparrow}(q;q)}{1 - \lambda^2 D_{\uparrow}(0)D_{\downarrow}(0)} \right\}_{q_0=\omega_B(q)} + \delta\mu(T) \frac{\partial n_{\downarrow}}{\partial \mu} (T=0)$$

$$+ \ldots \qquad \text{(B.12b)}$$

The last terms appearing in Eq. (B.12a) and Eq. (B.12b) represents the shift in the chemical potential and is determined by the requirement, that the total number density $n(= n_{\uparrow}(T) + n_{\downarrow}(T))$ remain independent of temperature.

To obtain the low temperature behaviour we expand the term in the curly brackets in powers of momenta, we therefore define

$$R_{\uparrow}(q;q)\Big|_{q_0=\omega_B^0(\vec{q})} = R_{\uparrow}^{(1)} + R_{\uparrow}^{(2)}|\vec{q}|^2 + \ldots , \qquad \text{(B.13a)}$$

$$R_{\downarrow}(q;q)\Big|_{q_0=\omega_B(\vec{q})} = R_{\downarrow}^{(1)} + R_{\downarrow}^{(2)}|\vec{q}|^2 + \ldots \qquad \text{(B.13b)}$$

$$Z_B^0(\vec{q}) = M_0 + Z_B^{(2)}|\vec{q}|^2 + \ldots$$

and

$$\omega_B^0 = D|\vec{q}|^2 + \ldots . \qquad \text{(B.13c)}$$

Where D is generally referred to as the spin wave stiffness. We thus obtain,

$$n_{\uparrow}(T) = n_{\uparrow}(T=0) - \frac{\lambda^2 M_0}{(2\pi)^3} \frac{R_{\uparrow}^{(1)} - \lambda D_{\uparrow}(0)R_{\downarrow}^{(1)}}{1 - \lambda^2 D_{\uparrow}(0)D_{\downarrow}(0)} \left\{ \left(\frac{\pi}{D}\right)^{3/2} \zeta\left(\frac{3}{2}\right) \beta^{-3/2} \right.$$

$$\left. + \left\{ \frac{R_{\uparrow}^{(2)} - \lambda D_{\uparrow}(0)R_{\downarrow}^{(2)}}{R_{\uparrow}^{(1)} - \lambda D_{\uparrow}(0)R_{\downarrow}^{(1)}} + \frac{Z_B^{(2)}}{M_0} \right\} \frac{3}{4\pi} \left\{\frac{\pi}{D}\right\}^{5/2} \zeta\left(\frac{5}{2}\right) \beta^{-5/2} + \ldots \right\} + \delta\mu(T) \frac{\partial n_{\uparrow}}{\partial \mu} (T=0) \qquad \text{(B.14a)}$$

and

$$n_{\downarrow}(T) = n_{\downarrow}(T=0) - \frac{\lambda^2 M_0}{(2\pi)^3} \frac{R_{\downarrow}^{(1)} - \lambda D_{\downarrow}(0)R_{\uparrow}^{(1)}}{1 - \lambda^2 D_{\uparrow}(0)D_{\downarrow}(0)} \left\{ \left(\frac{\pi}{D}\right)^{3/2} \zeta\left(\frac{3}{2}\right) \beta^{-3/2} \right.$$

$$+ \left\{ \frac{R_{\downarrow}^{(2)} - \lambda D_{\downarrow}(0) R_{\uparrow}^{(2)}}{R_{\downarrow}^{(1)} - \lambda D_{\uparrow}(0) R_{\uparrow}^{(1)}} + \frac{Z_B^{(2)}}{M_0} \right\} \frac{3}{4\pi} \left(\frac{\pi}{D}\right)^{5/2} \zeta\left(\frac{5}{2}\right) \beta^{-5/2} + \ldots \right\} + \delta\mu(T) \frac{\partial n_{\downarrow}}{\partial \mu} (T=0) \tag{B.14b}$$

It remains therefore to calculate the coefficients appearing in the expansion in Eqs. (B.13a, B.13b and B.13c). While this is perfectly straightforward it is nevertheless somewhat tedious. However a number of simplifications may be realised if we define

$$\varepsilon_F^{\pm} = \mu_0 \pm \frac{\lambda M_0}{2} , \tag{B.15}$$

where μ_0 is the zero temperature chemical potential. Then by means of the relations

$$\frac{\partial}{\partial \varepsilon_F^{+}} G_{\uparrow}^{0}(p) = - G_{\uparrow}^{0}(p) G_{\uparrow}^{0}(p) \tag{B.16a}$$

$$\frac{\partial}{\partial \varepsilon_F^{-}} G_{\downarrow}^{0}(p) = - G_{\downarrow}^{0}(p)\, G_{\downarrow}^{0}(p) \tag{B.16b}$$

and

$$\frac{\partial}{\partial \varepsilon_F^{+}} G_{\downarrow}^{0}(p) = \frac{\partial}{\partial \varepsilon_F^{-}} G_{\uparrow}^{0}(p) = 0 , \tag{B.16c}$$

we obtain the following result for $R_{\uparrow}(q;q)$

$$R_{\uparrow}(q;q) = - \frac{\partial}{\partial \varepsilon_F^{+}} D(q) \tag{B.17a}$$

and similarly for $R_{\downarrow}(q;q)$,

$$R_{\downarrow}(q;q) = - \frac{\partial}{\partial \varepsilon_F^{-}} D(q) . \tag{B.17b}$$

where $D(q)$ is given by

$$D(q) = \frac{i}{(2\pi)^4} \int d^4p \; G_{\uparrow}^{0}(p-q/2) G_{\downarrow}^{0}(p+q/2) . \tag{B.18}$$

Equations (B.16a and B.16b) also allow us to write

$$D_{\uparrow}(0) = \frac{\partial}{\partial\varepsilon_F^+} n(\varepsilon_F^+) \tag{B.19a}$$

and

$$D_{\downarrow}(0) = \frac{\partial}{\partial\varepsilon_F^-} n(\varepsilon_F^-) , \tag{B.19b}$$

where

$$n(\varepsilon_F^+) = -\frac{i}{(2\pi)^4} \oint_{+} d^4p \cdot G^0_{\uparrow}(p) \tag{B.20a}$$

and

$$n(\varepsilon_F^-) = -\frac{i}{(2\pi)^4} \oint_{+} d^4p \; G^0_{\downarrow}(p). \tag{B.20b}$$

Now

$$-\frac{i}{(2\pi)^4} \oint^{+} d^4p \; G^0_{\uparrow}(p) = \int \frac{d^3\vec{p}}{(2\pi)^3} \theta[\varepsilon_F^+ - \tilde{\varepsilon}(\vec{p})] \tag{B.21a}$$

and

$$-\frac{i}{(2\pi)^4} \oint^{+} d^4p \; G^0_{\downarrow}(p) = \int \frac{d^3\vec{p}}{(2\pi)^3} \theta[\varepsilon_F^- - \tilde{\varepsilon}(p)], \tag{B.21b}$$

where we have defined $\tilde{\varepsilon} = \varepsilon + \mu$. Thus

$$D_{\uparrow}(0) = \int \frac{d^3\vec{p}}{(2\pi)^3} \delta[\varepsilon_F^+ - \tilde{\varepsilon}(\vec{p})]$$

$$\equiv N(\varepsilon_F^+) \tag{B.22a}$$

and

$$D_{\downarrow}(0) = \int \frac{d^3p}{(2\pi)^3} \delta(\varepsilon_F^- - \tilde{\varepsilon}(\vec{p}))$$

$$\equiv N(\varepsilon_F^-), \tag{B.22b}$$

where $N(\varepsilon)$ denotes the density of states at energy ε.

The expression for $D(q)$ may be computed, in a low momentum expansion, by means of the finite momentum generalisation of Eq. (B.7).

$$G^o_\uparrow(p-q/2)^{-1} - G^o_\downarrow(p+q/2)^{-1} = \varepsilon_F^+ - \varepsilon_F^- - q_o - \tilde{\varepsilon}(\vec{p}-\vec{q}/2) + \tilde{\varepsilon}(\vec{p}+\vec{q}/2)$$

$$= \varepsilon_F^+ - \varepsilon_F^- - q_o + \vec{q}\cdot\vec{\nabla}_{\vec{p}}\varepsilon(\vec{p}) + \ldots \qquad \text{(B.23)}$$

$$G^o_\uparrow(p-q/2)G^o_\downarrow(p+q/2) = -\frac{1}{\varepsilon_F^+ - \varepsilon_F^- - q_o}\{G^o_\uparrow(p-q/2) - G^o_\downarrow(p+q/2)\}$$

$$-\frac{\vec{q}\cdot\vec{\nabla}_p\varepsilon(p)}{\varepsilon_F^+ - \varepsilon_F^- - q_o} G^o_\uparrow(p-q/2)G^o_\downarrow(p-q/2)$$

$$+ \ldots$$

$$= -\frac{1}{(\varepsilon_F^+ - \varepsilon_F^- - q_o)}[G^o_\uparrow(p-q/2) - G^o_\downarrow(p+q/2)]$$

$$+\frac{\vec{q}\cdot\vec{\nabla}_p\tilde{\varepsilon}(\vec{p})}{(\varepsilon_F^+ - \varepsilon_F^- - q_o)^2}\{G^o_\uparrow(p-q/2) - G^o_\downarrow(p+q/2)\}$$

$$-\frac{[\vec{q}\cdot\vec{\nabla}_{\vec{p}}\tilde{\varepsilon}(\vec{p})]^2}{(\varepsilon_F^+ - \varepsilon_F^- - q_o)^2} G^o_\uparrow(p-q/2)G^o_\downarrow(p+q/2)$$

$$+ \ldots \qquad \text{(B.24)}$$

Thus we have to order $|\vec{q}|^2$ that

$$\frac{i}{(2\pi)^4}\int d^4p\, G^o_\uparrow(p-q/2)G^o_\downarrow(p+q/2)$$

$$= -\frac{1}{\varepsilon_F^+ - \varepsilon_F^- - q_o}\frac{i}{(2\pi)^4}\int d^4p\{G^o_\uparrow(p-q/2) - G^o_\downarrow(p+q/2)\}$$

$$+\frac{1}{(\varepsilon_F^+ - \varepsilon_F^- - q_o)^2}\frac{i}{(2\pi)^4}\int d^4p\,[\vec{q}\cdot\nabla_{\vec{p}}\tilde{\varepsilon}(\vec{p})]\{G^o_\uparrow(p-q/2) - G^o_\downarrow(p+q/2)\}$$

$$-\frac{1}{(\varepsilon_F^+ - \varepsilon_F^- - q_o)^2}\frac{i}{(2\pi)^4}\int d^4p[\vec{q}\cdot\nabla_p\tilde{\varepsilon}(\vec{p})]^2\, G^o_\uparrow(p-q/2)G^o_\downarrow(p+q/2)$$

$$+ \ldots$$

$$= \frac{1}{\varepsilon_F^+ - \varepsilon_F^- - q_o} \{n(\varepsilon_F^+) - n(\varepsilon_F^-)\}$$

$$- \frac{|\vec{q}|^2}{\varepsilon_F^+ - \varepsilon_F^- - q_o} \int \frac{d^3\vec{p}}{(2\pi)^3} [\nabla^2_{\vec{p}}\tilde{\varepsilon}(\vec{p})]\{\theta[\varepsilon_F^+ - \tilde{\varepsilon}\text{[illegible]}\theta[\varepsilon_F^- - \tilde{\varepsilon}(\vec{p})]$$

$$+ \frac{|q|^2}{(\varepsilon_F^+ - \varepsilon_F^- - q_o)^3} \int \frac{d^3\vec{p}}{(2\pi)^3} [\vec{\nabla}_{\vec{p}}\tilde{\varepsilon}(\vec{p}) \cdot \vec{\nabla}_{\vec{p}}\tilde{\varepsilon}(\vec{p})]$$

$$\{\theta[\varepsilon_F^+ - \tilde{\varepsilon}(\vec{p})] - \theta[\varepsilon_F^- - \tilde{\varepsilon}(\vec{p})]\} + O\{|q|^4\} . \qquad (B.25)$$

Thus if we define the following band parameters

$$a(\varepsilon_F^{\pm}) = \int \frac{d^3\vec{p}}{(2\pi)^3} [\nabla^2_{\vec{p}}\tilde{\varepsilon}(\vec{p})]\theta[\varepsilon_F^{\pm} - \tilde{\varepsilon}(\vec{p})] \qquad (B.26a)$$

and

$$b(\varepsilon_F^{\pm}) = \int \frac{d^3\vec{p}}{(2\pi)^3} [\vec{\nabla}_{\vec{p}}\tilde{\varepsilon}(\vec{p}) \cdot \vec{\nabla}_{\vec{p}}\tilde{\varepsilon}(\vec{p})]\theta[\varepsilon_F^{\pm} - \varepsilon(\vec{p})] \qquad (B.26b)$$

together with their derivatives.

$$\Lambda(\varepsilon_F^{\pm}) = a'(\varepsilon_F^{\pm}) \cdot$$

$$= \int \frac{d^3\vec{p}}{(2\pi)^3} [\nabla^2_p\tilde{\varepsilon}(\vec{p})]\delta[\varepsilon_F^{\pm} - \tilde{\varepsilon}(\vec{p})] \qquad (B.27a)$$

and

$$B(\varepsilon_F^{\pm}) = b'(\varepsilon_F^{\pm}) .$$

$$= \int \frac{d^3\vec{p}}{(2\pi)^3} [\vec{\nabla}_p\varepsilon(\vec{p}) \cdot \vec{\nabla}_p\varepsilon(\vec{p})]\delta(\varepsilon_F^{\pm} - \tilde{\varepsilon}(\vec{p})), \qquad (B.27b)$$

then we obtain the following expression for $D, R_\uparrow$ and $R_\downarrow$

$$\text{Re } D(q) \simeq \frac{n(\varepsilon_F^+) - n(\varepsilon_F^-)}{(\varepsilon_F^+ - \varepsilon_F^- - q_o)} - \frac{a(\varepsilon_F^+) - (\varepsilon_F^-)}{(\varepsilon_F^+ - \varepsilon_F^- - q_o)^2} |\vec{q}|^2$$

$$+ \frac{b(\varepsilon_F^+) - b(\varepsilon_F^-)}{(\varepsilon_F^+ - \varepsilon_F^- - q_o)^2} |\vec{q}|^2 + \ldots . \tag{B.28}$$

$$\begin{aligned} \text{Re } R_\uparrow(q;q) &= -\frac{\partial}{\partial \varepsilon_F^+} D(q) \\ &= \frac{n(\varepsilon_F^+) - n(\varepsilon_F^-)}{(\varepsilon_F^+ - \varepsilon_F^- - q_o)^2} - \frac{N(\varepsilon_F^+)}{\varepsilon_F^+ - \varepsilon_F^- - q_o} \\ &- \left| \frac{2(a(\varepsilon_F^+) - a(\varepsilon_F^-))}{(\varepsilon_F^+ - \varepsilon_F^- - q_o)^3} - \frac{A(\varepsilon_F^+)}{(\varepsilon_F^+ - \varepsilon_F^- - q_o)^2} \right| |\vec{q}|^2 \\ &+ \left| \frac{3(b(\varepsilon_F^+) - b(\varepsilon_F^-))}{(\varepsilon_F^+ - \varepsilon_F^- - q_o)^4} - \frac{B(\varepsilon_F^+)}{(\varepsilon_F^+ - \varepsilon_F^- - q_o)^3} \right| |\vec{q}|^2 \\ &+ \ldots . \end{aligned} \tag{B.29a}$$

and

$$\begin{aligned} \text{Re } R_\downarrow(q;q) &= -\frac{\partial}{\partial \varepsilon_F^-} D(q) \\ &= -\frac{n(\varepsilon_F^+) - n(\varepsilon_F^-)}{(\varepsilon_F^+ - \varepsilon_F^- - q_o)^2} + \frac{N(\varepsilon_F^-)}{(\varepsilon_F^+ - \varepsilon_F^- - q_o)} \\ &+ \left| \frac{2(a(\varepsilon_F^+) - a(\varepsilon_F^-))}{(\varepsilon_F^+ - \varepsilon_F^- - q_o)^3} - \frac{A(\varepsilon_F^-)}{(\varepsilon_F^+ - \varepsilon_F^- - q_o)^2} \right| |\vec{q}|^2 \\ &- \left| \frac{3(b(\varepsilon_F^+) - b(\varepsilon_F^-))}{(\varepsilon_F^+ - \varepsilon_F^- - q_o)^4} - \frac{B(\varepsilon_F^-)}{(\varepsilon_F^+ - \varepsilon_F^- - q_o)^3} \right| |\vec{q}|^2 \\ &+ \ldots . \end{aligned} \tag{B.29b}$$

If we now consider the quantities $R_\uparrow$ and $R_\downarrow$ on shell, that is for

$q_o = \omega_B^o(\vec{q})$ and expanding $\omega_B^o(\vec{q})$ in low momentum as given by Eq. (B.13c), we can expand Eqs. (B.29a and B.29b) and thus obtain an expression for the coefficients defined by the expansion in Eqs. (B.13a and B.13b).

We thus obtain the following results,

$$R_{\uparrow}^{(1)} = \frac{n(\varepsilon_F^+) - n(\varepsilon_F^-)}{(\varepsilon_F^+ - \varepsilon_F^-)^2} - \frac{N(\varepsilon_F^+)}{\varepsilon_F^+ - \varepsilon_F^-} \tag{B.30a}$$

$$R_{\downarrow}^{(1)} = -\frac{n(\varepsilon_F^+) - n(\varepsilon_F^-)}{(\varepsilon_F^+ - \varepsilon_F^-)^2} + \frac{N(\varepsilon_F^-)}{\varepsilon_F^+ - \varepsilon_F^-} \tag{B.30b}$$

$$R_{\uparrow}^{(2)} = -\frac{D}{(\varepsilon_F^+ - \varepsilon_F^-)^2} \quad N(\varepsilon_F^+) - 2\,\frac{n(\varepsilon_F^+ - n(\varepsilon_F^-)}{\varepsilon_F^+ - \varepsilon_F^-}$$

$$+ \frac{2}{(\varepsilon_F^+ - \varepsilon_F^-)^3} \quad A(\varepsilon_F^+) - 3\,\frac{(a(\varepsilon_F^+) - a(\varepsilon_F^-))}{\varepsilon_F^+ - \varepsilon_F^-}$$

$$- \frac{3}{(\varepsilon_F^+ - \varepsilon_F^-)^4} \quad B(\varepsilon_F^+) - 4\,\frac{b(\varepsilon_F^+) - b(\varepsilon_F^-)}{\varepsilon_F^+ - \varepsilon_F^-} \tag{B.30c}$$

and

$$R_{\downarrow}^{(2)} = \frac{D}{(\varepsilon_F^+ - \varepsilon_F^-)^2} \quad N(\varepsilon_F^-) - 2\,\frac{n(\varepsilon_F^+) - n(\varepsilon_F^-)}{\varepsilon_F^+ - \varepsilon_F^-}$$

$$- \frac{2}{(\varepsilon_F^+ - \varepsilon_F^-)^3} \quad A(\varepsilon_F^-) - 3\,\frac{a(\varepsilon_F^+) - a(\varepsilon_F^-)}{\varepsilon_F^+ - \varepsilon_F^-}$$

$$+ \frac{2}{(\varepsilon_F^+ - \varepsilon_F^-)^4} \quad B(\varepsilon_F^-) - 4\,\frac{b(\varepsilon_F^+) - b(\varepsilon_F^-)}{\varepsilon_F^+ - \varepsilon_F^-} \tag{B.30d}$$

Now, since ε_F^+ and ε_F^- are determined in such a way that

$$\varepsilon_F^+ - \varepsilon_F^- = \lambda M_o$$

$$= \lambda\{n(\varepsilon_F^+) - n(\varepsilon_F^-)\}, \tag{B.31}$$

then the coefficients $R_\uparrow^{(1)}$ and $R_\downarrow^{(1)}$ simplify somewhat to give

$$R_\uparrow^{(1)} = \frac{1}{\lambda^2 M_o} - \frac{N(\varepsilon_F^+)}{\lambda M_o} \tag{B.32a}$$

and

$$R_\downarrow^{(1)} = -\frac{1}{\lambda^2 M_o} + \frac{N(\varepsilon_F^-)}{\lambda M_o}, \tag{B.32b}$$

which of course is simply the result given by Eqs. (B.6 and B.8) together with Eqs. (B.22a and B.22b).

We thus find, as expected, that the terms in the low temperature expansion simplify somewhat. From Eq. (B.32a) and Eq. (B.32b) we obtain that

$$\frac{R_\uparrow^{(1)} - \lambda D_\uparrow(0) R_\downarrow^{(1)}}{1 - \lambda^2 D_\uparrow(0) D_\downarrow(0)} = \frac{1}{\lambda^2 M_o} \tag{B.33a}$$

and

$$\frac{R_\downarrow^{(1)} - \lambda D_\downarrow(0) R_\uparrow^{(1)}}{1 - \lambda^2 D_\uparrow(0) D_\downarrow(0)} = -\frac{1}{\lambda^2 M_o} \tag{B.33b}$$

Hence the expansion given by Eqs. (B.14a and B.14b) simplify somewhat to give

$$n_\uparrow(T) = n(\varepsilon_F^+) - \frac{1}{(2\pi)^3}\left\{\left(\frac{\pi}{D}\right)^{3/2}\xi\left(\frac{3}{2}\right)\beta^{-3/2} + \left\{\frac{\lambda^2 M_o (R_\uparrow^{(2)} - \lambda N(\varepsilon_F^+) R_\downarrow^{(2)})}{1 - \lambda^2 N(\varepsilon_F^+) N(\varepsilon_F^-)} - \frac{Z_B^{(2)}}{M_o}\right\}\right.$$

$$\left.\frac{3}{4\pi}\left(\frac{\pi}{D}\right)^{5/2}\xi\left(\frac{5}{2}\right)\beta^{-5/2} + \ldots\right\} + \delta\mu(T) N(\varepsilon_F^+) \tag{B.34a}$$

and

$$n_\downarrow(T) = n(\varepsilon_F^-) + \frac{1}{(2\pi)^3}\left\{\left(\frac{\pi}{D}\right)^{3/2}\xi\left(\frac{3}{2}\right)\beta^{-3/2} - \left\{\frac{\lambda^2 M_o(R_\downarrow^{(2)} - \lambda N(\varepsilon_F^-)R_\uparrow^{(2)})}{1 - \lambda^2 N(\varepsilon_F^+)N(\varepsilon_F^-)} + \frac{Z_B^{(2)}}{M_o}\right\}\right.$$

$$\left.\frac{3}{(4\pi)}\left(\frac{\pi}{D}\right)^{5/2}\xi\left(\frac{5}{2}\right)\beta^{-5/2} + \ldots\right\} + \delta\mu(T)N(\varepsilon_F^-) \qquad \text{(B.34b)}$$

From the results contained in Eqs. (B.34a and B.34b) we obtain, from the condition that

$$n_\uparrow(T) + n_\downarrow(T) = n(\varepsilon_F^+) + n(\varepsilon_F^-) \qquad \text{(B.35)}$$

the result that

$$\delta\mu(T) = \frac{1}{N(\varepsilon_F^+) + N(\varepsilon_F^-)}\,\frac{\lambda^2 M_o}{1 - \lambda^2 N(\varepsilon_F^+)N(\varepsilon_F^-)}\,\frac{1}{(2\pi)^3}\left\{R_\uparrow^{(2)}(1 - \lambda N(\varepsilon_F^-)) + R_\downarrow^{(2)}(1 - \lambda N(\varepsilon_F^+))\right\}$$

$$\frac{3}{4\pi}\left\{\frac{\pi}{D}\right\}^{5/2}\xi\left(\frac{5}{2}\right)\beta^{-5/2} + \ldots . \qquad \text{(B.36)}$$

We note that this expression does not contain any $\beta^{-3/2}$ contribution, as expected in the light of the discussion in Section (3.2). The resultant expression for the magnetisation is therefore given by

$$M(T) = M_o - \frac{2}{(2\pi)^3}\left\{\frac{\pi}{D}\right\}^{3/2}\beta^{-3/2} - \frac{1}{(2\pi)^3}\,\frac{3}{4\pi}\left\{\frac{\pi}{D}\right\}^{5/2}\frac{\beta^{-5/2}}{M_o}$$

$$\times\left\{2Z_B^{(2)} + \frac{\lambda^2 M_o^2}{1 - \lambda^2 N(\varepsilon_F^+)N(\varepsilon_F^-)}\left\{R_\uparrow^{(2)}\left\{1 - \frac{N(\varepsilon_F^+) - N(\varepsilon_F^-)}{N(\varepsilon_F^+) + N(\varepsilon_F^-)}\right\}\{1 - N(\varepsilon_F^-)\}\right.\right.$$

$$\left.\left. - R_\downarrow^{(2)}\left\{1 + \frac{N(\varepsilon_F^+) - N(\varepsilon_F^-)}{N(\varepsilon_F^+) + N(\varepsilon_F^-)}\right\}\{1 - \lambda N(\varepsilon_F^+)\}\right\}\right\} + \ldots . \qquad \text{(B.37)}$$

From the result contained in Eq. (B.37) we obtain the Bloch $T^{3/2}$ term in the magnetisation, explicitly. This of course is due to the fact that our approximation for the electron magnon vertex was chosen in such a fashion that the W-T identities Eqs. (3.105 and 3.106) were satisfied. The analysis presented in this section serves therefore to demonstrate in an explicit manner within the context of a particular model the argument regarding the role of symmetry in determing the temperature dependence of various physical quantities such as the magnetisation. It also serves, perhaps, as a useful basis for the analysis of magnon effects in metals.

APPENDIX C

The Electron Self Energy

In this appendix we discuss the derivation of the electron self energy given by Eq. (4.37). The derivation is in terms of the TFD formalism outlined in Chapter (2.1). From Eq. (4.8) we obtain the equation for the thermal doublet field ϕ^{α}, Eq. (2.29),

$$\{i\frac{\partial}{\partial t} - \varepsilon(i\nabla)\tau_3 + \Delta_o\tau_1 + \mu\sigma_3\}\phi^{\alpha} = I\{\vec{M}^{\alpha} - <\vec{M}>\}\cdot\vec{\sigma}\phi^{\alpha} - \mu_B\{\vec{B}^{\alpha} - <\vec{B}>\}\cdot\vec{\sigma}\phi^{\alpha}. \quad (C.1)$$

From Eq. (C.1) we obtain the following expression for the electron propagator $<\beta\Delta T\{\phi^{\alpha}(x)\phi^{\beta}(y)^{\dagger}\}|\beta>$

$$\{i\frac{\partial}{\partial t} - \varepsilon(-i\nabla)\tau_3 + \Delta_o\tau_1 + \mu\sigma_3\}<\beta|T\{\phi^{\alpha}(x)\phi^{\beta}(y)^{\dagger}\}|\beta>$$
$$= i\delta^{\alpha\beta}\delta(x-y) + I\sigma_i<\beta|T\{(M_i^{\alpha}(x) - <M_i(x)>)\phi^{\alpha}(x)\phi^{\beta}(y)^{\dagger}\}|\beta> . \quad (C.2)$$

where we have neglected the contribution from the B field. In the lowest order of perturbation we have that

$$<\beta|T\{(M_i^{\gamma}(x) - <M_i(x)>)\phi^{\alpha}(x)\phi^{\beta}(y)^{\dagger}\}|\beta>$$
$$\simeq -iI\int d^4z<\beta|T\{\sum_a \vec{M}^a(z)\psi^a(z)^{\dagger}\vec{\sigma}\psi(z)^a(M_i^{\gamma}(x) - <M_i(x)>)\phi^{\alpha}(x)\phi^{\beta}(y)^{\dagger}\}|\beta> .$$
$$\simeq -iI\int d^4z \sum_a <\beta|T\{M_i^a(x) - <M_i(x)>)(M_j^a(z) - <M_j(z)>)\}|\beta>$$
$$<\beta|T\{\phi^{\alpha}(x)\phi^a(z)^{\dagger}\}|\beta>\sigma_i<\beta|T\{\phi^a(z)\phi^{\beta}(y)^{\dagger}\}|\beta> , \quad (C.3)$$

where we have used the relation $\psi^{\dagger}\sigma\psi = \psi_c^{\dagger}\sigma\psi_c$.

If we now define the momentum Green's functions as

$$<\beta|T\{\phi^{\alpha}(x)\phi^{\beta}(y)^{\dagger}\}|\beta> = \frac{i}{(2\pi)^4}\int d^4p\ e^{-ip(x-y)}S^{\alpha\beta}(p) \quad (C.4)$$

and

$$<\beta|T\{(M_i^{\alpha}(x) - <M_i(x)>)(M_j^{\beta}(y) - <M_j(y)>)\}|\beta> = \frac{i}{(2\pi)^4} \int d^4k \; e^{-ik(x-y)} \; \chi_{ij}^{\alpha\beta}(k) \tag{C.5}$$

with $p\cdot x = \vec{p}\cdot\vec{x} - p_o t_x$, then Eq. (C.2) together with Eq. (C.3) yields

$$S^{-1}(p)^{\alpha\beta} = (p_o - \varepsilon(\vec{p})\tau_3 + \Delta_o\tau_1)S_{\alpha\beta} - \frac{iI^2}{(2\pi)^4}\int d^4k\cdot\sum_i \chi_{ij}^{\alpha\beta}(k)\sigma_i S^{\alpha\beta}(p-k)\sigma_j \; . \tag{C.6}$$

Now using the definitions of the spectral functions provided in Eqs. (4.38 and 4.41) we have that

$$S^{\alpha\beta}(p) = \int \delta(v;\vec{p})U_F(p_o)\{p_o - u + i\delta\tau\}^{-1}U_F^{\dagger}(p_o) \tag{C.7}$$

and

$$\chi_{ij}^{\alpha\beta}(k) = \int \rho_{ij}(\omega\vec{k})U_B(k_o)\tau\{k_o - \omega + i\delta\tau\}^{-1}U_B(k_o) \tag{C.8}$$

Then we obtain from Eq. (C.6) together with the definition of the self energy given by

$$S^{-1}(p)^{\alpha\beta} = (p_o - \varepsilon(\vec{p}) + \Delta\tau_1 + \mu\sigma_3)\delta_{\alpha\beta} - \Sigma^{\alpha\beta}(p), \tag{C.9}$$

the following result for $\Sigma^{\alpha\beta}(p)$.

$$\Sigma^{\alpha\beta}(p) \equiv \frac{iI^2}{(2\pi)^4}\int d^4k \; \chi_{ij}^{\alpha\beta}(k)\sigma_i S^{\alpha\beta}(p-k)\sigma_j$$

$$= \int d^4k \; \rho(k;\vec{p})\{U_F(k)[p_o - k + i\delta\tau]^{-1} \; U_F(k)\}^{\alpha\beta} \tag{C.10}$$

with

$$\rho(k;\vec{p}) = \frac{I^2}{(2\pi)^3}\int d^3k \int dw\cdot dv \; \rho_{ij}(w;\vec{k})\sigma_i \delta(v;\vec{p}-\vec{k})\sigma_j \delta(k-w-v) \; \frac{e^{\beta k}+1}{(e^{\beta w}-1)e^{\beta w}+1)} \; . \tag{C.11}$$

If we now define the matrices S(p) and Σ(p) as

$$S^{\alpha\beta}(p) = [U_F(p_o)S(p)U_F^{\dagger}(p_o)]_{\alpha\beta} \tag{C.12}$$

and

$$\Sigma^{\alpha\beta}(p) = [U_F(p_o)\Sigma(p)U_F(p_o)]_{\alpha\beta}, \tag{C.13}$$

then we can easily show that S(p) and Σ(p) are diagonal with respect to the thermal indices with the upper component given by the retarded function and the lower component given by the advanced function. We thus obtain the desired result contained in Eq. (4.37)

$$S^{-1}(p) = p_o - \varepsilon(\vec{p})\tau_3 + \Delta_o\tau_1 + \mu\sigma_3 - \Sigma(p) \tag{C.14}$$

with

$$\Sigma(p) = \frac{I^2}{(2\pi)^3}\int d^3\vec{k}\int dw\int dv\ \rho_{ij}(w;\vec{k})\sigma_i s(v;\vec{p}-\vec{k})\sigma_j\ \frac{e^{\beta(v+w)}+1}{(e^{\beta w}-1)(e^{\beta v}+1)}\ \frac{1}{p_o - w - v + i\varepsilon}\ . \tag{C.15}$$

APPENDIX D

Spin Fluctuations and the Surface Impedance in Magnetic Superconductors

In the analysis of the magnetic properties of $ErRh_4B_4$ presented in Chapter 4, we found that nearly all of the observed phenomena arose largely from the Zeeman splitting of the electron spins by the mean field created by the magnetic ions through the d-f interaction. The results therefore seemed to indicate that it would be difficult to draw any quantitative conclusions regarding the nature of the spin fluctuations solely from the magnetisation measurements. Instead it was shown how the effect of the spin fluctuations could be more readily observed by means of the various Meissner state quantities such as the superconducting gap, the condensation energy and the London penetration depth. This is clearly seen from the graphs presented in Figs. (4,5 and 6) and is confirmed by recent estimates of the condensation energy obtained from the single crystal magnetisation curves[122].

In this appendix we consider how the spin fluctuations affect the electromagnetic fields generated at the surface of a magnetic superconductor in the Meissner state. We begin with a brief discussion of the surface impedance and show to what extent it may be used to characterise surface phenomena in metals. We then go on to show how the resonant frequency in a microwave cavity is affected by changes in the surface impedance, thus providing us with an excellent means whereby it can be measured. Finally we present the results of some calculations of the effective penetration depth, defined in terms of the surface impedance, for the case of $ErRh_4B_4$ together with the results of some recent measurements[136].

The results of the calculation together with the experimental results are interesting in that not only do they clearly show the effect of the spin fluctuations but they also suggest that the surface impedance measurements could be useful in confirming the existence of the predicted surface magnetisation states[110,111].

We begin by defining the surface impedance on a surface S as the two-dimensional dyadic

$$\hat{n} \wedge \vec{E} = \frac{c}{4\pi}\overleftrightarrow{Z}_S\{\vec{H} - \hat{n}(\hat{n}\cdot\vec{H})\} \qquad (D.1)$$

where $\hat{n}$ denotes the unit vector normal to the surface and $\vec{E}$ and $\vec{H}$ the corresponding values of the macroscopic electric and magnetic fields respectively. The physical importance of the surface impedance Z_S, defined by Eq. (D.1), depends on the fact that it is continuous across any surface S[148]. Hence the electromagnetic fields on either side of a surface S are related solely through the boundary condition expressed by Eq. (D.1). This is of considerable importance when one wishes to consider, for example, various surface phenomena in either normal or superconducting metals, since it allows one to characterise the electromagnetic behaviour in the region close to surface entirely in terms of the surface impedance Z_S.

In order to make our considerations somewhat more specific, we consider how the surface currents generated in the walls of a microwave cavity affect the electromagnetic characteristics of that cavity.

Assuming the time dependence of the fields to be sinusoidal we can write

$$\vec{E}(\vec{x};t) = \vec{E}(\vec{x})e^{-i\omega t}, \qquad (D.2a)$$

$$\vec{B}(\vec{x};t) = B(\vec{x})e^{-i\omega t} \qquad (D.2b)$$

and

$$\vec{H}(\vec{x};t) = \vec{H}(\vec{x};t), \tag{D.2c}$$

then Maxwells equations inside the cavity are given by

$$\nabla \wedge \vec{E} = \frac{i\omega}{c} \vec{B} , \tag{D.3a}$$

$$\nabla \wedge \vec{B} = - \frac{i\omega}{c} \vec{E} , \tag{D.3b}$$

$$\nabla \cdot \vec{B} = \nabla \cdot \vec{E} = 0 \tag{D.3c}$$

and

$$\vec{B} = \vec{H} . \tag{D.3d}$$

Equations (D.3a and D.3b) may be combined to give

$$\{\nabla^2 + \frac{\omega^2}{c^2}\} \begin{bmatrix} \vec{E} \\ \vec{B} \end{bmatrix} = 0 . \tag{D.4}$$

Equation (D.4) together with Eqs. (D.3b and D.3c) and the boundary condition, expressed in terms of the surface impedance Z_s and given by Eq. (D.1) provide us with an eigenvalue equation for the frequency ω. The solutions to the eigenvalue problem determine the resonant modes of the cavity. What we wish to do is to determine how the various eigenvalues are affected by the finite value of Z_s. This is best achieved by comparing the eigenvalue solution obtained from the boundary condition expressed in Eq. (D.1), with those of an ideal cavity whose eigenvalues are determined from the boundary conditions,

$$\hat{n} \wedge \vec{E}_0 = 0 \tag{D.5a}$$

and

$$\hat{n} \cdot \vec{B}_0 = 0 , \tag{D.5b}$$

on S. Where $\vec{E}_0$ $\vec{B}_0$ and ω_0 correspond to the solutions of the eigenvalue problem in the case of an ideal conduction.

In order to determine the shift in frequency induced by the finite value of Z_s we make use of the vector generalisation of Green's first identity[148]

$$\int d^3\vec{x}\{\vec{F}_1\cdot\nabla^2 \vec{F}_2 - \vec{F}_2\cdot\nabla^2 F_1\} = \oint dA\{\vec{F}_1\nabla\cdot F_2 - \vec{F}_2\nabla\cdot\vec{F}_1\}\cdot\hat{n}$$
$$- \oint dA\{\vec{F}_1\cdot(\hat{n}\wedge\nabla\wedge F_2) - \nabla\wedge\vec{F}_1\cdot(\hat{n}\wedge\vec{F}_2)\} \qquad \text{(D.6)}$$

Thus we obtain

$$\int d^3\vec{x}\{\vec{E}\cdot\nabla^2 \vec{E}_o - \vec{E}_o\cdot\nabla^2\vec{E}\} = -\oint dA\{(\hat{n}\wedge\vec{E})\cdot\nabla\wedge\vec{E}_o - \nabla\wedge\vec{E}\cdot(\hat{n}\wedge\vec{E}_o)\}_S$$
$$= -i\frac{i\omega_o}{c}\oint dA(\hat{n}\wedge\vec{E})\cdot\vec{B}_o \ , \qquad \text{(D.7)}$$

where Eqs. (D.3a, D.3c and D.5a) were used together with Eq. (D.6). From the definition of the surface impedance given in Eq. (D.1) together with Eq. (D.4) we obtain the following equation for the resonant frequency ω.

$$\left[\frac{\omega^2}{c^2} - \frac{\omega_o^2}{c^2}\right]\int d^3x\ \vec{E}\cdot E_o = -\frac{i\omega_o}{4\pi}\oint dA\ \vec{B}\cdot\overleftrightarrow{Z}_s\cdot B_o \qquad \text{(D.8)}$$

$$(\omega^2 - \omega_o^2) = \frac{-i\omega_o c^2/4\pi \oint dA\ \vec{B}\cdot\overleftrightarrow{Z}_s\cdot\vec{B}_o}{\int d^3x\ \vec{E}\cdot\vec{E}_o} \qquad \text{(D.9)}$$

In cases where Z_s is both diagonal and constant over the surface S this simplifies to give

$$\omega^2 = \omega_o^2 - \frac{i\omega_o c^2}{4\pi} Z_s \frac{\oint dA\ \vec{B}\cdot\vec{B}_o}{\int d^3x\ \vec{E}\cdot\vec{E}_o} \qquad \text{(D.10)}$$

$$\simeq \omega_o^2 - \frac{i\omega_o c^2}{4\pi} Z_s \frac{\oint dA|B_o|^2}{\int d^3x|E_o|^2} + \ldots , \qquad \text{(D.11)}$$

where we have neglected higher order corrections in Z_s which we assume to be small.

The reason for including such a detailed analysis is twofold.

Firstly measurements regarding the shift in the resonant frequency of a microwave cavity as a function of temperature have been made in a cavity with superconducting "walls", this analysis shows that the measured quantity is in fact the surface impedance defined by Eq. (D.1) at the cavity/wall interface. Secondly it serves to emphasise the fact that the fundamental quantity that can be measured, by means of electromagnetic radiation is the surface impedance. This is important since it provides us with a precise definition of the penetration depth in conducting surfaces, based on a mathematically well defined, experimentally accessible quantity, the surface impedance.

In order to see how the surface impedance may be used to define the effective penetration depth we consider the geometry shown in Fig. (23), and if we assume that the system is isotropic then we write the fields for $z > 0$ (i.e. inside the metal) as

$$\vec{E}(\vec{x};t) = e(\omega;z)e^{-i\omega t}\,\hat{x}\ , \tag{D.12a}$$

$$\vec{H}(\vec{x},t) = h(\omega;z)e^{-i\omega t}\,\hat{y}\ , \tag{D.12b}$$

$$\vec{B}(\vec{x};t) = b(\omega;z)e^{-i\omega t}\,\hat{y} \tag{D.12c}$$

and

$$\vec{M}(\vec{x};t) = M(\omega;z)e^{-i\omega t}\,\hat{y}\ . \tag{D.12d}$$

Now Maxwell's equations in the metal are given by

$$\nabla \wedge \vec{H} = \frac{4\pi}{c}\vec{J} \tag{D.13a}$$

$$\nabla \wedge \vec{E} = \frac{i\omega}{c}\vec{B} \tag{D.13b}$$

and

$$\vec{B} = \vec{H} + 4\pi\vec{M} \tag{D.13c}$$

where we have neglected the effect of the displacement current. From Eq. (D.13b) together with Eqs. (D.12a and D.12c) we obtain

$$\frac{d}{dz} e(\omega;z) = \frac{i\omega}{c} b(\omega;z) \tag{D.14}$$

and hence

$$e(\omega;0^+) = \frac{i\omega}{c}\int_{0^+}^{\infty} b(\omega;z)dz \ . \tag{D.15}$$

[The notation $z = 0^+$ means that z is taken to be positive yet infinitesimally close to the surface z = 0.] From our definition of Z_s given by Eq. (D.1) we obtain the following result for the value of the surface impedance Z_s on the surface $z = 0^+$.

$$Z_s(\omega) = \frac{4\pi}{c}\frac{e(\omega;0)}{h(\omega;0)} = -\ i\ \frac{4\pi\omega}{c^2}\int_{0^+}^{\infty} dz\ b(\omega;z)/h(\omega;0) \ . \tag{D.16}$$

The expression for the surface impedance given by Eq. (D.16) suggests the following definition for the effective penetration depth.

$$\lambda(\omega) = \mathrm{Re}\left[\int dz\ b(\omega;z)/h(\omega;0)\right]. \tag{D.17}$$

Since Z_s is continuous across the interface the resonant frequency of the cavity may be obtained from Eq. (D.16) together with Eq. (D.11)

$$\omega^2 = \omega_o^2\{1 - \frac{\lambda(\omega_o)}{L(\omega_o)} + O(\lambda^2/L^2)\} \ , \tag{D.18}$$

where we have defined the $L(\omega_o)$ as

$$L = \frac{\int d^3x|E_o|^2}{\oint dA|B_o|^2} \ . \tag{D.19}$$

Obviously L depends only on the geometry of the cavity and in particular mode that is being excited.

We briefly note that the definition of λ given by Eq. (D.17) differs somewhat from that contained in the earlier work of Kotani et al.[111,110,149] However as we demonstrated the definition given in Eq. (D.17) is an experimentally accessible quantity, as shown by the result of Eq. (D.18).

We now turn our attention to the calculation of the $\lambda(\omega)$ in the case of magnetic superconductors. We simplify the analysis somewhat and assume first of all that $\vec{M}$ and $\vec{H}$ are related linearly as

$$\vec{M} = \chi(\omega;-i\nabla)\vec{H}, \tag{D.20}$$

furthermore if we restrict our considerations to the paramagnetic domain, then the susceptibility may be assumed to have the hydrodynamical form

$$\chi(\omega;\vec{k}) = \chi(\vec{k}) . \frac{i\Gamma(\vec{k})}{\omega + i\Gamma(\vec{k})} \tag{D.21}$$

where $\chi(\vec{k})$ is the static susceptibility given by

$$\chi(\vec{k}) = \frac{C}{T - T_m' + Dk^2} . \tag{D.22}$$

Where, as in Chapter 4, C denotes the Curie constant, T_m the Curie constant of the normal phase, D the stiffness constant and $\Gamma(\vec{k})$ the decay width (i.e. the inverse of the spin relaxation time), which it is assumed may be written as

$$\Gamma(\vec{k})^{-1} = \tau\chi(\vec{k}) . \tag{D.23}$$

The superconducting current $\vec{J}(\omega;k)$ may be computed in the linear approximation as

$$\vec{J}(\omega;\vec{k}) = \{- \frac{c}{4\pi\lambda_L^2(T)} + \frac{i\omega}{c} \sigma(T)\}\vec{A}(\omega;\vec{k}) \tag{D.24}$$

where $\vec{A}$ is the vector potential for the magnetic induction field $\vec{B}$ (i.e. $\vec{B} = \nabla \wedge \vec{A}$). The expression for the current given in Eq. (D.24) differs from that used in Chapter 4 Eq. (4.21) in a number of ways; first of all we have simplified the expression by taking the London limit, $C(-i\nabla) \sim 1$, secondly we have included the low frequency part of the continuum contribution to the photon self energy which we have parameterised in terms of the constant σ. This term is included in order to allow us to treat the region in the vicinity of T_c in a realistic manner. Finally we note that, since we are considering the Meisner state, $f(x) = 0$.

We simplify the analysis somewhat further by assuming pair breaking effects, induced through the d-f interaction, are negligible and that $\lambda_L(T)$ may be computed using the standard BCS formula. By means of constitutive Eqs. (D.24 and D.20) together with the Maxwell equations Eqs. (D.13a, D.13b and D.13c) we obtain the following expression for magnetic field.

$$- \frac{d^2}{dz^2} h(\omega;z) = - \{\lambda_L^{-2} - i\delta^{-2}\}[1 + 4\pi\chi \{\omega; - i \frac{d}{cz}\}]h(\omega;z), \qquad (D.25)$$

where $\delta^2 \equiv c/4\pi\omega\sigma$.

Equation (D.25) may be solved subject to the boundary conditions that

$$\lim_{z\to\infty} h(\omega;z) = 0, \qquad (D.26a)$$

$$\lim_{z\to 0^+} h(\omega;z) = h_o(\omega). \qquad (D.26b)$$

and

$$\frac{d}{dz} m(\omega;z)\Big|_{z=0^+} = \mu m(\omega;0^+), \qquad (D.26c)$$

to give

$$h(\omega;z) = A_+ \exp\{-\frac{\alpha+z}{\lambda_L}\} + A_- \exp\{-\frac{\alpha-z}{\lambda}\}. \quad (D.27)$$

The term $\alpha_\pm$, appearing in the exponent, are determined from the roots of the equation.

$$\alpha_\pm^2 = \{\varepsilon - d\eta - ic\gamma \pm \sqrt{(\varepsilon - d\eta - ic\gamma)^2 - 4cd\eta}\}\frac{1}{2d} \quad (D.28)$$

where η is defined by $\eta = 1 - i\lambda_L^2/\delta^2$ and $\gamma = \omega\tau/4\pi$, while $d = D/T_m\lambda_L^2$, $\varepsilon = T/T_m - 1$ and $c = 4\pi c/T_m$, in a manner similar to the definitions presented in Chapter 4. The constants $A_\pm$ are determined in terms of $h_0(\omega)$ and the parameter μ. It is obvious from the boundary conditions that the root of $\alpha_\pm$ computed from Eq. (D.28) should have a positive real part. Since $b(\omega;z) \equiv [1 + 4\pi\chi(\omega;-i\partial_z)]h(\omega;z)$ and $1 + 4\pi\chi(\omega;-i\alpha_\pm/\lambda_L(T)) \cong \alpha_\pm^2/\eta$ which follows from Eq. (D.25), we obtain after some straightforward manipulation the result

$$\lambda(\omega) = \mathrm{Re}\left[\frac{\lambda_L(T)}{\eta}\;\frac{\alpha_+\alpha_-(\alpha_+ + \alpha_- + \mu\lambda_L(T) + \eta\mu\lambda_L(T)}{\alpha_+^2 + \alpha_+\alpha_- + \alpha^2 + \mu\lambda_L(T)(\alpha_+ + \alpha_-) - \eta}\right] \quad (D.29)$$

The result for the normal state may be obtained from Eq. (D.29) by taking the limit $\lambda_L \to \infty$.

Near T_c, $\lambda_L(T)$ is large and therefore the momentum dependence of $\chi(\omega;\vec{k})$ is negligible and may be approximated by the static susceptibility $\chi(T) = C/(T - T_m)$. In this case Eq. (D.25) shows that the behaviour of $h(\omega;z)$ may be obtained from the result of the non-magnetic case by means of the simple scaling rule: $\lambda_L(T) \to \lambda_L(T)/\sqrt{1+4\pi\chi}$ and $\delta \to \delta/\sqrt{1+4\pi\chi}$. Because $b = (1 + 4\pi\chi)h$, $\lambda(\omega)$ is given by

$$\lambda(\omega) \cong \sqrt{1+4\pi\chi(T)}\;\mathrm{Re}(1/\sqrt{\lambda_L^{-2}(T) - i\delta^{-2}}) . \quad (D.30)$$

In particular we have $\lambda(\omega) \simeq \sqrt{1+4\pi\chi(T)}\,(\delta/\sqrt{2})$ for $T > T_{c1}$, and $\lambda(\omega) \simeq \sqrt{1+4\pi\chi(T)}\,\lambda_L(T)$ for $T < T_{c1}$ with $\lambda_L \ll \delta$. This shows that the characteristic length $\lambda(\omega)$ obtained from the impedance may increase with decreasing temperature owing to the factor $[1+4\pi\chi(T)]^{1/2}$.

When the temperature is lowered, the frequency and momentum dependence of the susceptibility $\chi(\omega,k)$ becomes important and induces a shift of the magnetic transition temperature. To understand this let us note that, for $\omega = \mu = 0$, the roots $\alpha_\pm$ given by Eq. (D.28) have positive real parts only for $T > T_p$, where $T_p = T_m(1 + d$ [illegible] $\sqrt{dc})$, with $d = D/T_m\lambda_L^2(0)$, denotes the critical temperature for the onset of the spin periodic phase. However $\lambda(\omega)$ at $\omega = \mu = 0$ diverges at $T = T_s = T_m(1 + (1/2)d - \sqrt{dc + (1/4)d^2})$ signifying the onset of spontaneous surface magnetization;

$$\lambda(0) \underset{T\to T_s}{\sim} \frac{T_m}{T - T_s}\,\frac{d^{1/4}}{2\sqrt{2}}\,\frac{1}{\sqrt{d+4c}}\left(\sqrt{d+4c} - 1\right)^2 \times \left(\sqrt{d} + \sqrt{d+4c}\right)^{1/2} . \qquad (D.31)$$

At finite frequency, however, the critical behaviour at T_s is smeared out due to the effects of the skin depth and the relaxation rate $\gamma\left(= \frac{\omega\tau}{4\pi}\right)$.

In Fig. (24) we present the theoretical values for the inverse of the penetration depth $\lambda(\omega)$ (solid curve) calculated by means of Eq. (D.29) for $ErRh_4B_4$ together with the experimental values (circles) obtained from recent measurements[136] calculated from the observed shift in the resonant frequency of a cavity. The parameters used in the calculation differ slightly from those presented in Tables (1,2) here $T_{c1} = 8.7°K$, $T_m = 1.0°K$, $T_p = 0.85°K$ and $d(\equiv D/T_m\lambda_L(T=0)) \simeq 0.2529 \times 10^{-2}$. The values for $\lambda_L(0)$ and $\delta/\lambda_L(0)$ are determined in such a way that the maximum value of λ^{-1} agrees with the maximum experimental value (λ^{-1}_{max} = 7.7 μ^{-1}) and $\lambda^{-1}(T = T_c)$ is equal to the experimental value 0.149 μ^{-1}. This gives a value of $\lambda_L(T = 0)$ = 908Å and a ratio $\delta/\lambda_L(T = 0)$ = 91.8. In spite of the discrepancy around T_{c1} due to the finite value of the frequency 9.3 GHz (∿0.4°K), the agreement between theory and experiment is satisfactory. Furthermore it is worth noting that the value of $\lambda_L(0)$ = 908Å is very close to the value obtained in Chapter 4, Page from the analysis of the magnetic properties of single crystal $ErRh_4B_4$ (λ_{Lo} = 825Å). For comparison we also present the result of the static limit (dash dotted curve) calculated by the method described in Refs. [150] and [149] using a non-local kernel toegether with the parameters $\kappa_B = 4$, $d_o = 0.4254 \times 10^{-2}$ and $\lambda_L(0)$ = 749Å. The dashed curve is the BCS $\lambda_L^{-1}(T)$ with the parameter choice $\lambda_L(0)$ = 1184Å. We note that the effect of the spin fluctuations, as evidenced by the departure of the data from the BCS fitting, is quite pronounced in particular at low temperatures. The analysis suggests that, if T were to be further decreased, surface ferromagnetic effects would show up.

In Fig. (25) the experimental data of $\lambda^{-1}(\omega)$ for $Er_{0.5}Ho_{0.5}Rh_4B_4$ presented (circles) together with the BCS $\lambda_L^{-1}(T)$ (dashed curve) with the parameter choice $\lambda_L(0)$ = 1186Å. The experimental $\lambda^{-1}(\omega)$ shows a mild deviation from the BCS result above T_{c2} and jumps discontinuously to its normal value at $T = T_{c2}$, indicating that there is no additional magnetic transition above T_{c2} (i.e. $T_s < T_{c2}$). This is consistent with the neutron data[151] for $Er_{0.4}Ho_{0.6}Rh_4B_4$, in which a clear first order mean-field-type magnetic transition at T_{c2} is observed without showing any effect of spin fluctuation. This pseudo-ternary has a rather complicated spin-spin interaction because of the difference in the easy axes associated with the Er and Ho spins. Assuming that the value of T_m may be obtained from the extrapolation of the decrease of T_m with increasing x in the pseudo-ternary $Ho_{1-x}Er_xRh_4B_4$ and that the Curie constant C is given by the mean value of the value obtained in the Er and Ho case ($4\pi C_{ave}$ = 2.57K), the theory (solid curve) yields d = 1.0 and γ = 0.5, which are fairly large (this choice of d means that T_s is well below T_{c2}). For comparison, the theoretical curve for $\gamma = 0$ (i.e. $\omega = 0$) is also presented and shows a small decrease at lower temperature due to the fluctuation effect. Therefore the present analysis suggests that the apparent suppression of the spin fluctuations in the superconducting state is due to $T_s << T_{c2}$ and also to the effect of spin relaxation time.

To summarise we began this section with a brief discussion on the definition of the surface impedance in electrodynamics. In particular it was shown how, in a very general way, the electromagnetic properties of a resonant cavity could be determined from a knowledge of the surface impedance at the cavity walls, together with Maxwells equations. An explicit expression was given for the change in the resonant frequency of the cavity induced by the finite value of Z_s.

Having established the experimental importance of the surface impedance we then went on to show how it may be used to define in an entirely unambiguous fashion the penetration depth for a conducting half space Fig. (23). An explicit expression for the penetration depth was obtained for the case of a magnetic superconductor and examined for various limiting cases. In particular it was shown, in the case of $ErRh_4B_4$, how the penetration depth clearly manifests the effect of the critical fluctuations in the surface magnetisation around T_{c2}. A comparison of the analytical results with recent experimental measurements on polycrystalline $ErRh_4B_4$ is satisfactory suggesting that if the temperature range of the measurements were to be extended the surface ferromagnetic effect would show up.